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

Appendix to:
Weakly-bound clusters of atmospheric molecules: infrared spectra and structural calculations of $(CO_2)_n$-$(CO)_m$-$(N_2)_p$,
(n,m,p) = (2,1,0), (2,0,1), (1,2,0), (1,0,2), (1,1,1), (1,3,0), (1,0,3), (1,2,1), (1,1,2)

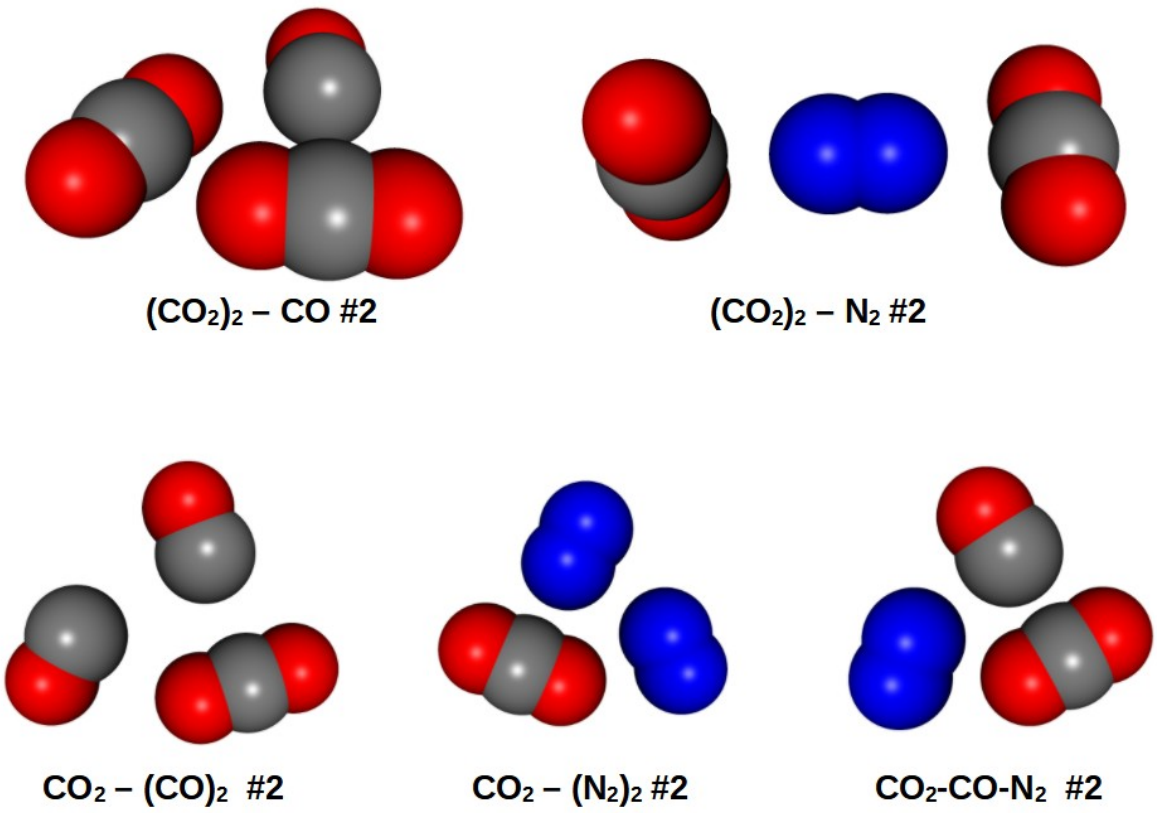

Figure A-1. Illustrations of the calculated structures of isomer #2 for clusters in Table 1 of the paper. See also Table A-10 of this Appendix, below.

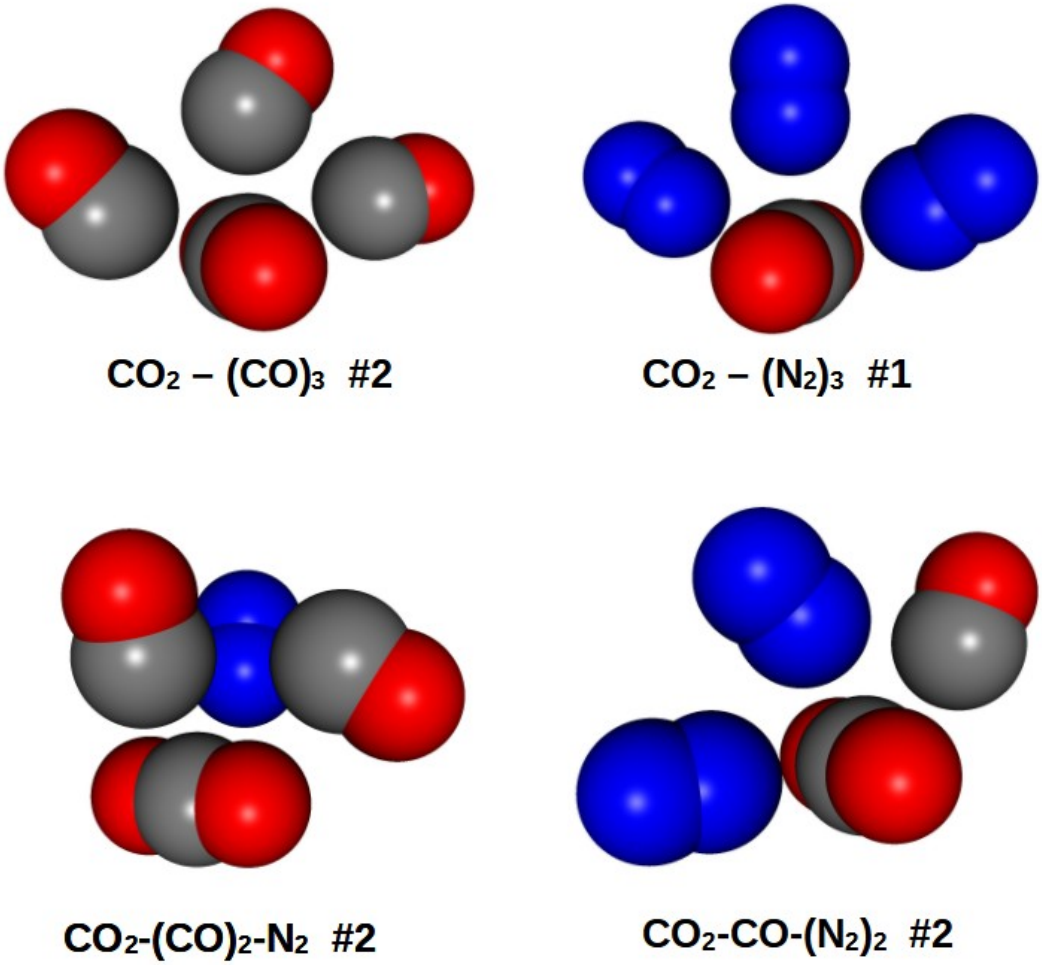

Figure A-2. Illustrations of the calculated structures of isomer #2 for clusters in Table 1 of the paper. See also Table A-10 of this Appendix, below. Note that calculated isomer #2 of CO_2-$(N_2)_3$ corresponds to the observed species and is illustrated in Fig. 1 of the paper. Calculated isomer #1 of CO_2-$(N_2)_3$ is illustrated here.

Table A-1. Observed and fitted transitions of $(CO_2)_2$-CO (cm^{-1}).
Int = calculated relative intensity, used to weight the blended lines.

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2345 > nu > 2348 = b-type fundamental band
2350 > nu > 2352 = a-, c-type fundamental band
2375 > nu > 2377 = b-type combination band

Note: Data from the fundamental band in the CO fundamental band region
(2149 - 2152 cm-1, not shown here) was also included in the combined fit.
See: Chem. Phys. Lett. 677, 127-130 (2017).
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J'	Ka'	Kc'	J"	Ka"	Kc"	Obs	Calc	Obs-Calc	Int
5	3	3	6	4	2	2345.5875	2345.5877	-0.0002	
7	6	2	8	5	3	2345.5921	2345.5924	-0.0002	
8	3	5	9	4	6	2345.6000	2345.5997	0.0003	
10	0	10	11	1	11	2345.6060	2345.6062	-0.0002	
6	5	1	7	6	2	2345.6102	2345.6096	0.0006	
7	5	3	8	4	4	2345.6194	2345.6190	0.0004	
9	2	8	10	1	9	2345.6232	2345.6231	0.0001	
5	4	2	6	5	1	2345.6403	2345.6392	0.0011	0.00033
8	2	6	9	3	7	2345.6403	2345.6406	-0.0003	0.00051
						Blend	2345.6400	0.0003	
7	4	4	8	3	5	2345.6588	2345.6585	0.0003	
9	1	9	10	0	10	2345.6644	2345.6644	0.0000	
8	1	7	9	2	8	2345.6818	2345.6815	0.0003	
7	3	5	8	2	6	2345.6993	2345.6992	0.0001	
6	3	3	7	4	4	2345.7160	2345.7164	-0.0005	
8	0	8	9	1	9	2345.7226	2345.7226	0.0000	
7	2	6	8	1	7	2345.7396	2345.7400	-0.0004	
6	2	4	7	3	5	2345.7580	2345.7579	0.0001	
4	4	0	5	5	1	2345.7764	2345.7767	-0.0003	
7	1	7	8	0	8	2345.7805	2345.7810	-0.0004	0.00140
5	4	2	6	3	3	2345.7805	2345.7803	0.0002	0.00061
						Blend	2345.7808	-0.0003	
6	1	5	7	2	6	2345.7985	2345.7986	-0.0001	
5	3	3	6	2	4	2345.8171	2345.8169	0.0002	
4	3	1	5	4	2	2345.8222	2345.8221	0.0001	
6	0	6	7	1	7	2345.8394	2345.8394	-0.0001	
3	3	1	4	4	0	2345.8572	2345.8580	-0.0008	0.00104
5	2	4	6	1	5	2345.8572	2345.8573	-0.0001	0.00139
						Blend	2345.8576	-0.0004	
4	2	2	5	3	3	2345.8738	2345.8734	0.0004	
5	1	5	6	0	6	2345.8977	2345.8980	-0.0002	
4	1	3	5	2	4	2345.9158	2345.9160	-0.0001	
10	1	9	10	2	8	2345.9338	2345.9337	0.0001	0.00009
11	3	9	11	4	8	2345.9338	2345.9334	0.0003	0.00006
9	1	9	9	2	8	2345.9338	2345.9340	-0.0002	0.00010
12	3	9	12	4	8	2345.9338	2345.9332	0.0006	0.00003
						Blend	2345.9337	0.0001	
4	0	4	5	1	5	2345.9566	2345.9566	0.0000	
3	1	3	4	0	4	2346.0146	2346.0153	-0.0007	
2	1	1	3	2	2	2346.0293	2346.0299	-0.0006	
1	1	1	2	2	0	2346.0522	2346.0537	-0.0015	0.00047
7	2	6	7	3	5	2346.0522	2346.0522	0.0000	0.00036
6	0	6	6	1	5	2346.0522	2346.0523	-0.0001	0.00031
8	2	6	8	3	5	2346.0522	2346.0522	0.0001	0.00029
9	4	6	9	5	5	2346.0522	2346.0522	0.0000	0.00020

						Blend	2346.0526	-0.0004	
2	0	2	3	1	3	2346.0739	2346.0740	-0.0001	
8	3	5	8	4	4	2346.0920	2346.0925	-0.0004	0.00032
9	5	5	9	6	4	2346.0920	2346.0923	-0.0003	0.00020
5	1	5	5	2	4	2346.0920	2346.0919	0.0001	0.00041
6	1	5	6	2	4	2346.0920	2346.0919	0.0001	0.00050
7	3	5	7	4	4	2346.0920	2346.0919	0.0001	0.00044
						Blend	2346.0920	0.0000	
7	5	3	7	6	2	2346.1621	2346.1625	-0.0003	
8	5	3	8	6	2	2346.1901	2346.1900	0.0000	0.00044
0	0	0	1	1	1	2346.1901	2346.1907	-0.0006	0.00092
5	4	2	5	5	1	2346.1901	2346.1896	0.0005	0.00071
						Blend	2346.1902	-0.0001	
3	2	2	3	3	1	2346.2025	2346.2027	-0.0003	
4	2	2	4	3	1	2346.2203	2346.2199	0.0005	0.00146
6	4	2	6	5	1	2346.2203	2346.2206	-0.0003	0.00115
						Blend	2346.2202	0.0001	
4	3	1	4	4	0	2346.2347	2346.2348	-0.0001	
2	2	0	2	1	1	2346.2952	2346.2953	-0.0001	
4	4	0	4	3	1	2346.3067	2346.3067	0.0000	
3	3	1	3	2	2	2346.3394	2346.3389	0.0005	
1	1	1	0	0	0	2346.3509	2346.3515	-0.0006	0.00097
8	6	2	8	5	3	2346.3509	2346.3523	-0.0014	0.00049
5	5	1	5	4	2	2346.3509	2346.3505	0.0005	0.00076
						Blend	2346.3513	-0.0004	
7	7	1	7	6	2	2346.3692	2346.3671	0.0021	0.00035
4	2	2	4	1	3	2346.3692	2346.3688	0.0004	0.00096
						Blend	2346.3683	0.0008	
5	4	2	5	3	3	2346.3725	2346.3732	-0.0007	0.00092
3	2	2	3	1	3	2346.3725	2346.3717	0.0008	0.00068
						Blend	2346.3725	-0.0001	
6	2	4	6	1	5	2346.4510	2346.4513	-0.0003	0.00058
7	4	4	7	3	5	2346.4510	2346.4507	0.0003	0.00050
5	2	4	5	1	5	2346.4510	2346.4518	-0.0008	0.00047
8	4	4	8	3	5	2346.4510	2346.4497	0.0013	0.00037
						Blend	2346.4510	0.0000	
3	1	3	2	0	2	2346.4688	2346.4687	0.0001	
3	2	2	2	1	1	2346.5124	2346.5124	0.0000	
4	0	4	3	1	3	2346.5283	2346.5279	0.0004	
3	3	1	2	2	0	2346.5560	2346.5559	0.0001	
4	1	3	3	2	2	2346.5672	2346.5669	0.0003	
5	1	5	4	0	4	2346.5876	2346.5873	0.0003	
10	2	8	10	1	9	2346.6136	2346.6135	0.0001	0.00012
11	4	8	11	3	9	2346.6136	2346.6129	0.0007	0.00008
12	4	8	12	3	9	2346.6136	2346.6122	0.0015	0.00004
9	2	8	9	1	9	2346.6136	2346.6141	-0.0005	0.00013
						Blend	2346.6134	0.0002	
5	2	4	4	1	3	2346.6270	2346.6269	0.0001	
6	0	6	5	1	5	2346.6470	2346.6468	0.0001	
5	3	3	4	2	2	2346.6691	2346.6688	0.0003	
7	1	7	6	0	6	2346.7066	2346.7064	0.0002	
7	2	6	6	1	5	2346.7457	2346.7456	0.0001	
8	0	8	7	1	7	2346.7662	2346.7661	0.0001	
7	3	5	6	2	4	2346.7851	2346.7851	0.0000	
8	1	7	7	2	6	2346.8052	2346.8052	0.0001	
9	1	9	8	0	8	2346.8259	2346.8259	0.0000	0.00159
7	4	4	6	3	3	2346.8259	2346.8256	0.0003	0.00089
						Blend	2346.8258	0.0001	
8	2	6	7	3	5	2346.8445	2346.8444	0.0000	

9	2	8	8	1	7	2346.8650	2346.8648	0.0002	
9	3	7	8	2	6	2346.9034	2346.9039	-0.0005	0.00081
6	5	1	5	4	2	2346.9034	2346.9023	0.0011	0.00051
						Blend	2346.9033	0.0001	
11	2	10	10	1	9	2346.9838	2346.9844	-0.0006	0.00058
9	5	5	8	4	4	2346.9838	2346.9832	0.0006	0.00043
						Blend	2346.9839	-0.0001	
6	3	3	5	2	4	2347.0027	2347.0039	-0.0012	0.00011
10	3	7	9	4	6	2347.0027	2347.0027	0.0000	0.00043
						Blend	2347.0029	-0.0003	
12	0	12	11	1	11	2347.0057	2347.0057	0.0000	
11	3	9	10	2	8	2347.0230	2347.0232	-0.0002	
12	2	10	11	3	9	2347.0820	2347.0830	-0.0010	0.00027
10	5	5	9	6	4	2347.0820	2347.0816	0.0004	0.00023
						Blend	2347.0823	-0.0003	
8	7	1	7	6	2	2347.0874	2347.0882	-0.0008	0.00041
9	7	3	8	6	2	2347.0874	2347.0869	0.0006	0.00026
						Blend	2347.0877	-0.0003	
8	1	8	9	1	9	2350.1157	2350.1161	-0.0004	0.00108
6	4	3	7	4	4	2350.1157	2350.1163	-0.0006	0.00070
						Blend	2350.1162	-0.0005	
6	3	4	7	3	5	2350.1570	2350.1560	0.0011	
5	2	3	6	2	4	2350.2153	2350.2153	0.0000	
6	1	6	7	1	7	2350.2360	2350.2359	0.0001	
5	1	4	6	1	5	2350.2561	2350.2557	0.0004	
4	2	3	5	2	4	2350.3149	2350.3153	-0.0004	
4	1	4	5	1	5	2350.3552	2350.3553	-0.0001	
3	0	3	4	0	4	2350.4148	2350.4148	0.0001	
1	0	1	2	0	2	2350.5305	2350.5322	-0.0017	0.00132
5	1	4	5	3	3	2350.5305	2350.5299	0.0006	0.00056
6	3	4	6	3	3	2350.5305	2350.5309	-0.0003	0.00051
4	1	4	4	1	3	2350.5305	2350.5304	0.0002	0.00045
						Blend	2350.5312	-0.0007	
4	3	2	4	3	1	2350.6237	2350.6232	0.0004	
2	2	1	2	2	0	2350.6550	2350.6553	-0.0002	
5	0	5	5	1	5	2350.6693	2350.6698	-0.0006	0.00438
4	1	4	4	0	4	2350.6693	2350.6704	-0.0012	0.00431
6	1	6	6	0	6	2350.6693	2350.6691	0.0001	0.00406
3	0	3	3	1	3	2350.6693	2350.6709	-0.0016	0.00378
7	0	7	7	1	7	2350.6693	2350.6683	0.0010	0.00351
8	1	8	8	0	8	2350.6693	2350.6673	0.0019	0.00283
5	1	4	5	2	4	2350.6693	2350.6700	-0.0007	0.00245
6	2	5	6	1	5	2350.6693	2350.6693	0.0000	0.00240
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3	3	0	3	3	1	2350.6851	2350.6846	0.0005	
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5	2	3	5	2	4	2350.8088	2350.8096	-0.0008	0.00063
6	4	3	6	2	4	2350.8088	2350.8094	-0.0007	0.00057
4	2	3	4	0	4	2350.8088	2350.8107	-0.0020	0.00050
						Blend	2350.8091	-0.0003	
3	1	2	2	1	1	2350.9113	2350.9109	0.0004	
4	1	4	3	1	3	2350.9271	2350.9266	0.0005	
3	2	1	2	2	0	2350.9401	2350.9401	0.0000	
5	0	5	4	0	4	2350.9850	2350.9850	0.0000	
5	1	4	4	1	3	2351.0256	2351.0253	0.0003	

4	4	1	3	3	1	2351.0747	2351.0744	0.0003	
6	2	5	5	2	4	2351.0829	2351.0836	-0.0007	
7	0	7	6	0	6	2351.1017	2351.1015	0.0002	
6	3	4	5	3	3	2351.1233	2351.1237	-0.0004	0.00151
5	4	1	4	4	0	2351.1233	2351.1237	-0.0004	0.00116
						Blend	2351.1237	-0.0004	
7	1	6	6	1	5	2351.1418	2351.1418	0.0000	
5	4	1	4	3	1	2351.1605	2351.1601	0.0004	0.00232
5	3	2	4	2	2	2351.1605	2351.1614	-0.0009	0.00212
8	1	8	7	1	7	2351.1605	2351.1595	0.0009	0.00201
6	4	3	5	4	2	2351.1605	2351.1611	-0.0006	0.00116
						Blend	2351.1604	0.0000	
6	6	1	5	5	1	2351.2767	2351.2772	-0.0005	0.00193
10	1	10	9	1	9	2351.2767	2351.2753	0.0014	0.00120
						Blend	2351.2764	0.0003	
11	1	11	12	0	12	2375.0177	2375.0182	-0.0005	0.00034
9	4	6	10	3	7	2375.0177	2375.0174	0.0003	0.00025
						Blend	2375.0178	-0.0002	
10	1	9	11	2	10	2375.0386	2375.0388	-0.0002	0.00035
8	4	4	9	5	5	2375.0386	2375.0385	0.0001	0.00026
						Blend	2375.0387	-0.0001	
6	6	0	7	7	1	2375.0668	2375.0666	0.0002	
9	1	9	10	0	10	2375.1456	2375.1459	-0.0003	0.00077
7	4	4	8	3	5	2375.1456	2375.1453	0.0003	0.00049
						Blend	2375.1457	-0.0001	
6	4	2	7	5	3	2375.1537	2375.1536	0.0000	
7	3	5	8	2	6	2375.1868	2375.1874	-0.0005	
8	0	8	9	1	9	2375.2084	2375.2091	-0.0007	0.00107
6	3	3	7	4	4	2375.2084	2375.2069	0.0015	0.00059
						Blend	2375.2084	0.0001	
7	1	7	8	0	8	2375.2717	2375.2719	-0.0002	
4	4	0	5	5	1	2375.2778	2375.2784	-0.0006	0.00120
5	4	2	6	3	3	2375.2778	2375.2774	0.0004	0.00061
						Blend	2375.2781	-0.0003	
6	1	5	7	2	6	2375.2922	2375.2922	0.0000	
5	3	3	6	2	4	2375.3134	2375.3132	0.0002	
4	3	1	5	4	2	2375.3187	2375.3191	-0.0004	
6	0	6	7	1	7	2375.3338	2375.3342	-0.0005	
5	2	4	6	1	5	2375.3537	2375.3544	-0.0007	
4	2	2	5	3	3	2375.3719	2375.3716	0.0002	
5	1	5	6	0	6	2375.3960	2375.3961	-0.0001	
4	1	3	5	2	4	2375.4157	2375.4160	-0.0004	
4	0	4	5	1	5	2375.4577	2375.4575	0.0001	
3	2	2	4	1	3	2375.4780	2375.4784	-0.0004	
2	2	0	3	3	1	2375.4904	2375.4904	0.0001	
3	1	3	4	0	4	2375.5184	2375.5185	-0.0001	
2	1	1	3	2	2	2375.5337	2375.5336	0.0000	
1	1	1	2	2	0	2375.5598	2375.5601	-0.0003	0.00047
10	5	5	10	6	4	2375.5598	2375.5609	-0.0011	0.00013
						Blend	2375.5603	-0.0005	
2	0	2	3	1	3	2375.5789	2375.5788	0.0000	0.00177
7	3	5	7	4	4	2375.5789	2375.5801	-0.0012	0.00046
						Blend	2375.5791	-0.0002	
1	1	1	2	0	2	2375.6414	2375.6410	0.0004	
5	3	3	5	4	2	2375.6654	2375.6648	0.0006	0.00088
8	5	3	8	6	2	2375.6654	2375.6650	0.0004	0.00053
						Blend	2375.6649	0.0005	
6	4	2	6	5	1	2375.7065	2375.7068	-0.0004	0.00126
3	2	2	3	3	1	2375.7065	2375.7056	0.0009	0.00089

						Blend	2375.7063	0.0001	
4	2	2	4	3	1	2375.7187	2375.7181	0.0006	0.00160
2	0	2	2	1	1	2375.7187	2375.7196	-0.0009	0.00083
						Blend	2375.7186	0.0001	
4	3	1	4	4	0	2375.7317	2375.7317	0.0000	
2	1	1	2	2	0	2375.7505	2375.7506	-0.0001	
4	3	1	4	2	2	2375.8192	2375.8194	-0.0002	
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7	7	1	7	6	2	2375.8673	2375.8667	0.0006	0.00033
						Blend	2375.8671	0.0002	
2	0	2	1	1	1	2375.9126	2375.9126	0.0000	0.00126
4	1	3	4	0	4	2375.9126	2375.9114	0.0012	0.00058
						Blend	2375.9123	0.0003	
3	1	3	2	0	2	2375.9721	2375.9719	0.0001	
3	2	2	2	1	1	2376.0154	2376.0153	0.0001	
4	0	4	3	1	3	2376.0289	2376.0288	0.0001	
3	3	1	2	2	0	2376.0607	2376.0607	0.0000	
4	1	3	3	2	2	2376.0670	2376.0670	0.0000	
5	1	5	4	0	4	2376.0855	2376.0854	0.0001	
5	2	4	4	1	3	2376.1242	2376.1240	0.0002	
6	0	6	5	1	5	2376.1417	2376.1416	0.0000	
5	3	3	4	2	2	2376.1649	2376.1651	-0.0003	
6	1	5	5	2	4	2376.1803	2376.1798	0.0006	
4	4	0	3	3	1	2376.1847	2376.1846	0.0001	
7	1	7	6	0	6	2376.1977	2376.1973	0.0004	
6	2	4	5	3	3	2376.2173	2376.2180	-0.0006	0.00131
5	4	2	4	3	1	2376.2173	2376.2167	0.0007	0.00108
						Blend	2376.2174	0.0000	
7	2	6	6	1	5	2376.2356	2376.2351	0.0005	
8	0	8	7	1	7	2376.2527	2376.2526	0.0000	0.00199
6	3	3	5	4	2	2376.2527	2376.2517	0.0009	0.00080
						Blend	2376.2524	0.0003	
5	5	1	4	4	0	2376.2652	2376.2654	-0.0002	
7	3	5	6	2	4	2376.2732	2376.2732	0.0000	

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Table A-2. Observed and fitted transitions of $(CO_2)_2$-N_2 (cm^{-1}).
Int = calculated relative intensity, used to weight the blended lines.

2345 > nu > 2348 = b-type fundamental band
2350 > nu > 2352 = a-, c-type fundamental band

J'	Ka'	Kc'	J"	Ka"	Kc"	Obs	Calc	Obs-Calc	Int
10	3	7	11	4	8	2345.5671	2345.5669	0.0001	
12	0	12	13	1	13	2345.5718	2345.5725	-0.0006	
11	2	10	12	1	11	2345.5900	2345.5906	-0.0006	0.00139
9	5	5	10	4	6	2345.5900	2345.5895	0.0005	0.00089
						Blend	2345.5902	-0.0001	
10	2	8	11	3	9	2345.6097	2345.6093	0.0004	
9	3	7	10	2	8	2345.6706	2345.6705	0.0002	
8	3	5	9	4	6	2345.6882	2345.6879	0.0002	
10	0	10	11	1	11	2345.6937	2345.6940	-0.0003	
9	2	8	10	1	9	2345.7126	2345.7126	-0.0001	
6	4	2	7	5	3	2345.7168	2345.7175	-0.0007	
5	5	1	6	6	0	2345.7290	2345.7281	0.0009	
5	4	2	6	5	1	2345.7483	2345.7480	0.0003	
9	1	9	10	0	10	2345.7557	2345.7549	0.0008	0.00374
7	4	4	8	3	5	2345.7557	2345.7558	-0.0001	0.00189
						Blend	2345.7552	0.0005	
8	1	7	9	2	8	2345.7741	2345.7738	0.0003	
6	3	3	7	4	4	2345.7942	2345.7946	-0.0004	0.00588
7	3	5	8	2	6	2345.7942	2345.7934	0.0009	0.00802
						Blend	2345.7939	0.0004	
8	0	8	9	1	9	2345.8160	2345.8159	0.0001	
7	2	6	8	1	7	2345.8353	2345.8351	0.0002	
4	4	0	5	5	1	2345.8445	2345.8441	0.0004	
6	2	4	7	3	5	2345.8536	2345.8527	0.0009	
7	1	7	8	0	8	2345.8774	2345.8771	0.0004	
4	3	1	5	4	2	2345.8941	2345.8937	0.0004	
6	1	5	7	2	6	2345.8961	2345.8963	-0.0002	
5	3	3	6	2	4	2345.9227	2345.9221	0.0006	
6	0	6	7	1	7	2345.9389	2345.9383	0.0006	
5	1	5	6	0	6	2346.0001	2345.9996	0.0004	
4	1	3	5	2	4	2346.0168	2346.0176	-0.0008	
4	0	4	5	1	5	2346.0599	2346.0610	-0.0011	
2	2	0	3	3	1	2346.0749	2346.0757	-0.0009	
3	2	2	4	1	3	2346.0874	2346.0879	-0.0005	
3	1	3	4	0	4	2346.1221	2346.1228	-0.0008	
1	1	1	2	2	0	2346.1635	2346.1635	0.0001	
8	2	6	8	3	5	2346.1732	2346.1733	-0.0001	0.00160
9	4	6	9	5	5	2346.1732	2346.1729	0.0004	0.00125
11	6	6	11	7	5	2346.1732	2346.1726	0.0007	0.00055
						Blend	2346.1730	0.0002	
5	3	3	5	4	2	2346.2681	2346.2687	-0.0006	0.00898
6	2	4	6	3	3	2346.2681	2346.2682	-0.0001	0.00915
						Blend	2346.2684	-0.0003	
3	1	3	3	2	2	2346.2855	2346.2847	0.0008	0.00652
8	5	3	8	6	2	2346.2855	2346.2870	-0.0014	0.00650
						Blend	2346.2858	-0.0003	
4	1	3	4	2	2	2346.3034	2346.3041	-0.0007	0.00404
0	0	0	1	1	1	2346.3034	2346.3033	0.0001	0.00280
						Blend	2346.3038	-0.0004	
6	3	3	6	4	2	2346.3145	2346.3145	0.0000	

4	2	2	4	3	1	2346.3363	2346.3355	0.0008	0.00620
2	0	2	2	1	1	2346.3363	2346.3378	-0.0015	0.00334
						Blend	2346.3363	0.0000	
2	1	1	2	2	0	2346.3549	2346.3547	0.0002	
2	2	0	2	1	1	2346.4259	2346.4257	0.0002	
4	3	1	4	2	2	2346.4442	2346.4457	-0.0015	0.00644
2	1	1	2	0	2	2346.4442	2346.4432	0.0009	0.00345
						Blend	2346.4449	-0.0007	
6	4	2	6	3	3	2346.4688	2346.4681	0.0007	0.00510
4	4	0	4	3	1	2346.4688	2346.4705	-0.0018	0.00317
						Blend	2346.4690	-0.0003	
4	2	2	4	1	3	2346.4780	2346.4776	0.0004	0.00428
1	1	1	0	0	0	2346.4780	2346.4772	0.0009	0.00293
3	3	1	3	2	2	2346.4780	2346.4781	0.0000	0.00278
						Blend	2346.4776	0.0004	
7	5	3	7	4	4	2346.5427	2346.5427	0.0000	0.00754
7	6	2	7	5	3	2346.5427	2346.5421	0.0006	0.00585
						Blend	2346.5425	0.0002	
4	1	3	3	2	2	2346.6927	2346.6930	-0.0003	
3	3	1	2	2	0	2346.7040	2346.7032	0.0008	
7	1	7	6	0	6	2346.8470	2346.8465	0.0005	
6	2	4	5	3	3	2346.8600	2346.8591	0.0009	0.01127
6	3	3	5	4	2	2346.8600	2346.8609	-0.0008	0.00417
						Blend	2346.8596	0.0004	
8	0	8	7	1	7	2346.9095	2346.9092	0.0003	
9	1	9	8	0	8	2346.9720	2346.9719	0.0000	
8	2	6	7	3	5	2346.9881	2346.9894	-0.0013	0.01121
7	4	4	6	3	3	2346.9881	2346.9874	0.0007	0.00817
						Blend	2346.9885	-0.0004	
9	2	8	8	1	7	2347.0116	2347.0118	-0.0002	
8	3	5	7	4	4	2347.0262	2347.0259	0.0003	
6	5	1	5	4	2	2347.0289	2347.0293	-0.0004	
10	0	10	9	1	9	2347.0345	2347.0348	-0.0003	
6	6	0	5	5	1	2347.0435	2347.0434	0.0001	
9	3	7	8	2	6	2347.0521	2347.0521	0.0000	
10	1	9	9	2	8	2347.0742	2347.0745	-0.0003	
11	1	11	10	0	10	2347.0976	2347.0978	-0.0002	
10	2	8	9	3	7	2347.1145	2347.1145	0.0000	
7	6	2	6	5	1	2347.1211	2347.1211	0.0001	
7	7	1	6	6	0	2347.1520	2347.1525	-0.0005	
12	0	12	11	1	11	2347.1616	2347.1608	0.0007	
11	3	9	10	2	8	2347.1764	2347.1771	-0.0007	
8	8	0	7	7	1	2347.2623	2347.2625	-0.0001	0.01089
13	2	12	12	1	11	2347.2623	2347.2632	-0.0009	0.00430
						Blend	2347.2627	-0.0004	
6	2	5	7	3	5	2350.3645	2350.3643	0.0003	0.02371
6	3	4	7	4	4	2350.3645	2350.3651	-0.0006	0.02939
						Blend	2350.3647	-0.0002	
5	2	3	6	3	3	2350.4808	2350.4802	0.0006	0.03960
7	2	5	8	2	6	2350.4808	2350.4823	-0.0014	0.01558
5	3	2	6	4	2	2350.4808	2350.4815	-0.0006	0.04395
						Blend	2350.4811	-0.0003	
4	4	1	5	5	1	2350.5392	2350.5396	-0.0004	
4	3	2	5	4	2	2350.5591	2350.5602	-0.0011	0.04612
5	3	2	6	3	3	2350.5591	2350.5585	0.0006	0.01964
						Blend	2350.5597	-0.0006	
3	3	0	4	4	0	2350.6530	2350.6531	-0.0001	
3	2	1	4	3	1	2350.6791	2350.6791	0.0001	
5	0	5	6	0	6	2350.6902	2350.6909	-0.0006	

3	0	3	4	0	4	2350.8162	2350.8158	0.0004		
1	1	0	2	2	0	2350.8750	2350.8751	0.0000		
1	1	0	2	1	1	2350.9117	2350.9108	0.0008		
1	0	1	2	0	2	2350.9373	2350.9383	-0.0010	0.01993	
5	1	4	5	3	3	2350.9373	2350.9381	-0.0008	0.00724	
						Blend	2350.9383	-0.0009		
5	1	4	5	2	4	2351.0813	2351.0821	-0.0008	0.07334	
5	0	5	5	1	5	2351.0813	2351.0828	-0.0015	0.13039	
6	1	6	6	0	6	2351.0813	2351.0819	-0.0006	0.12777	
7	0	7	7	1	7	2351.0813	2351.0808	0.0005	0.11718	
8	1	8	8	0	8	2351.0813	2351.0796	0.0017	0.10147	
6	2	5	6	1	5	2351.0813	2351.0820	-0.0007	0.07700	
7	1	6	7	2	6	2351.0813	2351.0808	0.0004	0.07337	
8	2	7	8	1	7	2351.0813	2351.0797	0.0016	0.06491	
						Blend	2351.0813	0.0000		
3	2	1	3	2	2	2351.1228	2351.1235	-0.0007		
3	2	1	2	1	1	2351.3860	2351.3844	0.0016	0.05719	
3	1	2	2	0	2	2351.3860	2351.3865	-0.0005	0.03755	
						Blend	2351.3852	0.0008		
3	3	0	2	2	0	2351.4056	2351.4051	0.0005		
5	0	5	4	0	4	2351.4131	2351.4128	0.0003	0.04033	
4	3	2	3	3	1	2351.4131	2351.4122	0.0009	0.01651	
						Blend	2351.4126	0.0005		
6	2	5	5	2	4	2351.5143	2351.5147	-0.0004	0.03224	
5	4	1	4	4	0	2351.5143	2351.5138	0.0005	0.01405	
						Blend	2351.5144	-0.0001		
4	4	1	3	3	1	2351.5219	2351.5215	0.0004		
5	2	3	4	1	3	2351.5885	2351.5883	0.0001		
5	5	0	4	4	0	2351.6320	2351.6318	0.0001		
7	4	3	6	3	3	2351.7766	2351.7759	0.0006	0.05004	
11	0	11	10	0	10	2351.7766	2351.7763	0.0002	0.01858	
						Blend	2351.7760	0.0005		
7	6	1	6	5	1	2351.8228	2351.8229	-0.0001		

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Table A-3. Observed and fitted transitions of CO_2-$(CO)_2$ (cm^{-1}).
Int = calculated relative intensity, used to weight the blended lines.

2348 > nu > 2351 = fundamental band
2364 > nu > 2367 = combination band

J'	Ka'	Kc'	J"	Ka"	Kc"	Obs	Calc	Obs-Calc	Int
7	3	4	8	4	4	2348.6429	2348.6415	0.0015	0.00054
7	5	2	8	6	2	2348.6429	2348.6437	-0.0007	0.00056
						Blend	2348.6426	0.0003	
6	3	4	7	4	4	2348.7387	2348.7383	0.0004	0.00077
6	2	5	7	3	5	2348.7387	2348.7375	0.0012	0.00065
						Blend	2348.7380	0.0007	
5	5	0	6	6	0	2348.8076	2348.8080	-0.0003	
5	4	1	6	5	1	2348.8399	2348.8395	0.0004	
4	4	1	5	5	1	2348.9193	2348.9192	0.0001	
4	3	2	5	4	2	2348.9387	2348.9389	-0.0002	
4	1	4	5	2	4	2348.9464	2348.9468	-0.0004	0.00079
4	2	3	5	3	3	2348.9464	2348.9464	0.0000	0.00124
						Blend	2348.9466	-0.0001	
3	3	0	4	4	0	2349.0355	2349.0352	0.0002	
3	0	3	4	1	3	2349.0529	2349.0530	0.0000	
3	1	2	4	2	2	2349.0595	2349.0604	-0.0009	0.00160
3	2	1	4	3	1	2349.0595	2349.0587	0.0008	0.00186
						Blend	2349.0595	0.0000	
2	2	1	3	3	1	2349.1429	2349.1426	0.0003	
2	1	2	3	2	2	2349.1545	2349.1545	0.0000	
1	1	0	2	2	0	2349.2590	2349.2586	0.0004	
1	0	1	2	1	1	2349.2675	2349.2676	-0.0001	
3	1	2	3	2	2	2349.4653	2349.4639	0.0013	0.00153
5	2	3	5	3	3	2349.4653	2349.4649	0.0004	0.00117
1	0	1	1	1	1	2349.4653	2349.4648	0.0004	0.00147
7	3	4	7	4	4	2349.4653	2349.4660	-0.0007	0.00064
						Blend	2349.4647	0.0005	
5	0	5	5	1	5	2349.4715	2349.4720	-0.0005	0.00459
9	0	9	9	1	9	2349.4715	2349.4722	-0.0007	0.00219
7	1	6	7	2	6	2349.4715	2349.4713	0.0002	0.00214
5	1	4	5	2	4	2349.4715	2349.4712	0.0003	0.00250
6	2	5	6	1	5	2349.4715	2349.4715	0.0001	0.00244
3	0	3	3	1	3	2349.4715	2349.4717	-0.0002	0.00399
7	0	7	7	1	7	2349.4715	2349.4721	-0.0005	0.00362
4	1	4	4	0	4	2349.4715	2349.4720	-0.0005	0.00454
6	1	6	6	0	6	2349.4715	2349.4720	-0.0005	0.00423
8	1	8	8	0	8	2349.4715	2349.4721	-0.0006	0.00290
						Blend	2349.4719	-0.0003	
4	3	2	4	2	2	2349.4917	2349.4921	-0.0004	0.00081
2	2	1	2	1	1	2349.4917	2349.4933	-0.0017	0.00071
						Blend	2349.4927	-0.0010	
1	1	0	0	0	0	2349.5782	2349.5778	0.0004	
3	2	1	2	1	1	2349.7798	2349.7795	0.0003	
3	1	2	2	0	2	2349.7832	2349.7831	0.0002	
3	3	0	2	2	0	2349.7946	2349.7948	-0.0002	
4	3	2	3	2	2	2349.8953	2349.8956	-0.0004	
5	5	0	4	4	0	2350.0186	2350.0189	-0.0004	
6	4	3	5	3	3	2350.1005	2350.1007	-0.0002	0.00174
6	2	5	5	1	5	2350.1005	2350.1017	-0.0012	0.00093
6	3	4	5	2	4	2350.1005	2350.0999	0.0006	0.00145

						Blend	2350.1007	-0.0002		
6	6	1	5	5	1	2350.1309	2350.1316	-0.0007		
7	5	2	6	4	2	2350.1880	2350.1888	-0.0007	0.00150	
7	4	3	6	3	3	2350.1880	2350.1886	-0.0006	0.00144	
						Blend	2350.1887	-0.0007		
7	6	1	6	5	1	2350.2130	2350.2128	0.0002		
7	7	0	6	6	0	2350.2413	2350.2413	0.0000		
8	5	4	7	4	4	2350.3063	2350.3057	0.0006	0.00098	
8	4	5	7	3	5	2350.3063	2350.3070	-0.0007	0.00092	
						Blend	2350.3063	0.0000		
8	2	7	7	1	7	2350.3116	2350.3115	0.0001	0.00052	
8	6	3	7	5	3	2350.3116	2350.3116	0.0000	0.00099	
						Blend	2350.3116	0.0001		
8	8	1	7	7	1	2350.3520	2350.3514	0.0006		
8	6	3	9	6	4	2364.4811	2364.4805	0.0006		
10	3	8	11	3	9	2364.4855	2364.4857	-0.0001		
10	2	9	11	2	10	2364.5262	2364.5262	0.0001	0.00035	
7	7	0	8	7	1	2364.5262	2364.5251	0.0012	0.00015	
						Blend	2364.5258	0.0004		
7	5	2	8	5	3	2364.5324	2364.5315	0.0009		
9	2	7	10	2	8	2364.5406	2364.5411	-0.0005		
5	3	2	6	5	1	2364.5504	2364.5515	-0.0011		
8	4	5	9	4	6	2364.5565	2364.5559	0.0006		
7	4	3	8	4	4	2364.5664	2364.5660	0.0003	0.00050	
10	1	10	11	1	11	2364.5664	2364.5670	-0.0006	0.00053	
						Blend	2364.5665	-0.0001		
9	1	8	10	1	9	2364.5821	2364.5820	0.0000		
8	3	6	9	3	7	2364.5965	2364.5971	-0.0006		
7	3	4	8	3	5	2364.6114	2364.6111	0.0002		
9	0	9	10	0	10	2364.6230	2364.6231	-0.0001		
8	2	7	9	2	8	2364.6383	2364.6383	-0.0001	0.00076	
6	5	2	7	5	3	2364.6383	2364.6380	0.0003	0.00054	
						Blend	2364.6382	0.0001		
8	1	8	9	1	9	2364.6801	2364.6798	0.0003		
5	4	1	6	4	2	2364.6953	2364.6955	-0.0002	0.00095	
7	1	6	8	1	7	2364.6953	2364.6951	0.0002	0.00103	
						Blend	2364.6953	0.0000		
6	3	4	7	3	5	2364.7098	2364.7101	-0.0003		
5	3	2	6	3	3	2364.7194	2364.7199	-0.0004		
7	0	7	8	0	8	2364.7369	2364.7369	0.0000		
6	2	5	7	2	6	2364.7522	2364.7522	0.0000		
5	2	3	6	2	4	2364.7656	2364.7659	-0.0003		
5	1	4	6	1	5	2364.8099	2364.8096	0.0003		
4	3	2	5	3	3	2364.8281	2364.8284	-0.0003		
5	0	5	6	0	6	2364.8525	2364.8523	0.0002		
3	3	0	4	3	1	2364.8677	2364.8688	-0.0012	0.00106	
4	2	3	5	2	4	2364.8677	2364.8678	-0.0001	0.00167	
						Blend	2364.8682	-0.0005		
3	2	1	4	2	2	2364.8812	2364.8816	-0.0004		
4	1	4	5	1	5	2364.9108	2364.9106	0.0002		
3	1	2	4	1	3	2364.9243	2364.9240	0.0003		
3	0	3	4	0	4	2364.9691	2364.9693	-0.0002		
2	2	1	3	2	2	2364.9911	2364.9912	-0.0001		
2	1	2	3	1	3	2365.0290	2365.0287	0.0002		
1	1	0	2	1	1	2365.0522	2365.0526	-0.0004		
1	0	1	2	0	2	2365.0855	2365.0860	-0.0005		
6	3	4	6	3	3	2365.1019	2365.1020	-0.0001		
5	2	3	5	4	2	2365.1098	2365.1105	-0.0007		
4	2	3	4	2	2	2365.1372	2365.1379	-0.0007	0.00071	

3	1	2	3	3	1	2365.1372	2365.1370	0.0002	0.00044
						Blend	2365.1376	-0.0003	
6	4	3	6	4	2	2365.1745	2365.1758	-0.0013	0.00064
2	1	2	2	1	1	2365.1745	2365.1737	0.0007	0.00071
						Blend	2365.1747	-0.0002	
4	3	2	4	3	1	2365.1975	2365.1983	-0.0008	
2	2	1	2	2	0	2365.2156	2365.2159	-0.0002	
6	5	2	6	5	1	2365.2221	2365.2224	-0.0003	0.00127
6	6	1	6	6	0	2365.2221	2365.2212	0.0009	0.00211
4	4	1	4	4	0	2365.2221	2365.2232	-0.0011	0.00312
						Blend	2365.2224	-0.0003	
5	5	0	5	5	1	2365.2283	2365.2281	0.0002	
3	3	0	3	3	1	2365.2387	2365.2389	-0.0002	
1	1	0	1	1	1	2365.2500	2365.2498	0.0002	0.00147
7	6	1	7	6	2	2365.2500	2365.2509	-0.0009	0.00093
						Blend	2365.2503	-0.0002	
5	4	1	5	4	2	2365.2677	2365.2682	-0.0005	
3	2	1	3	2	2	2365.2855	2365.2852	0.0003	
1	0	1	0	0	0	2365.3108	2365.3107	0.0001	0.00104
2	2	1	2	0	2	2365.3108	2365.3104	0.0004	0.00043
						Blend	2365.3106	0.0002	
5	3	2	5	3	3	2365.3338	2365.3335	0.0003	
3	1	2	3	1	3	2365.3438	2365.3427	0.0011	
4	3	2	4	1	3	2365.3557	2365.3553	0.0004	0.00059
4	4	1	4	2	2	2365.3557	2365.3546	0.0011	0.00018
						Blend	2365.3552	0.0006	
2	1	2	1	1	1	2365.3719	2365.3710	0.0009	
3	0	3	2	0	2	2365.4367	2365.4369	-0.0002	
3	1	2	2	1	1	2365.4877	2365.4878	-0.0001	
4	1	4	3	1	3	2365.4976	2365.4977	-0.0001	
3	2	1	2	2	0	2365.5103	2365.5098	0.0005	
4	2	3	3	2	2	2365.5417	2365.5415	0.0002	
5	0	5	4	0	4	2365.5602	2365.5599	0.0003	
4	3	2	3	3	1	2365.5692	2365.5684	0.0008	
3	3	0	2	1	1	2365.5889	2365.5897	-0.0007	0.00040
9	2	7	9	2	8	2365.5889	2365.5895	-0.0006	0.00014
						Blend	2365.5896	-0.0007	
5	1	4	4	1	3	2365.6086	2365.6081	0.0005	
6	1	6	5	1	5	2365.6228	2365.6223	0.0005	
5	2	3	4	2	2	2365.6636	2365.6637	-0.0001	
6	2	5	5	2	4	2365.6702	2365.6698	0.0004	
7	0	7	6	0	6	2365.6853	2365.6850	0.0003	
5	4	1	4	4	0	2365.6904	2365.6900	0.0005	
5	3	2	4	3	1	2365.7031	2365.7033	-0.0002	
6	3	4	5	3	3	2365.7155	2365.7156	-0.0001	
7	1	6	6	1	5	2365.7329	2365.7330	0.0000	
8	1	8	7	1	7	2365.7485	2365.7481	0.0003	0.00209
6	4	3	5	4	2	2365.7485	2365.7484	0.0001	0.00117
						Blend	2365.7482	0.0002	
7	2	5	6	2	4	2365.7822	2365.7820	0.0002	
8	2	7	7	2	6	2365.7963	2365.7963	0.0000	
9	0	9	8	0	8	2365.8115	2365.8117	-0.0001	
7	3	4	6	3	3	2365.8388	2365.8391	-0.0003	
8	3	6	7	3	5	2365.8449	2365.8447	0.0002	
9	1	8	8	1	7	2365.8602	2365.8600	0.0002	
10	1	10	9	1	9	2365.8751	2365.8756	-0.0005	
9	2	7	8	2	6	2365.9083	2365.9087	-0.0004	
10	2	9	9	2	8	2365.9243	2365.9241	0.0003	
9	3	6	8	3	5	2365.9583	2365.9586	-0.0002	

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  10    3    8       9    3    7 2365.9726    2365.9729 -0.0002
  11    1   10      10    1    9 2365.9888    2365.9885  0.0002
   9    4    5       8    4    4 2366.0160    2366.0155  0.0005
  10    4    7       9    4    6 2366.0217    2366.0222 -0.0005
  11    2    9      10    2    8 2366.0375    2366.0374  0.0000
  12    2   11      11    2   10 2366.0533    2366.0534 -0.0001
*********************************************************************
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Table A-4. Ground state combination difference fit to CO_2-$(N_2)_2$ (cm^{-1}).

J'	Ka'	Kc'	J"	Ka"	Kc"	Obs	Calc	Obs-Calc
3	0	3	1	0	1	0.3926	0.3922	0.0003
4	2	2	2	0	2	0.8212	0.8201	0.0012
4	0	4	2	0	2	0.5274	0.5279	-0.0005
4	1	4	2	1	2	0.5274	0.5277	-0.0004
5	2	3	3	0	3	1.0557	1.0561	-0.0004
5	4	1	3	2	1	1.0476	1.0474	0.0002
5	0	5	3	0	3	0.6643	0.6646	-0.0003
4	1	4	3	1	2	0.1765	0.1761	0.0004
5	3	3	3	1	3	1.0557	1.0563	-0.0007
5	1	5	3	1	3	0.6643	0.6646	-0.0003
6	4	3	4	2	3	1.2904	1.2904	0.0001
6	6	1	4	4	1	1.3070	1.3068	0.0002
6	2	5	4	2	3	0.8989	0.8991	-0.0002
6	2	4	4	0	4	1.2904	1.2908	-0.0004
6	0	6	4	0	4	0.8015	0.8014	0.0001
6	3	4	4	1	4	1.2904	1.2908	-0.0004
6	1	6	4	1	4	0.8015	0.8014	0.0001
6	3	3	4	1	3	1.2904	1.2898	0.0007
6	5	1	4	3	1	1.2819	1.2809	0.0010
6	1	5	4	1	3	0.8989	0.8991	-0.0002
7	2	5	5	0	5	1.5244	1.5251	-0.0008
6	2	5	5	2	3	0.3135	0.3126	0.0009
7	4	4	5	2	4	1.5244	1.5245	-0.0002
7	3	4	5	1	4	1.5244	1.5245	-0.0002
7	7	0	5	5	0	1.5387	1.5387	0.0001
7	3	5	5	1	5	1.5244	1.5251	-0.0008
7	5	3	5	3	3	1.5244	1.5240	0.0003
6	1	5	5	3	3	0.3135	0.3124	0.0011
8	4	5	6	2	5	1.7581	1.7586	-0.0005
8	4	4	6	2	4	1.7581	1.7577	0.0003
8	6	2	6	4	2	1.7457	1.7458	-0.0001
8	8	0	6	6	0	1.7776	1.7768	0.0008
8	5	4	6	3	4	1.7581	1.7578	0.0002
8	3	5	6	1	5	1.7581	1.7586	-0.0005
9	1	9	7	0	7	1.2117	1.2122	-0.0005
9	0	9	7	1	7	1.2117	1.2122	-0.0005
10	6	5	8	4	5	2.2238	2.2242	-0.0004
10	6	4	8	4	4	2.2238	2.2225	0.0012
10	8	2	8	6	2	2.2076	2.2078	-0.0002
10	10	0	8	8	0	2.2516	2.2511	0.0005
10	0	10	8	0	8	1.3494	1.3492	0.0002
10	7	4	8	5	4	2.2238	2.2230	0.0008
10	1	10	8	1	8	1.3494	1.3492	0.0002
10	5	5	8	3	5	2.2238	2.2241	-0.0004
10	9	1	8	7	1	2.2191	2.2192	0.0000
11	11	0	9	9	0	2.4871	2.4868	0.0003
11	11	1	9	9	1	2.4871	2.4882	-0.0011

Table A-5. Fundamental band fit of CO_2-$(N_2)_2$ (cm^{-1}).
Int = calculated relative intensity, used to weight the blended lines.

J'	Ka'	Kc'	J"	Ka"	Kc"	Obs	Calc	Obs-Calc	Int
11	5	7	12	6	7	2348.6227	2348.6230	-0.0003	0.01632
11	5	6	12	6	6	2348.6227	2348.6225	0.0001	0.01623
11	6	6	12	7	6	2348.6227	2348.6225	0.0001	0.01623
11	3	8	12	4	8	2348.6227	2348.6236	-0.0009	0.01603
11	4	8	12	5	8	2348.6227	2348.6236	-0.0009	0.01603
11	6	5	12	7	5	2348.6227	2348.6224	0.0003	0.01599
11	7	5	12	8	5	2348.6227	2348.6223	0.0003	0.01598
11	7	4	12	8	4	2348.6227	2348.6229	-0.0002	0.01573
11	4	7	12	5	7	2348.6227	2348.6230	-0.0003	0.01632
					Blend		2348.6229	-0.0002	
10	10	1	11	11	1	2348.7260	2348.7258	0.0003	0.02407
10	10	0	11	11	0	2348.7260	2348.7262	-0.0001	0.02409
					Blend		2348.7260	0.0001	
9	9	0	10	10	0	2348.8446	2348.8448	-0.0002	0.01126
9	9	1	10	10	1	2348.8446	2348.8442	0.0004	0.01125
					Blend		2348.8445	0.0001	
9	3	7	10	4	7	2348.8580	2348.8588	-0.0008	0.01270
9	2	7	10	3	7	2348.8580	2348.8588	-0.0008	0.01270
9	4	6	10	5	6	2348.8580	2348.8583	-0.0002	0.01308
9	3	6	10	4	6	2348.8580	2348.8583	-0.0002	0.01308
9	4	5	10	5	5	2348.8580	2348.8579	0.0001	0.01297
9	6	4	10	7	4	2348.8580	2348.8579	0.0002	0.01268
9	5	5	10	6	5	2348.8580	2348.8579	0.0001	0.01297
9	5	4	10	6	4	2348.8580	2348.8581	-0.0001	0.01268
					Blend		2348.8582	-0.0002	
9	7	2	10	8	2	2348.8632	2348.8632	0.0000	
8	8	1	9	9	1	2348.9637	2348.9629	0.0007	
8	8	0	9	9	0	2348.9637	2348.9639	-0.0002	
8	4	4	9	5	4	2348.9762	2348.9758	0.0004	0.05705
8	2	6	9	3	6	2348.9762	2348.9762	0.0000	0.04851
8	6	3	9	7	3	2348.9762	2348.9753	0.0010	0.05871
8	2	7	9	3	7	2348.9762	2348.9768	-0.0006	0.03945
8	3	6	9	4	6	2348.9762	2348.9762	0.0000	0.04851
8	5	4	9	6	4	2348.9762	2348.9757	0.0006	0.05703
8	3	5	9	4	5	2348.9762	2348.9758	0.0004	0.05390
8	4	5	9	5	5	2348.9762	2348.9758	0.0004	0.05390
8	1	7	9	2	7	2348.9762	2348.9768	-0.0006	0.03945
					Blend		2348.9760	0.0003	
7	7	0	8	8	0	2349.0827	2349.0833	-0.0007	
7	7	1	8	8	1	2349.0827	2349.0819	0.0008	
7	6	2	8	7	2	2349.0898	2349.0904	-0.0006	
7	4	4	8	5	4	2349.0940	2349.0936	0.0004	0.03627
7	2	6	8	3	6	2349.0940	2349.0942	-0.0003	0.02862
7	3	4	8	4	4	2349.0940	2349.0936	0.0004	0.03627
7	5	3	8	6	3	2349.0940	2349.0933	0.0007	0.03738
7	2	5	8	3	5	2349.0940	2349.0938	0.0002	0.03376
7	3	5	8	4	5	2349.0940	2349.0938	0.0002	0.03376
7	1	6	8	2	6	2349.0940	2349.0942	-0.0003	0.02862
7	4	3	8	5	3	2349.0940	2349.0946	-0.0006	0.03741
					Blend		2349.0939	0.0001	
7	5	2	8	6	2	2349.0988	2349.0984	0.0004	
6	6	0	7	7	0	2349.2025	2349.2031	-0.0006	
6	0	6	7	1	6	2349.2117	2349.2123	-0.0006	0.02732

6	1	6	7	2	6	2349.2117	2349.2123	-0.0006	0.02732
6	1	5	7	2	5	2349.2117	2349.2118	-0.0001	0.04271
6	2	5	7	3	5	2349.2117	2349.2118	-0.0001	0.04271
6	3	4	7	4	4	2349.2117	2349.2115	0.0002	0.05126
6	3	3	7	4	3	2349.2117	2349.2120	-0.0003	0.05592
6	4	3	7	5	3	2349.2117	2349.2112	0.0005	0.05590
6	2	4	7	3	4	2349.2117	2349.2115	0.0002	0.05126
					Blend		2349.2117	0.0000	
5	5	1	6	6	1	2349.3209	2349.3204	0.0004	
5	5	0	6	6	0	2349.3232	2349.3230	0.0002	
5	1	4	6	2	4	2349.3295	2349.3294	0.0001	0.06059
5	0	5	6	1	5	2349.3295	2349.3298	-0.0003	0.03818
5	1	5	6	2	5	2349.3295	2349.3298	-0.0003	0.03818
5	3	3	6	4	3	2349.3295	2349.3292	0.0003	0.07358
5	2	4	6	3	4	2349.3295	2349.3294	0.0001	0.06059
5	2	3	6	3	3	2349.3295	2349.3296	-0.0001	0.07360
					Blend		2349.3295	0.0000	
5	4	1	6	5	1	2349.3326	2349.3329	-0.0003	
4	4	1	5	5	1	2349.4399	2349.4398	0.0002	
4	4	0	5	5	0	2349.4430	2349.4428	0.0002	
4	1	4	5	2	4	2349.4472	2349.4474	-0.0002	0.05083
4	2	3	5	3	3	2349.4472	2349.4471	0.0001	0.08128
4	0	4	5	1	4	2349.4472	2349.4474	-0.0002	0.05083
4	1	3	5	2	3	2349.4472	2349.4472	-0.0001	0.08129
					Blend		2349.4472	-0.0001	
4	3	1	5	4	1	2349.4505	2349.4508	-0.0003	
3	0	3	4	1	3	2349.5654	2349.5650	0.0004	0.06417
3	1	2	4	2	2	2349.5654	2349.5659	-0.0005	0.10203
3	1	3	4	2	3	2349.5654	2349.5649	0.0004	0.06417
					Blend		2349.5654	0.0000	
2	2	1	3	3	1	2349.6788	2349.6783	0.0005	
2	1	2	3	2	2	2349.6822	2349.6823	-0.0001	0.07598
2	0	2	3	1	2	2349.6822	2349.6830	-0.0008	0.07601
2	2	0	3	3	0	2349.6822	2349.6812	0.0009	0.12849
					Blend		2349.6820	0.0002	
2	1	1	3	2	1	2349.6850	2349.6856	-0.0006	
1	1	0	0	0	0	2350.1523	2350.1525	-0.0002	
3	2	1	2	1	1	2350.3829	2350.3827	0.0002	
3	3	0	2	2	0	2350.3866	2350.3874	-0.0007	0.16014
3	1	2	2	0	2	2350.3866	2350.3860	0.0007	0.09469
3	2	2	2	1	2	2350.3866	2350.3868	-0.0002	0.09470
					Blend		2350.3868	-0.0002	
3	3	1	2	2	1	2350.3903	2350.3908	-0.0005	
4	3	1	3	2	1	2350.4981	2350.4982	-0.0001	
4	1	3	3	0	3	2350.5028	2350.5034	-0.0005	0.08606
4	3	2	3	2	2	2350.5028	2350.5036	-0.0007	0.13674
4	2	3	3	1	3	2350.5028	2350.5034	-0.0006	0.08606
					Blend		2350.5035	-0.0006	
5	4	1	4	3	1	2350.6144	2350.6138	0.0007	
5	3	3	4	2	3	2350.6199	2350.6195	0.0004	0.11731
5	4	2	4	3	2	2350.6199	2350.6202	-0.0003	0.14266
5	2	4	4	1	4	2350.6199	2350.6202	-0.0003	0.07337
5	1	4	4	0	4	2350.6199	2350.6202	-0.0003	0.07337
5	2	3	4	1	3	2350.6199	2350.6193	0.0006	0.11731
					Blend		2350.6199	0.0001	
5	5	1	4	4	1	2350.6279	2350.6272	0.0007	
6	5	1	5	4	1	2350.7298	2350.7293	0.0005	
6	2	4	5	1	4	2350.7361	2350.7360	0.0001	0.09414
6	2	5	5	1	5	2350.7361	2350.7369	-0.0008	0.05934

6	4	3	5	3	3	2350.7361	2350.7353	0.0008	0.11427
6	3	4	5	2	4	2350.7361	2350.7360	0.0001	0.09414
6	1	5	5	0	5	2350.7361	2350.7369	-0.0008	0.05934
					Blend		2350.7361	0.0000	
6	6	0	5	5	0	2350.7413	2350.7418	-0.0005	
6	6	1	5	5	1	2350.7448	2350.7452	-0.0004	
7	5	2	6	4	2	2350.8445	2350.8442	0.0003	0.09738
7	6	1	6	5	1	2350.8445	2350.8450	-0.0005	0.09982
					Blend		2350.8446	-0.0001	
7	3	5	6	2	5	2350.8521	2350.8524	-0.0003	0.07140
7	4	4	6	3	4	2350.8521	2350.8514	0.0007	0.08567
7	2	5	6	1	5	2350.8521	2350.8524	-0.0003	0.07140
7	3	4	6	2	4	2350.8521	2350.8514	0.0007	0.08567
					Blend		2350.8519	0.0002	
7	7	0	6	6	0	2350.8603	2350.8602	0.0001	
7	7	1	6	6	1	2350.8619	2350.8629	-0.0010	
8	6	2	7	5	2	2350.9573	2350.9576	-0.0003	
8	7	1	7	6	1	2350.9616	2350.9609	0.0007	
8	8	0	7	7	0	2350.9791	2350.9783	0.0008	
9	7	2	8	6	2	2351.0708	2351.0710	-0.0002	
9	8	1	8	7	1	2351.0772	2351.0768	0.0003	0.04299
9	6	3	8	5	3	2351.0772	2351.0771	0.0001	0.04356
					Blend		2351.0769	0.0002	
9	5	5	8	4	5	2351.0818	2351.0821	-0.0003	0.04323
9	6	4	8	5	4	2351.0818	2351.0808	0.0010	0.04375
9	7	3	8	6	3	2351.0818	2351.0803	0.0014	0.04353
9	4	5	8	3	5	2351.0818	2351.0821	-0.0003	0.04323
9	5	4	8	4	4	2351.0818	2351.0806	0.0012	0.04375
					Blend		2351.0812	0.0006	
9	9	0	8	8	0	2351.0962	2351.0959	0.0002	
10	8	2	9	7	2	2351.1840	2351.1843	-0.0003	
10	7	3	9	6	3	2351.1889	2351.1897	-0.0008	
10	10	1	9	9	1	2351.2131	2351.2140	-0.0009	0.11083
10	10	0	9	9	0	2351.2131	2351.2130	0.0002	0.11082
					Blend		2351.2135	-0.0004	
11	9	2	10	8	2	2351.2980	2351.2976	0.0004	
11	11	1	10	10	1	2351.3295	2351.3301	-0.0006	0.04245
11	11	0	10	10	0	2351.3295	2351.3294	0.0001	0.04241
					Blend		2351.3298	-0.0003	
12	9	3	11	8	3	2351.4121	2351.4133	-0.0012	0.02853
12	10	2	11	9	2	2351.4121	2351.4108	0.0012	0.02833
					Blend		2351.4121	0.0000	

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Table A-6. Combination band fit of CO_2-$(N2)_2$ (cm^{-1}).
Int = calculated relative intensity, used to weight the blended lines.

J'	Ka'	Kc'	J"	Ka"	Kc"	Obs	Calc	Obs-Calc	Int
5	1	4	6	1	5	2364.9676	2364.9670	0.0006	0.01639
5	2	4	6	2	5	2364.9676	2364.9670	0.0006	0.01639
					Blend		2364.9670	0.0006	
5	0	5	6	0	6	2365.0037	2365.0037	0.0001	0.02358
5	1	5	6	1	6	2365.0037	2365.0037	0.0001	0.02358
					Blend		2365.0037	0.0001	
4	0	4	5	0	5	2365.0700	2365.0700	0.0000	0.02622
4	1	4	5	1	5	2365.0700	2365.0700	0.0000	0.02622
					Blend		2365.0700	0.0000	
3	0	3	4	0	4	2365.1364	2365.1364	-0.0001	0.02681
3	1	3	4	1	4	2365.1364	2365.1364	-0.0001	0.02681
					Blend		2365.1364	-0.0001	
2	0	2	3	0	3	2365.2028	2365.2030	-0.0002	
2	1	2	1	1	1	2365.5916	2365.5927	-0.0011	
2	0	2	1	0	1	2365.5954	2365.5952	0.0002	
4	1	3	4	1	4	2365.6166	2365.6173	-0.0007	0.00644
4	2	3	4	0	4	2365.6166	2365.6173	-0.0007	0.00644
					Blend		2365.6173	-0.0007	
3	0	3	2	0	2	2365.6637	2365.6643	-0.0006	0.02809
3	1	3	2	1	2	2365.6637	2365.6641	-0.0004	0.02806
					Blend		2365.6642	-0.0005	
3	1	2	2	1	1	2365.7255	2365.7234	0.0022	
4	0	4	3	0	3	2365.7343	2365.7346	-0.0003	0.03275
4	1	4	3	1	3	2365.7343	2365.7345	-0.0003	0.03274
					Blend		2365.7345	-0.0003	
4	1	3	3	1	2	2365.7932	2365.7934	-0.0002	
5	0	5	4	0	4	2365.8052	2365.8051	0.0001	0.03423
5	1	5	4	1	4	2365.8052	2365.8051	0.0001	0.03423
					Blend		2365.8051	0.0001	
5	1	4	4	1	3	2365.8665	2365.8661	0.0004	0.02476
5	2	4	4	2	3	2365.8665	2365.8660	0.0004	0.02475
					Blend		2365.8661	0.0004	
6	0	6	5	0	5	2365.8762	2365.8757	0.0004	0.03201
6	1	6	5	1	5	2365.8762	2365.8757	0.0004	0.03201
					Blend		2365.8757	0.0004	
6	1	5	5	1	4	2365.9405	2365.9395	0.0010	
6	3	4	5	3	3	2365.9992	2366.0007	-0.0015	0.01614
6	2	4	5	2	3	2365.9992	2366.0009	-0.0017	0.01610
					Blend		2366.0008	-0.0016	
7	3	5	6	3	4	2366.0780	2366.0772	0.0008	0.01393
7	2	5	6	2	4	2366.0780	2366.0772	0.0008	0.01393
					Blend		2366.0772	0.0008	
8	0	8	7	0	7	2366.0165	2366.0174	-0.0009	
8	1	8	9	1	9	2364.8048	2364.8053	-0.0005	
8	1	8	7	1	7	2366.0165	2366.0174	-0.0009	
8	0	8	9	0	9	2364.8048	2364.8053	-0.0005	
9	2	8	8	2	7	2366.1605	2366.1612	-0.0008	
9	0	9	8	0	8	2366.0891	2366.0884	0.0006	
9	0	9	10	0	10	2364.7397	2364.7392	0.0005	
9	1	9	8	1	8	2366.0891	2366.0884	0.0006	
9	1	9	10	1	10	2364.7397	2364.7392	0.0005	
9	1	8	8	1	7	2366.1605	2366.1612	-0.0008	0.01140
6	5	1	5	5	0	2366.1605	2366.1596	0.0009	0.00954

Blend	2366.1605	0.0000

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Table A-7. Fundamental band fit of CO_2-CO-N_2 (cm^{-1}).
Int = calculated relative intensity, used to weight the blended lines.

J'	Ka'	Kc'	J"	Ka"	Kc"	Obs	Calc	Obs-Calc	Int
7	4	4	8	5	4	2348.8665	2348.8663	0.0003	0.45343
7	2	5	8	3	5	2348.8665	2348.8662	0.0004	0.42803
7	3	5	8	4	5	2348.8665	2348.8660	0.0005	0.42796
7	1	6	8	2	6	2348.8665	2348.8659	0.0006	0.36908
7	2	6	8	3	6	2348.8665	2348.8659	0.0006	0.36907
7	0	7	8	1	7	2348.8665	2348.8664	0.0002	0.24577
7	1	7	8	2	7	2348.8665	2348.8664	0.0002	0.24577
						Blend	2348.8661	0.0004	
5	3	3	6	4	3	2349.0882	2349.0875	0.0008	0.99683
5	1	4	6	2	4	2349.0882	2349.0886	-0.0004	0.83237
5	2	4	6	3	4	2349.0882	2349.0883	-0.0001	0.83211
5	0	5	6	1	5	2349.0882	2349.0884	-0.0001	0.53203
5	1	5	6	2	5	2349.0882	2349.0883	-0.0001	0.53203
						Blend	2349.0882	0.0001	
4	4	1	5	5	1	2349.1784	2349.1781	0.0003	
4	2	2	5	3	2	2349.2083	2349.2082	0.0001	
3	3	1	4	4	1	2349.2949	2349.2947	0.0002	
3	3	0	4	4	0	2349.2989	2349.2993	-0.0005	
3	2	2	4	3	2	2349.3073	2349.3073	0.0000	
3	1	3	4	2	3	2349.3095	2349.3101	-0.0007	0.93369
3	0	3	4	1	3	2349.3095	2349.3108	-0.0013	0.93421
						Blend	2349.3104	-0.0010	
3	2	1	4	3	1	2349.3166	2349.3170	-0.0004	1.75458
3	1	2	4	2	2	2349.3166	2349.3156	0.0010	1.48298
						Blend	2349.3163	0.0002	
2	2	1	3	3	1	2349.4102	2349.4105	-0.0002	
1	1	0	2	2	0	2349.5301	2349.5300	0.0000	
0	0	0	1	1	0	2349.6420	2349.6424	-0.0004	
3	3	0	2	2	0	2350.0898	2350.0896	0.0002	
3	3	1	2	2	1	2350.0950	2350.0948	0.0001	
4	4	1	3	3	1	2350.2095	2350.2090	0.0005	
5	5	0	4	4	0	2350.3203	2350.3203	0.0000	
5	5	1	4	4	1	2350.3230	2350.3234	-0.0004	
6	4	2	5	3	2	2350.4033	2350.4026	0.0007	
6	2	4	5	1	4	2350.4157	2350.4152	0.0006	1.34225
6	3	4	5	2	4	2350.4157	2350.4155	0.0003	1.34220
6	2	5	5	1	5	2350.4157	2350.4169	-0.0012	0.85868
6	4	3	5	3	3	2350.4157	2350.4151	0.0006	1.60806
6	1	5	5	0	5	2350.4157	2350.4169	-0.0012	0.85868
						Blend	2350.4157	0.0000	
6	6	0	5	5	0	2350.4373	2350.4361	0.0012	1.74313
6	6	1	5	5	1	2350.4373	2350.4380	-0.0007	1.74033
						Blend	2350.4370	0.0002	
7	4	3	6	3	3	2350.5158	2350.5158	0.0000	
7	6	1	6	5	1	2350.5254	2350.5251	0.0003	1.30089
7	5	3	6	4	3	2350.5254	2350.5249	0.0005	1.26314
7	4	4	6	3	4	2350.5254	2350.5243	0.0011	1.17619
7	3	5	6	2	5	2350.5254	2350.5260	-0.0005	0.99476
7	2	5	6	1	5	2350.5254	2350.5259	-0.0005	0.99476
						Blend	2350.5252	0.0002	
7	6	2	6	5	2	2350.5341	2350.5340	0.0001	
8	7	2	7	6	2	2350.6467	2350.6471	-0.0004	
9	5	5	8	4	5	2350.7417	2350.7428	-0.0011	0.54595

9	6	4	8	5	4	2350.7417	2350.7415	0.0002	0.54504
9	4	5	8	3	5	2350.7417	2350.7424	-0.0007	0.54600
					Blend		2350.7422	-0.0005	
9	7	3	8	6	3	2350.7452	2350.7460	-0.0007	0.53104
9	3	6	8	2	6	2350.7452	2350.7450	0.0002	0.52711
9	4	6	8	3	6	2350.7452	2350.7451	0.0002	0.52711
					Blend		2350.7454	-0.0001	
9	8	1	8	7	1	2350.7561	2350.7563	-0.0002	
9	9	1	8	8	1	2350.7816	2350.7815	0.0000	0.46585
9	9	0	8	8	0	2350.7816	2350.7813	0.0003	0.46577
					Blend		2350.7814	0.0002	

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Table A-8. Fundamental band fit of CO_2-$(CO)_3$ (cm^{-1}).
Int = calculated relative intensity, used to weight the blended lines.

J'	Ka'	Kc'	J"	Ka"	Kc"	Obs	Calc	Obs-Calc	Int
12	2	11	13	2	12	2348.4688	2348.4712	-0.0024	0.00006
12	2	10	13	2	11	2348.4688	2348.4671	0.0017	0.00006
12	3	10	13	3	11	2348.4688	2348.4691	-0.0003	0.00006
12	3	9	13	3	10	2348.4688	2348.4661	0.0026	0.00006
12	4	9	13	4	10	2348.4688	2348.4684	0.0004	0.00005
12	4	8	13	4	9	2348.4688	2348.4675	0.0013	0.00005
12	5	8	13	5	9	2348.4688	2348.4684	0.0004	0.00005
12	5	7	13	5	8	2348.4688	2348.4683	0.0005	0.00005
12	1	11	13	1	12	2348.4688	2348.4707	-0.0019	0.00006
					Blend		2348.4686	0.0002	
10	3	8	11	3	9	2348.5780	2348.5753	0.0027	0.00013
10	3	7	11	3	8	2348.5780	2348.5771	0.0008	0.00013
10	2	8	11	2	9	2348.5780	2348.5751	0.0029	0.00013
10	1	9	11	1	10	2348.5780	2348.5814	-0.0034	0.00014
10	2	9	11	2	10	2348.5780	2348.5787	-0.0007	0.00013
					Blend		2348.5776	0.0004	
8	4	4	9	4	5	2348.6856	2348.6850	0.0007	0.00020
8	5	4	9	5	5	2348.6856	2348.6851	0.0005	0.00016
8	2	7	9	2	8	2348.6856	2348.6862	-0.0005	0.00024
8	3	5	9	3	6	2348.6856	2348.6851	0.0005	0.00022
8	4	5	9	4	6	2348.6856	2348.6850	0.0006	0.00020
8	0	8	9	0	9	2348.6856	2348.6883	-0.0027	0.00026
8	1	8	9	1	9	2348.6856	2348.6849	0.0008	0.00026
8	3	6	9	3	7	2348.6856	2348.6843	0.0013	0.00022
8	1	7	9	1	8	2348.6856	2348.6885	-0.0029	0.00025
8	2	6	9	2	7	2348.6856	2348.6834	0.0022	0.00024
					Blend		2348.6857	0.0000	
7	1	6	8	1	7	2348.7387	2348.7420	-0.0033	0.00032
7	1	7	8	1	8	2348.7387	2348.7385	0.0002	0.00032
7	2	5	8	2	6	2348.7387	2348.7377	0.0011	0.00030
7	3	4	8	3	5	2348.7387	2348.7392	-0.0004	0.00027
7	4	4	8	4	5	2348.7387	2348.7391	-0.0004	0.00023
7	3	5	8	3	6	2348.7387	2348.7387	0.0001	0.00027
7	0	7	8	0	8	2348.7387	2348.7417	-0.0030	0.00033
7	2	6	8	2	7	2348.7387	2348.7399	-0.0012	0.00030
					Blend		2348.7397	-0.0010	
4	2	3	5	2	4	2348.9015	2348.9013	0.0002	0.00038
4	1	3	5	1	4	2348.9015	2348.9026	-0.0011	0.00044
4	1	4	5	1	5	2348.9015	2348.9001	0.0014	0.00044
4	3	2	5	3	3	2348.9015	2348.9010	0.0005	0.00029
4	2	2	5	2	3	2348.9015	2348.9005	0.0010	0.00038
4	0	4	5	0	5	2348.9015	2348.9019	-0.0004	0.00046
4	4	0	5	4	1	2348.9015	2348.9010	0.0005	0.00016
4	3	1	5	3	2	2348.9015	2348.9010	0.0005	0.00029
4	4	1	5	4	2	2348.9015	2348.9010	0.0005	0.00016
					Blend		2348.9012	0.0003	
3	0	3	4	0	4	2348.9549	2348.9554	-0.0006	0.00045
3	1	3	4	1	4	2348.9549	2348.9541	0.0008	0.00042
3	2	1	4	2	2	2348.9549	2348.9546	0.0002	0.00033
3	3	1	4	3	2	2348.9549	2348.9549	0.0000	0.00019
3	3	0	4	3	1	2348.9549	2348.9549	-0.0001	0.00019
3	1	2	4	1	3	2348.9549	2348.9561	-0.0012	0.00042
3	2	2	4	2	3	2348.9549	2348.9550	-0.0002	0.00033

					Blend		2348.9550	-0.0002	
5	5	0	5	5	1	2349.1693	2349.1694	-0.0001	0.00077
3	3	0	3	3	1	2349.1693	2349.1697	-0.0004	0.00066
4	4	1	4	4	0	2349.1693	2349.1696	-0.0003	0.00076
6	6	0	6	6	1	2349.1693	2349.1691	0.0002	0.00071
6	6	1	6	6	0	2349.1693	2349.1691	0.0002	0.00071
3	3	1	3	3	0	2349.1693	2349.1697	-0.0004	0.00066
7	7	0	7	7	1	2349.1693	2349.1688	0.0005	0.00060
7	7	1	7	7	0	2349.1693	2349.1688	0.0005	0.00060
5	5	1	5	5	0	2349.1693	2349.1694	-0.0001	0.00077
4	4	0	4	4	1	2349.1693	2349.1696	-0.0003	0.00076
					Blend		2349.1693	0.0000	
4	3	2	3	3	1	2349.3845	2349.3844	0.0001	0.00022
4	3	1	3	3	0	2349.3845	2349.3844	0.0001	0.00022
4	1	3	3	1	2	2349.3845	2349.3833	0.0012	0.00049
4	2	2	3	2	1	2349.3845	2349.3847	-0.0002	0.00039
4	0	4	3	0	3	2349.3845	2349.3840	0.0005	0.00052
4	1	4	3	1	3	2349.3845	2349.3853	-0.0008	0.00049
4	2	3	3	2	2	2349.3845	2349.3843	0.0002	0.00039
					Blend		2349.3843	0.0002	
5	4	2	4	4	1	2349.4379	2349.4379	0.0000	0.00019
5	0	5	4	0	4	2349.4379	2349.4371	0.0008	0.00056
5	1	5	4	1	4	2349.4379	2349.4389	-0.0010	0.00054
5	2	4	4	2	3	2349.4379	2349.4378	0.0001	0.00046
5	3	3	4	3	2	2349.4379	2349.4380	-0.0001	0.00035
5	1	4	4	1	3	2349.4379	2349.4365	0.0014	0.00053
5	3	2	4	3	1	2349.4379	2349.4380	-0.0001	0.00035
5	4	1	4	4	0	2349.4379	2349.4379	0.0000	0.00019
5	2	3	4	2	2	2349.4379	2349.4385	-0.0006	0.00046
					Blend		2349.4378	0.0001	
7	0	7	6	0	6	2349.5449	2349.5430	0.0019	0.00051
7	3	4	6	3	3	2349.5449	2349.5450	0.0000	0.00040
7	2	5	6	2	4	2349.5449	2349.5462	-0.0012	0.00046
7	2	6	6	2	5	2349.5449	2349.5444	0.0005	0.00046
7	3	5	6	3	4	2349.5449	2349.5452	-0.0003	0.00040
7	4	4	6	4	3	2349.5449	2349.5449	0.0000	0.00032
7	4	3	6	4	2	2349.5449	2349.5449	0.0000	0.00032
7	5	3	6	5	2	2349.5449	2349.5449	0.0001	0.00023
7	1	7	6	1	6	2349.5449	2349.5458	-0.0009	0.00050
7	1	6	6	1	5	2349.5449	2349.5426	0.0024	0.00050
					Blend		2349.5446	0.0003	
8	1	7	7	1	6	2349.5980	2349.5955	0.0024	0.00044
8	2	6	7	2	5	2349.5980	2349.5999	-0.0019	0.00041
8	2	7	7	2	6	2349.5980	2349.5976	0.0003	0.00041
8	3	6	7	3	5	2349.5980	2349.5989	-0.0009	0.00037
8	3	5	7	3	4	2349.5980	2349.5984	-0.0004	0.00037
8	4	5	7	4	4	2349.5980	2349.5984	-0.0004	0.00032
8	4	4	7	4	3	2349.5980	2349.5984	-0.0004	0.00032
8	5	4	7	5	3	2349.5980	2349.5983	-0.0003	0.00025
8	0	8	7	0	7	2349.5980	2349.5959	0.0021	0.00044
8	1	8	7	1	7	2349.5980	2349.5991	-0.0011	0.00044
					Blend		2349.5980	0.0000	
9	0	9	8	0	8	2349.6514	2349.6487	0.0027	0.00037
9	3	6	8	3	5	2349.6514	2349.6518	-0.0004	0.00032
9	2	7	8	2	6	2349.6514	2349.6536	-0.0022	0.00035
9	2	8	8	2	7	2349.6514	2349.6508	0.0006	0.00035
9	3	7	8	3	6	2349.6514	2349.6526	-0.0012	0.00032
9	4	6	8	4	5	2349.6514	2349.6518	-0.0005	0.00028
9	4	5	8	4	4	2349.6514	2349.6519	-0.0005	0.00028

9	5	5	8	5	4	2349.6514	2349.6517	-0.0004	0.00023
9	1	9	8	1	8	2349.6514	2349.6521	-0.0007	0.00037
9	1	8	8	1	7	2349.6514	2349.6485	0.0029	0.00036
					Blend		2349.6513	0.0001	
12	1	11	11	1	10	2349.8115	2349.8104	0.0011	0.00015
12	2	11	11	2	10	2349.8115	2349.8097	0.0019	0.00015
12	2	10	11	2	9	2349.8115	2349.8136	-0.0020	0.00015
12	3	9	11	3	8	2349.8115	2349.8139	-0.0024	0.00014
12	3	10	11	3	9	2349.8115	2349.8115	0.0001	0.00014
12	4	9	11	4	8	2349.8115	2349.8120	-0.0005	0.00013
12	4	8	11	4	7	2349.8115	2349.8125	-0.0010	0.00013
					Blend		2349.8119	-0.0004	

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Table A-9. Fundamental band fit of CO_2-$(N_2)_3$ (cm^{-1}).
Int = calculated relative intensity, used to weight the blended lines.

J'	Ka'	Kc'	J"	Ka"	Kc"	Obs	Calc	Obs-Calc	Int
12	0	12	13	0	13	2349.0451	2349.0491	-0.0040	0.00069
12	1	11	13	1	12	2349.0451	2349.0445	0.0005	0.00068
12	2	11	13	2	12	2349.0451	2349.0459	-0.0008	0.00066
12	2	10	13	2	11	2349.0451	2349.0417	0.0034	0.00066
12	3	10	13	3	11	2349.0451	2349.0440	0.0011	0.00063
12	3	9	13	3	10	2349.0451	2349.0422	0.0028	0.00063
12	4	9	13	4	10	2349.0451	2349.0434	0.0016	0.00058
12	4	8	13	4	9	2349.0451	2349.0432	0.0018	0.00058
12	5	8	13	5	9	2349.0451	2349.0432	0.0018	0.00053
12	5	7	13	5	8	2349.0451	2349.0432	0.0019	0.00053
					Blend		2349.0441	0.0009	
11	0	11	12	0	12	2349.1032	2349.1069	-0.0037	0.00110
11	1	11	12	1	12	2349.1032	2349.1071	-0.0040	0.00109
11	1	10	12	1	11	2349.1032	2349.1024	0.0007	0.00107
11	2	10	12	2	11	2349.1032	2349.1040	-0.0008	0.00105
11	2	9	12	2	10	2349.1032	2349.1002	0.0030	0.00104
11	3	9	12	3	10	2349.1032	2349.1024	0.0008	0.00099
11	3	8	12	3	9	2349.1032	2349.1011	0.0021	0.00099
11	4	8	12	4	9	2349.1032	2349.1019	0.0013	0.00091
11	4	7	12	4	8	2349.1032	2349.1018	0.0014	0.00091
11	5	7	12	5	8	2349.1032	2349.1017	0.0015	0.00081
					Blend		2349.1031	0.0001	
10	0	10	11	0	11	2349.1613	2349.1647	-0.0034	0.00165
10	1	10	11	1	11	2349.1613	2349.1650	-0.0037	0.00165
10	1	9	11	1	10	2349.1613	2349.1604	0.0009	0.00162
10	2	9	11	2	10	2349.1613	2349.1620	-0.0007	0.00157
10	2	8	11	2	9	2349.1613	2349.1588	0.0026	0.00157
10	3	8	11	3	9	2349.1613	2349.1607	0.0006	0.00147
10	3	7	11	3	8	2349.1613	2349.1598	0.0015	0.00147
10	4	7	11	4	8	2349.1613	2349.1603	0.0010	0.00134
10	4	6	11	4	7	2349.1613	2349.1602	0.0011	0.00134
10	5	6	11	5	7	2349.1613	2349.1601	0.0013	0.00118
					Blend		2349.1613	0.0000	
6	0	6	7	0	7	2349.3934	2349.3952	-0.0018	0.00508
6	1	6	7	1	7	2349.3934	2349.3960	-0.0026	0.00499
6	1	5	7	1	6	2349.3934	2349.3926	0.0008	0.00496
6	2	5	7	2	6	2349.3934	2349.3940	-0.0006	0.00461
6	2	4	7	2	5	2349.3934	2349.3928	0.0006	0.00460
6	3	4	7	3	5	2349.3934	2349.3935	0.0000	0.00401
6	3	3	7	3	4	2349.3934	2349.3934	0.0001	0.00401
6	4	3	7	4	4	2349.3934	2349.3932	0.0002	0.00320
6	4	2	7	4	3	2349.3934	2349.3932	0.0002	0.00320
6	5	2	7	5	3	2349.3934	2349.3929	0.0005	0.00224
					Blend		2349.3938	-0.0004	
5	0	5	6	0	6	2349.4504	2349.4528	-0.0024	0.00583
5	1	5	6	1	6	2349.4504	2349.4536	-0.0032	0.00568
5	1	4	6	1	5	2349.4504	2349.4507	-0.0003	0.00565
5	2	4	6	2	5	2349.4504	2349.4519	-0.0015	0.00511
5	2	3	6	2	4	2349.4504	2349.4511	-0.0007	0.00511
5	3	3	6	3	4	2349.4504	2349.4515	-0.0011	0.00422
5	3	2	6	3	3	2349.4504	2349.4515	-0.0011	0.00422
5	4	2	6	4	3	2349.4504	2349.4513	-0.0008	0.00303
5	4	1	6	4	2	2349.4504	2349.4513	-0.0008	0.00303

					Blend		2349.4518	-0.0014	
2	0	2	3	0	3	2349.6252	2349.6258	-0.0006	0.00545
2	1	2	3	1	3	2349.6252	2349.6264	-0.0012	0.00483
2	1	1	3	1	2	2349.6252	2349.6249	0.0003	0.00482
2	2	1	3	2	2	2349.6252	2349.6255	-0.0003	0.00298
2	2	0	3	2	1	2349.6252	2349.6254	-0.0002	0.00298
					Blend		2349.6256	-0.0005	
4	4	0	4	4	1	2349.7972	2349.7975	-0.0003	0.01033
4	4	1	4	4	0	2349.7972	2349.7975	-0.0003	0.01033
5	5	0	5	5	1	2349.7972	2349.7968	0.0004	0.01027
5	5	1	5	5	0	2349.7972	2349.7968	0.0004	0.01027
6	6	0	6	6	1	2349.7972	2349.7960	0.0012	0.00927
6	6	1	6	6	0	2349.7972	2349.7960	0.0012	0.00927
3	3	0	3	3	1	2349.7972	2349.7980	-0.0008	0.00917
3	3	1	3	3	0	2349.7972	2349.7980	-0.0008	0.00917
					Blend		2349.7971	0.0001	
5	0	5	4	0	4	2350.0861	2350.0856	0.0005	0.00768
5	1	5	4	1	4	2350.0861	2350.0847	0.0014	0.00737
5	1	4	4	1	3	2350.0861	2350.0872	-0.0011	0.00735
5	2	4	4	2	3	2350.0861	2350.0859	0.0002	0.00635
5	2	3	4	2	2	2350.0861	2350.0864	-0.0003	0.00635
5	3	3	4	3	2	2350.0861	2350.0858	0.0002	0.00474
5	3	2	4	3	1	2350.0861	2350.0858	0.0002	0.00474
5	4	2	4	4	1	2350.0861	2350.0855	0.0006	0.00258
5	4	1	4	4	0	2350.0861	2350.0855	0.0006	0.00258
					Blend		2350.0859	0.0002	
6	0	6	5	0	5	2350.1433	2350.1425	0.0007	0.00748
6	1	6	5	1	5	2350.1433	2350.1417	0.0016	0.00728
6	1	5	5	1	4	2350.1433	2350.1446	-0.0014	0.00725
6	2	5	5	2	4	2350.1433	2350.1431	0.0002	0.00656
6	2	4	5	2	3	2350.1433	2350.1439	-0.0007	0.00656
6	3	4	5	3	3	2350.1433	2350.1431	0.0001	0.00541
6	3	3	5	3	2	2350.1433	2350.1432	0.0001	0.00541
6	4	3	5	4	2	2350.1433	2350.1428	0.0004	0.00389
6	4	2	5	4	1	2350.1433	2350.1428	0.0004	0.00389
6	5	2	5	5	1	2350.1433	2350.1424	0.0008	0.00206
					Blend		2350.1431	0.0002	
7	0	7	6	0	6	2350.2008	2350.1993	0.0015	0.00679
7	1	7	6	1	6	2350.2008	2350.1985	0.0023	0.00667
7	1	6	6	1	5	2350.2008	2350.2019	-0.0011	0.00664
7	2	6	6	2	5	2350.2008	2350.2002	0.0006	0.00616
7	2	5	6	2	4	2350.2008	2350.2015	-0.0007	0.00616
7	3	5	6	3	4	2350.2008	2350.2004	0.0004	0.00536
7	3	4	6	3	3	2350.2008	2350.2005	0.0003	0.00536
7	4	4	6	4	3	2350.2008	2350.2001	0.0008	0.00429
7	4	3	6	4	2	2350.2008	2350.2001	0.0008	0.00429
					Blend		2350.2003	0.0006	
8	0	8	7	0	7	2350.2577	2350.2560	0.0017	0.00580
8	1	8	7	1	7	2350.2577	2350.2553	0.0024	0.00573
8	1	7	7	1	6	2350.2577	2350.2591	-0.0014	0.00569
8	2	6	7	2	5	2350.2577	2350.2591	-0.0013	0.00537
8	2	7	7	2	6	2350.2577	2350.2573	0.0004	0.00537
8	3	6	7	3	5	2350.2577	2350.2576	0.0001	0.00482
8	3	5	7	3	4	2350.2577	2350.2578	-0.0001	0.00482
8	4	5	7	4	4	2350.2577	2350.2573	0.0004	0.00408
8	4	4	7	4	3	2350.2577	2350.2573	0.0004	0.00408
8	5	4	7	5	3	2350.2577	2350.2569	0.0008	0.00318
					Blend		2350.2574	0.0003	
9	0	9	8	0	8	2350.3149	2350.3126	0.0023	0.00468

9	1	9	8	1	8	2350.3149	2350.3120	0.0029	0.00464
9	1	8	8	1	7	2350.3149	2350.3161	-0.0013	0.00460
9	2	7	8	2	6	2350.3149	2350.3165	-0.0017	0.00440
9	2	8	8	2	7	2350.3149	2350.3143	0.0006	0.00439
9	3	7	8	3	6	2350.3149	2350.3148	0.0001	0.00402
9	3	6	8	3	5	2350.3149	2350.3151	-0.0002	0.00402
9	4	6	8	4	5	2350.3149	2350.3145	0.0004	0.00352
9	4	5	8	4	4	2350.3149	2350.3145	0.0004	0.00352
9	5	5	8	5	4	2350.3149	2350.3140	0.0009	0.00292
					Blend		2350.3144	0.0005	
11	0	11	10	0	10	2350.4291	2350.4255	0.0036	0.00260
11	1	11	10	1	10	2350.4291	2350.4252	0.0039	0.00259
11	1	10	10	1	9	2350.4291	2350.4297	-0.0007	0.00256
11	2	10	10	2	9	2350.4291	2350.4279	0.0012	0.00248
11	2	9	10	2	8	2350.4291	2350.4312	-0.0022	0.00248
11	3	9	10	3	8	2350.4291	2350.4289	0.0002	0.00233
11	3	8	10	3	7	2350.4291	2350.4298	-0.0007	0.00232
11	4	8	10	4	7	2350.4291	2350.4286	0.0004	0.00211
11	4	7	10	4	6	2350.4291	2350.4287	0.0003	0.00211
11	5	7	10	5	6	2350.4291	2350.4282	0.0009	0.00186
					Blend		2350.4283	0.0007	
13	1	12	12	1	11	2350.5425	2350.5426	-0.0001	0.00116
13	2	12	12	2	11	2350.5425	2350.5411	0.0014	0.00114
13	2	11	12	2	10	2350.5425	2350.5454	-0.0029	0.00114
13	3	11	12	3	10	2350.5425	2350.5426	-0.0001	0.00108
13	3	10	12	3	9	2350.5425	2350.5445	-0.0019	0.00108
13	4	10	12	4	9	2350.5425	2350.5426	-0.0001	0.00100
13	4	9	12	4	8	2350.5425	2350.5429	-0.0003	0.00100
13	5	9	12	5	8	2350.5425	2350.5421	0.0004	0.00091
13	5	8	12	5	7	2350.5425	2350.5421	0.0004	0.00091
13	6	8	12	6	7	2350.5425	2350.5415	0.0010	0.00080
					Blend		2350.5428	-0.0003	
15	1	14	14	1	13	2350.6553	2350.6550	0.0002	0.00044
15	2	14	14	2	13	2350.6553	2350.6540	0.0013	0.00043
15	2	13	14	2	12	2350.6553	2350.6589	-0.0036	0.00043
15	3	13	14	3	12	2350.6553	2350.6560	-0.0007	0.00041
15	3	12	14	3	11	2350.6553	2350.6590	-0.0037	0.00041
15	4	12	14	4	11	2350.6553	2350.6564	-0.0011	0.00039
15	4	11	14	4	10	2350.6553	2350.6570	-0.0017	0.00039
15	5	11	14	5	10	2350.6553	2350.6559	-0.0006	0.00036
15	5	10	14	5	9	2350.6553	2350.6559	-0.0006	0.00036
15	6	10	14	6	9	2350.6553	2350.6552	0.0000	0.00032
					Blend		2350.6564	-0.0011	

****

Table A-10. Cartesian structural coordinates for the clusters in Table 1 of the paper.

PLEASE NOTE THAT: all the geometries here listed were optimised at B2PLYP-D3BJ/m-aug-cc-pVTZ(-dH) level (no CP-corrections); the corresponding rotational constants (at equilibrium geometry) are reported.

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#########                    (CO2)2-CO complexes                        #########
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|
Geometry Set #1 Geo# 50

                        (Angstrom)
C     1.732388   -0.835332   -0.241947
O     2.393286   -0.463828    0.640842
O     1.077540   -1.206533   -1.131400
C    -1.732680   -0.834735    0.241962
O    -1.077994   -1.206053    1.131487
O    -2.393415   -0.463113   -0.640899
C     0.000337    1.978014   -0.000030
O     0.000551    3.108567   -0.000019

Equilibrium rotational constants (in GHz)
A = 1.5447251         B = 1.4525026         C =   0.8958886

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|
Geometry Set #1 Geo#56

                        (Angstrom)
C       1.353628   -1.597216   -0.000003
O       0.191819   -1.507064   -0.000010
O       2.512082   -1.702484    0.000004
C      -2.305543    0.157313   -0.000047
O      -1.652292    1.122280   -0.000040
O      -2.968305   -0.799059   -0.000054
C       1.527114    1.620706    0.000066
O       1.485296    2.750725    0.000088

Equilibrium rotational constants (in GHz)
A = 1.7044650         B =  1.1613463         C = 0.6907203

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#########                    (CO2)2-N2 complexes                        #########
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|
Geometry Set #1 Geo#3

                        (Angstrom)
C    -1.739089   -0.785216    0.246980
O    -2.411908   -0.443773   -0.638765
O    -1.070178   -1.124605    1.138848
C     1.739105   -0.785225   -0.246845
```

```
O     1.070215   -1.124769   -1.138669
O     2.411904   -0.443627    0.638856
N    -0.000033    3.015204   -0.000254
N    -0.000019    1.915773   -0.000169

Equilibrium rotational constants (in GHz)
A = 1.7058437         B = 1.4385116         C =  0.9436070

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|
Geometry Set #1 Geo#31

                        (Angstrom)
C   -3.711510    0.000005    0.000028
O   -3.714117    0.823807   -0.823004
O   -3.714120   -0.823798    0.823061
C    3.711511    0.000007   -0.000022
O    3.714135   -0.823786   -0.823064
O    3.714103    0.823800    0.823020
N    0.549625   -0.000023   -0.000022
N   -0.549626   -0.000015    0.000003

Equilibrium rotational constants (in GHz)
A = 5.8251218         B = 0.3995136         C =  0.3994883

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#########                   CO2-(CO)2 complexes                      #########
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|
Geometry Set #1 Geo#18

                        (Angstrom)
C    -1.934703   -0.841044   -0.000018
O    -2.504672   -1.818076   -0.000024
C     1.934554   -0.841614    0.000017
O     2.503856   -1.819035    0.000019
C     0.000337    1.775698    0.000002
O     0.000326    1.783665    1.164315
O     0.000348    1.783666   -1.164311

Equilibrium rotational constants (in GHz)
A =  1.6528569           B =   1.5139623        C =  0.9141495

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|
Geometry Set #1 Geo#8

                        (Angstrom)
C     -2.457331   -0.021793    0.000680
O     -3.017453   -1.004677   -0.000052
C      0.570342    1.877356   -0.000140
O      0.179082    2.938427   -0.000038
C      1.545734   -1.204532   -0.000115
O      2.663015   -0.878234    0.000903
```

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O      0.431297   -1.543790   -0.001133

Equilibrium rotational constants (in GHz)
A = 1.9112885   B =  1.3748465  C = 0.7996411

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#########                    (N2)2-CO2 complexes                     #########
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2_N2_CO2 Geo SET 4 Min_1 #22
(MOST STABLE ISOMER)

C    -1.745913   -0.000001    0.000017
O    -1.750666   -0.000010    1.164362
O    -1.750692    0.000008   -1.164328
N     1.861464   -2.259706   -0.000030
N     0.887562   -1.749372   -0.000021
N     0.887560    1.749374    0.000002
N     1.861462    2.259708   -0.000003

Rotational constants (in GHz) at equilibrium
A =   1.8574440          B =    1.7010585        C = 1.0475421

#####################################################################
2_N2_CO2 Geo Hint 1

C      -1.649456   -1.023020   -0.000142
O      -2.715588   -0.555434    0.001393
O      -0.585596   -1.497209   -0.001675
N       0.174946    2.813795   -0.000352
N      -0.335340    1.840016   -0.000370
N       2.893248   -1.219464    0.000187
N       2.453746   -0.211595    0.000978

Rotational constants (in GHz) at equilibrium
A =   2.1682897         B =    1.4053185       C = 0.8526784

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#########                   CO2-CO-N2 complexes                      #########
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|
Geometry Set #1 Geo#16

                        (Angstrom)
C        1.30441  -1.18717   0.00005
O        1.31005  -1.19048   1.16438
O        1.31024  -1.19035  -1.16428
C       -1.91349  -0.72469  -0.00019
O       -3.00935  -0.44471  -0.00026
```

```
N        0.31218   2.9564    0.00016
N        0.65454   1.91153   0.00015

Equilibrium rotational constants (in GHz)
A =   1.7509286          B =    1.6051473       C = 0.9779971

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|
Geometry Set #1 Geo#12

                        (Angstrom)
C       1.746298   -0.948253   -0.000011
O       2.778155   -0.409330   -0.000002
O       0.719451   -1.498097   -0.000021
C       0.178805    1.884663   -0.000019
O      -0.419687    2.844217   -0.000021
N      -2.762684   -1.456487    0.000041
N      -2.405027   -0.416768    0.000035

Equilibrium rotational constants (in GHz)
A = 1.9934431           B = 1.4061774         C = 0.8245434

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#########                    CO2-(CO)3 complexes                       #########
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|
Geometry Set #1 Geo#34

                        (Angstrom)
C   -0.384724    1.061581   -1.812228
O    0.037678    2.019209   -2.241158
C    2.359188   -0.324495    0.003838
O    2.963016   -1.281015    0.002469
C   -0.400150    0.954388    1.871725
O   -0.013506    1.922500    2.310784
C   -1.513285   -1.423206   -0.043270
O   -0.462762   -1.925790   -0.062976
O   -2.570198   -0.936105   -0.024168

Equilibrium rotational constants (in GHz)
A = 0.9695849           B = 0.8496632        C = 0.8132321

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|
Geometry Set #1 Geo#9

                        (Angstrom)
C     2.922556   -0.225886    0.000035
O     4.035607   -0.025284    0.000046
C    -0.147915    1.802276   -0.000298
O     0.496328    2.732196   -0.000470
C    -3.145595   -0.343778    0.000083
O    -3.930026    0.471481    0.000021
C    -0.119897   -1.488064    0.000195
```

```
O    -0.116880   -1.493237    1.164443
O    -0.116890   -1.493565   -1.164052

Equilibrium rotational constants (in GHz)
A =  1.6556038          B = 0.6504694        C = 0.5076757

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|
Geometry Set #1 Geo#47

                        (Angstrom)
C   -2.059418    0.000987    2.188262
O   -2.047950    0.000987    1.056240
C   -0.076527    1.866694   -0.969025
O   -0.895942    2.331972   -1.594686
C   -0.079107   -1.865072   -0.971050
O   -0.899443   -2.330984   -1.595029
C    1.997474   -0.001421    0.704259
O    1.261123   -0.001855    1.606667
O    2.745396   -0.001011   -0.187527

Equilibrium rotational constants (in GHz)
A = 1.0430766           B =  0.8947308         C = 0.8490564

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################################################################################
#########                    CO2-N2-(CO)2 complexes                    #########
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|
Geometry Set #1 Geo#69

                        (Angstrom)
C    -1.871555   -0.000922   -0.975213
O    -1.003186   -0.000994   -1.751303
O    -2.749998   -0.000869   -0.211500
C    -0.095627    1.863171    1.012919
O     0.601702    2.326005    1.773831
C    -0.093371   -1.862553    1.013399
O     0.605307   -2.327099    1.772025
N     2.163439    0.001443   -0.833780
N     2.512665    0.002197   -1.876369

Equilibrium rotational constants (in GHz)
A = 1.0070271            B =  0.8561160         C =  0.8404101

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|
Geometry Set #1 Geo#5

                        (Angstrom)
C    1.429115   -1.310780   -0.637658
O    2.498865   -0.957074   -0.345606
O    0.363707   -1.677962   -0.931956
C   -2.402472   -0.119298   -0.213077
O   -3.026760   -1.051295   -0.359017
```

```
C    0.498336    1.754273   -1.129839
O    0.097113    2.811646   -1.145626
N    0.124969    0.710921    2.846113
N    0.358849    0.010838    2.031185

Equilibrium rotational constants (in GHz)
A = 1.0119553            B = 0.8739755          C = 0.8203444

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|
Geometry Set #1 Geo#7

                        (Angstrom)
C   -0.082401   -1.501051    0.000009
O   -0.077606   -1.505941   -1.164241
O   -0.077604   -1.505926    1.164258
C   -0.064505    1.787873   -0.000011
O    0.534614    2.747372   -0.000017
C   -3.092348   -0.328334    0.000005
O   -3.873050    0.490457    0.000002
N    2.842878   -0.204891   -0.000002
N    3.926362   -0.017770   -0.000002

Equilibrium rotational constants (in GHz)
A = 1.6420736            B = 0.6904193           C = 0.5302841

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#########                   CO2-CO-(N2)2 complexes                    #########
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|
Geometry Set #1 Geo#16

                        (Angstrom)
C     1.800036   -0.687514   -0.778719
O     2.704196   -0.256211   -0.185852
O     0.903493   -1.128572   -1.377043
C     0.151229    2.078359   -0.393626
O    -0.521459    2.952049   -0.141784
N    -2.593436   -1.308678   -1.142270
N    -2.228899   -0.419706   -0.607689
N     0.102863   -0.727664    1.896308
N    -0.480159   -0.527266    2.806724

Equilibrium rotational constants (in GHz)
A = 1.0517241            B = 0.8943112          C =  0.8469144

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|
Geometry Set #1 Geo#36

                        (Angstrom)
C   -0.000829   -1.503104    0.000296
O    0.002584   -1.506894    1.164524
O    0.002583   -1.507367   -1.163930
```

```
C   -3.015675   -0.317428    0.000036
O   -3.857258    0.438536   -0.000143
N    0.282245    2.731186   -0.000330
N   -0.077471    1.692116   -0.000260
N    2.880294   -0.161593   -0.000023
N    3.902897    0.242431   -0.000187

Equilibrium rotational constants (in GHz)
A = 1.7239185            B = 0.7008012          C =  0.5448348

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|
Geometry Set #1 Geo#26

                        (Angstrom)
C       1.317921   -1.528207   -0.000083
O       0.212167   -1.894122   -0.000138
O       2.426164   -1.172523   -0.000028
C      -2.454811   -0.033302   -0.000070
O      -3.150879   -0.925075   -0.000187
N       0.526257    0.986760    1.734603
N       0.253758    1.963129    2.160329
N       0.526346    0.987037   -1.734405
N       0.253884    1.963476   -2.159992

Equilibrium rotational constants (in GHz)
A = 1.0723746             B =  0.8845689          C = 0.8248177

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#########                   CO2-(N2)3 complexes                        #########
#########        Preliminary results as at:  June 02, 2021             #########
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CO2-(N2)3 Geo 1

N     2.903092   -0.235074   -0.000002
N     3.831626    0.353813   -0.000004
N    -2.903092   -0.235074    0.000003
N    -3.831626    0.353813    0.000002
N     0.000000    2.781604   -0.000003
N     0.000000    1.682027   -0.000002
C     0.000000   -1.492542    0.000002
O    -0.000001   -1.497033   -1.164211
O     0.000001   -1.497030    1.164215

Equilibrium rotational constants (in GHz)
A = 1.7143055     B = 0.7318379     C = 0.5623790

################################################################

CO2-(N2)3 Geo 4
```

```
N   -0.361601    1.851870   -2.183044
N    0.206453    1.022162   -1.738387
N   -0.361436    1.852871    2.182283
N    0.206740    1.023123    1.737859
N   -2.753645   -1.570573    0.000271
N   -2.302269   -0.567967    0.000324
C    1.705438   -1.146099    0.000220
O    2.665235   -0.487434   -0.000106
O    0.750726   -1.813044    0.000549

Equilibrium rotational constants (in GHz)
A = 1.1116644     B = 0.9011364   C = 0.8722787

#########################################################################
```