

## Supporting Information to:

# *“Computational Study of the Rovibrational Spectrum of $CO_2-N_2$ ”*

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Table 1: Energies (in  $\text{cm}^{-1}$ ) for up to 40 of the levels below  $-100 \text{ cm}^{-1}$  in each symmetry block are listed. The two left-most columns of energies are allowed states, while the two columns at right are not, but transitions involving ro-vibrational states, whose vibrational parents do not exist, are allowed (see text)

$J = 0$				
	ee+ ( $A'_1$ )	eo+ ( $B'_2$ )	oo+ ( $A''_1$ )	oe+ ( $B''_2$ )
1	-229.461785	-229.461694	-208.389856	-208.389684
2	-188.143860	-188.142633	-170.003710	-170.004844
3	-182.956401	-182.954205	-167.797040	-167.791340
4	-166.189699	-166.087631	-157.139551	-157.142946
5	-154.322518	-154.320047	-145.621185	-145.643643
6	-149.123532	-149.104719	-140.433898	-140.438351
7	-141.799808	-141.795755	-132.091644	-132.106833
8	-136.403382	-136.381940	-130.736170	-130.673650
9	-129.373529	-129.102639	-121.743125	-122.209268
10	-128.928716	-127.107087	-117.894991	-118.622659
11	-127.168103	-126.612974	-115.537318	-116.518828
12	-119.562328	-119.148106	-114.292595	-115.636215
13	-118.904804	-116.662367	-111.830901	-114.512378
14	-117.352416	-113.312336	-110.869966	-110.722385
15	-114.484747	-112.625381	-106.608916	-107.790649
16	-111.926656	-108.856674	-103.638777	-106.276439
17	-108.398776	-106.179157	-101.470602	-105.929361
18	-105.394927	-104.007705		-101.716283
19	-103.982217	-102.020896		
20	-101.603280			
	ee- ( $A'_2$ )	eo- ( $B'_1$ )	oo- ( $A''_2$ )	oe- ( $B''_1$ )
1	-175.694427	-175.693283	-196.557007	-196.552601
2	-140.311571	-140.337268	-156.137235	-156.099396
3	-137.134802	-137.071128	-153.246052	-153.141233
4	-128.506275	-128.703868	-139.588177	-138.429367
5	-118.422587	-118.945604	-126.246523	-126.090433
6	-114.845160	-115.578369	-119.433428	-119.019890
7	-104.904931	-109.530918	-113.832763	-113.615169
8	-103.948465	-105.539339	-112.316724	-108.875794
9	-101.298511	-102.036071	-111.316295	-106.718126
10			-107.927598	-102.281922
11			-105.241997	-100.391514
12			-103.359891	

Table 2: Energies (in  $\text{cm}^{-1}$ ) for up to 40 of the levels below  $-100 \text{ cm}^{-1}$  in each symmetry block are listed. The two left-most columns of energies are allowed states, while the two columns at right are not, but transitions involving ro-vibrational states, whose vibrational parents do not exist, are allowed (see text)

$J = 1$				
	ee+ ( $A_1'$ )	eo+ ( $B_2'$ )	oo+ ( $A_1''$ )	oe+ ( $B_2''$ )
1	-207.934905	-207.935086	-228.996585	-228.996675
2	-196.086455	-196.090848	-196.428367	-196.423989
3	-175.565849	-175.564721	-187.689544	-187.690740
4	-169.531940	-169.530889	-182.489911	-182.492103
5	-167.328854	-167.334660	-175.256308	-175.258122
6	-156.716575	-156.713429	-165.587472	-165.688268
7	-155.658737	-155.694958	-156.009970	-155.972531
8	-152.652796	-152.756876	-153.834500	-153.836471
9	-145.220973	-145.227228	-153.118914	-153.015032
10	-140.211048	-140.235168	-148.645665	-148.664088
11	-139.901707	-139.901275	-141.336017	-141.339934
12	-137.887273	-139.017677	-139.870192	-139.845456
13	-137.005781	-136.943023	-139.452065	-138.302869
14	-131.620550	-131.607219	-136.624013	-136.701646
15	-130.205446	-130.268938	-135.939900	-135.957115
16	-128.380766	-128.577302	-128.604842	-128.880106
17	-125.627113	-125.758469	-128.318229	-128.587031
18	-121.260042	-121.246568	-126.672833	-127.913557
19	-118.613985	-118.983765	-126.120185	-126.599949
20	-118.290319	-118.812347	-126.010000	-125.944224
21	-117.575262	-117.673777	-119.306815	-118.961539
22	-115.244501	-115.479305	-118.797960	-118.787932
23	-114.731484	-115.185377	-118.418326	-118.617327
24	-114.062404	-115.100847	-117.388313	-116.454653
25	-113.106045	-113.781636	-114.760601	-116.074036
26	-111.980357	-113.286062	-113.711762	-114.426976
27	-110.203567	-112.167135	-113.691780	-113.495128
28	-108.769865	-110.216624	-112.443426	-113.005179
29	-107.216721	-109.549580	-111.848368	-108.817029
30	-106.235112	-108.551148	-111.215288	-108.707197
31	-105.476256	-107.397896	-111.166848	-106.759403
32	-104.780949	-107.065653	-107.803047	-106.499676
33	-103.886509	-105.544383	-107.727264	-105.820849
34	-102.902911	-105.410859	-105.682914	-104.447138
35	-101.692603	-103.447118	-105.105654	-103.969159
36	-101.240849	-102.835975	-104.551344	-103.073499
37	-100.876607	-101.943105	-103.606124	-102.162444
38	-100.239169		-103.241651	-102.118579
39			-101.890778	-100.298343
40			-101.042376	

Table 3: Energies (in  $\text{cm}^{-1}$ ) for up to 40 of the levels below  $-100 \text{ cm}^{-1}$  in each symmetry block are listed. The two left-most columns of energies are allowed states, while the two columns at right are not, but transitions involving ro-vibrational states, whose vibrational parents do not exist, are allowed (see text)

$J = 1$				
	ee- ( $A'_2$ )	eo- ( $B'_1$ )	oo- ( $A''_2$ )	oe- ( $B''_1$ )
1	-229.334857	-229.334766	-229.007230	-229.007321
2	-207.946452	-207.946633	-208.262036	-208.261865
3	-196.076065	-196.080437	-187.702223	-187.703419
4	-188.015351	-188.014132	-182.500036	-182.502237
5	-182.833897	-182.831717	-175.245810	-175.247644
6	-169.544878	-169.543824	-169.877983	-169.879110
7	-167.341578	-167.347307	-167.670105	-167.664469
8	-166.059123	-165.957769	-165.597062	-165.698357
9	-156.726769	-156.723604	-157.016167	-157.019541
10	-155.650084	-155.686014	-153.848275	-153.850462
11	-154.196144	-154.193819	-148.660250	-148.678695
12	-152.642765	-152.746264	-145.492214	-145.514764
13	-148.994602	-148.976061	-141.345752	-141.349698
14	-145.230631	-145.236111	-140.326995	-140.330592
15	-141.682488	-141.678468	-139.838212	-139.817188
16	-139.940807	-139.938256	-136.614303	-136.691346
17	-137.881742	-139.006677	-135.951184	-135.968517
18	-136.279214	-136.258093	-131.969169	-131.984367
19	-131.633697	-131.620363	-130.609061	-130.547485
20	-130.220998	-130.283560	-128.615201	-128.894517
21	-129.243053	-128.983064	-128.311793	-128.596591
22	-128.798452	-126.991723	-126.658616	-127.911349
23	-127.049549	-126.491100	-126.038604	-126.591385
24	-125.602415	-125.730526	-121.626755	-122.088704
25	-121.291928	-121.259839	-118.804639	-118.859547
26	-119.442889	-119.041962	-118.412879	-118.630361
27	-118.783117	-118.955488	-117.780976	-118.515804
28	-118.598294	-117.681838	-117.380501	-116.709229
29	-117.581235	-116.584478	-115.417502	-116.194962
30	-117.218891	-115.183077	-114.755503	-116.041567
31	-115.244793	-115.095181	-114.149886	-115.514202
32	-114.395829	-113.798346	-113.718323	-114.513029
33	-114.088121	-113.282469	-112.132128	-114.280707
34	-113.096540	-113.183363	-111.853962	-113.014379
35	-112.245159	-112.670015	-111.090197	-110.596927
36	-111.526971	-111.976441	-110.698766	-108.831739
37	-110.208472	-110.214894	-107.735167	-107.723318
38	-108.767853	-108.781674	-106.490486	-106.652308
39	-108.279858	-108.658143	-105.495604	-106.179608
40	-107.221497	-107.412191	-104.687260	-105.883127