

Supporting Information for:

Ab initio study of the CO-N₂ complex: A new highly accurate intermolecular potential energy surface and rovibrational spectrum

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The following lists the lowest 10 levels for each symmetry case up to $J = 20$. Units are cm^{-1} . The first column of energies is with respect to dissociation, the second column is relative to the lowest level of that list (specific to symmetry and J), the third is relative to the lowest level for each of ortho or para N_2 .

Ortho N_2

Energy							
J0e-N2-even				J0o-N2-even			
1	-76.1252	0.0000	0.0000	1	-60.0651	0.0000	16.0601
2	-71.4388	4.6863	4.6863	2	-52.3504	7.7147	23.7748
3	-66.9581	9.1671	9.1671	3	-43.1135	16.9516	33.0117
4	-62.1757	13.9495	13.9495	4	-40.2118	19.8533	35.9134
5	-59.7001	16.4251	16.4251	5	-37.5301	22.5350	38.5951
6	-53.8239	22.3012	22.3012	6	-31.6175	28.4476	44.5077
7	-51.4472	24.6780	24.6780	7	-27.9072	32.1579	48.2180
8	-48.0427	28.0825	28.0825	8	-26.4902	33.5749	49.6350
9	-46.1147	30.0105	30.0105	9	-23.4369	36.6282	52.6882
10	-44.0925	32.0326	32.0326	10	-22.3798	37.6853	53.7453
J1e-N2-even				J1o-N2-even			
1	-72.4919	0.0000	3.6333	1	-75.9771	0.0000	0.1480
2	-67.2738	5.2181	8.8514	2	-72.5003	3.4769	3.6249
3	-62.5367	9.9552	13.5885	3	-71.3005	4.6766	4.8246
4	-60.6557	11.8362	15.4695	4	-67.2827	8.6945	8.8425
5	-59.9112	12.5807	16.2139	5	-66.8337	9.1434	9.2914
6	-56.5998	15.8920	19.5253	6	-62.5210	13.4561	13.6041
7	-53.3098	19.1820	22.8153	7	-62.0412	13.9359	14.0839
8	-52.9173	19.5746	23.2079	8	-60.6545	15.3226	15.4706
9	-52.1830	20.3089	23.9421	9	-59.5508	16.4263	16.5743
10	-50.2441	22.2478	25.8811	10	-56.5989	19.3782	19.5262
J2e-N2-even				J2o-N2-even			
1	-75.6812	0.0000	0.4439	1	-72.1990	0.0000	3.9262
2	-72.2242	3.4570	3.9010	2	-67.0096	5.1894	9.1155
3	-71.0239	4.6573	5.1013	3	-66.1336	6.0654	9.9916
4	-67.0358	8.6454	9.0893	4	-64.7517	7.4473	11.3735
5	-66.5851	9.0961	9.5401	5	-62.2778	9.9211	13.8473
6	-66.1339	9.5473	9.9913	6	-61.0526	11.1463	15.0725
7	-64.7516	10.9296	11.3735	7	-60.3637	11.8353	15.7615
8	-62.2322	13.4490	13.8929	8	-59.6044	12.5946	16.5208
9	-61.7719	13.9093	14.3533	9	-57.8769	14.3221	18.2482
10	-61.0527	14.6285	15.0724	10	-56.3278	15.8712	19.7974

J3e-N2-even				J3o-N2-even			
1	-71.7600	0.0000	4.3652	1	-75.2376	0.0000	0.8875
2	-66.6124	5.1476	9.5128	2	-71.8106	3.4271	4.3146
3	-65.6893	6.0707	10.4358	3	-70.6090	4.6286	5.5162
4	-64.3186	7.4414	11.8065	4	-66.6635	8.5741	9.4616
5	-61.8885	9.8715	14.2367	5	-66.2122	9.0254	9.9129
6	-60.6788	11.0812	15.4464	6	-65.6908	9.5468	10.4343
7	-59.9276	11.8324	16.1976	7	-64.3183	10.9193	11.8069
8	-59.2549	12.5051	16.8702	8	-61.8012	13.4364	14.3240
9	-59.1463	12.6137	16.9788	9	-61.3668	13.8708	14.7584
10	-57.4915	14.2685	18.6337	10	-60.6793	14.5584	15.4459
J4e-N2-even				J4o-N2-even			
1	-74.6467	0.0000	1.4785	1	-71.1755	0.0000	4.9497
2	-71.2600	3.3867	4.8652	2	-66.0812	5.0942	10.0439
3	-70.0559	4.5908	6.0693	3	-65.0990	6.0765	11.0262
4	-66.1641	8.4826	9.9611	4	-63.7418	7.4336	12.3833
5	-65.7151	8.9316	10.4100	5	-61.3675	9.8079	14.7576
6	-65.1029	9.5438	11.0222	6	-60.1763	10.9991	15.9488
7	-63.7409	10.9058	12.3843	7	-59.3489	11.8266	16.7763
8	-61.2306	13.4161	14.8945	8	-58.6254	12.5501	17.4998
9	-60.8244	13.8223	15.3008	9	-58.5393	12.6362	17.5859
10	-60.1779	14.4688	15.9472	10	-56.9782	14.1972	19.1469
J5e-N2-even				J5o-N2-even			
1	-70.4460	0.0000	5.6792	1	-73.9089	0.0000	2.2163
2	-65.4153	5.0307	10.7099	2	-70.5733	3.3356	5.5519
3	-64.3637	6.0823	11.7615	3	-69.3646	4.5443	6.7606
4	-63.0219	7.4241	13.1033	4	-65.5361	8.3728	10.5890
5	-60.7140	9.7320	15.4112	5	-65.0937	8.8152	11.0314
6	-59.5436	10.9024	16.5815	6	-64.3715	9.5374	11.7536
7	-58.6288	11.8172	17.4964	7	-63.0198	10.8891	13.1054
8	-57.8419	12.6041	18.2832	8	-60.5244	13.3845	15.6008
9	-57.7859	12.6602	18.3393	9	-60.1425	13.7664	15.9827
10	-56.3375	14.1085	19.7877	10	-59.5473	14.3616	16.5779
J6e-N2-even				J6o-N2-even			
1	-73.0248	0.0000	3.1003	1	-69.5725	0.0000	6.5527
2	-69.7513	3.2735	6.3738	2	-64.6138	4.9587	11.5114
3	-68.5351	4.4897	7.5900	3	-63.4845	6.0879	12.6406
4	-64.7785	8.2464	11.3467	4	-62.1594	7.4130	13.9657
5	-64.3481	8.6768	11.7771	5	-59.9269	9.6455	16.1983
6	-63.4978	9.5270	12.6274	6	-58.7794	10.7930	17.3458

7	-62.1555	10.8693	13.9696
8	-59.6870	13.3378	16.4381
9	-59.3183	13.7065	16.8069
10	-58.7866	14.2382	17.3386

7	-57.7683	11.8042	18.3569
8	-56.9073	12.6652	19.2179
9	-56.8878	12.6846	19.2373
10	-55.5696	14.0028	20.5555

J7e-N2-even

1	-68.5558	0.0000	7.5694
2	-63.6763	4.8795	12.4489
3	-62.4625	6.0934	13.6627
4	-61.1553	7.4005	14.9699
5	-59.0058	9.5500	17.1194
6	-57.8829	10.6729	18.2423
7	-56.7683	11.7875	19.3568
8	-55.8537	12.7021	20.2714
9	-55.8174	12.7384	20.3078
10	-54.6746	13.8812	21.4506

J7o-N2-even

1	-71.9952	0.0000	4.1300
2	-68.7953	3.1998	7.3298
3	-67.5677	4.4274	8.5574
4	-63.8904	8.1048	12.2348
5	-63.4780	8.5172	12.6472
6	-62.4825	9.5126	13.6426
7	-61.1488	10.8464	14.9764
8	-58.7231	13.2720	17.4020
9	-58.3498	13.6454	17.7754
10	-57.8954	14.0998	18.2298

J8e-N2-even

1	-70.8209	0.0000	5.3043
2	-67.7065	3.1144	8.4187
3	-66.4626	4.3583	9.6626
4	-62.8714	7.9494	13.2537
5	-62.4833	8.3376	13.6419
6	-61.3265	9.4944	14.7987
7	-60.0004	10.8205	16.1248
8	-57.6354	13.1855	18.4898
9	-57.2367	13.5841	18.8884
10	-56.8733	13.9475	19.2518

J8o-N2-even

1	-67.3973	0.0000	8.7279
2	-62.6024	4.7948	13.5227
3	-61.2983	6.0990	14.8269
4	-60.0105	7.3868	16.1147
5	-57.9503	9.4469	18.1748
6	-56.8537	10.5436	19.2715
7	-55.6299	11.7674	20.4953
8	-54.6785	12.7187	21.4466
9	-54.5817	12.8156	21.5435
10	-53.6521	13.7452	22.4731

J9e-N2-even

1	-66.0982	0.0000	10.0270
2	-61.3921	4.7061	14.7331
3	-59.9928	6.1054	16.1324
4	-58.7261	7.3721	17.3991
5	-56.7608	9.3374	19.3644
6	-55.6915	10.4067	20.4337
7	-54.3539	11.7443	21.7712
8	-53.3695	12.7287	22.7556
9	-53.1975	12.9007	22.9277
10	-52.5009	13.5972	23.6242

J9o-N2-even

1	-69.5029	0.0000	6.6222
2	-66.4861	3.0169	9.6391
3	-65.2199	4.2830	10.9052
4	-61.7217	7.7813	14.4035
5	-61.3638	8.1392	14.7614
6	-60.0302	9.4728	16.0950
7	-58.7115	10.7914	17.4137
8	-56.4242	13.0788	19.7010
9	-55.9819	13.5211	20.1433
10	-55.7202	13.7828	20.4050

J10e-N2-even

1	-68.0427	0.0000	8.0825
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J10o-N2-even

1	-64.6601	0.0000	11.4650
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2	-65.1354	2.9073	10.9897
3	-63.8403	4.2024	12.2848
4	-60.4414	7.6013	15.6838
5	-60.1188	7.9239	16.0064
6	-58.5942	9.4485	17.5309
7	-57.2833	10.7594	18.8419
8	-55.0886	12.9541	21.0366
9	-54.5903	13.4524	21.5349
10	-54.4347	13.6080	21.6905

2	-60.0451	4.6150	16.0800
3	-58.5466	6.1135	17.5785
4	-57.3035	7.3567	18.8217
5	-55.4376	9.2226	20.6876
6	-54.3965	10.2637	21.7287
7	-52.9415	11.7186	23.1836
8	-51.9303	12.7299	24.1949
9	-51.6669	12.9933	24.4583
10	-51.2183	13.4419	24.9069

J11e-N2-even

1	-63.0849	0.0000	13.0402
2	-58.5617	4.5232	17.5634
3	-56.9604	6.1245	19.1648
4	-55.7442	7.3407	20.3810
5	-53.9816	9.1033	22.1435
6	-52.9688	10.1162	23.1564
7	-51.3938	11.6911	24.7313
8	-50.3666	12.7183	25.7586
9	-49.9950	13.0899	26.1301
10	-49.7952	13.2897	26.3300

J11o-N2-even

1	-66.4416	0.0000	9.6836
2	-63.6558	2.7858	12.4694
3	-62.3243	4.1172	13.8008
4	-59.0318	7.4098	17.0934
5	-58.7471	7.6944	17.3780
6	-57.0193	9.4222	19.1058
7	-55.7173	10.7242	20.4078
8	-53.6277	12.8139	22.4975
9	-53.0756	13.3660	23.0496
10	-53.0071	13.4345	23.1180

J12e-N2-even

1	-64.7014	0.0000	11.4237
2	-62.0484	2.6531	14.0768
3	-60.6730	4.0284	15.4522
4	-57.4955	7.2060	18.6297
5	-57.2461	7.4553	18.8790
6	-55.3064	9.3950	20.8188
7	-54.0153	10.6861	22.1099
8	-52.0411	12.6603	24.0840
9	-51.4927	13.2088	24.6325
10	-51.3857	13.3157	24.7394

J12o-N2-even

1	-61.3744	0.0000	14.7507
2	-56.9421	4.4323	19.1830
3	-55.2347	6.1397	20.8904
4	-54.0499	7.3246	22.0753
5	-52.3941	8.9804	23.7311
6	-51.4086	9.9658	24.7165
7	-49.7120	11.6624	26.4132
8	-48.6897	12.6847	27.4354
9	-48.2646	13.1098	27.8605
10	-48.1395	13.2349	27.9856

J13e-N2-even

1	-59.5309	0.0000	16.5943
2	-55.1866	4.3443	20.9386
3	-53.3704	6.1604	22.7547
4	-52.2225	7.3084	23.9027
5	-50.6763	8.8546	25.4489
6	-49.7165	9.8144	26.4087
7	-47.8974	11.6335	28.2278
8	-46.9187	12.6122	29.2065

J13o-N2-even

1	-62.8244	0.0000	13.3008
2	-60.3141	2.5103	15.8111
3	-58.8874	3.9369	17.2377
4	-55.8373	6.9870	20.2878
5	-55.6107	7.2137	20.5144
6	-53.4564	9.3679	22.6687
7	-52.1792	10.6452	23.9460
8	-50.3295	12.4949	25.7957

9	-46.5219	13.0090	29.6033
10	-46.1872	13.3437	29.9380

9	-49.8100	13.0144	26.3152
10	-49.6042	13.2202	26.5209
			76.1252

J14e-N2-even

1	-60.8131	0.0000	15.3121
2	-58.4537	2.3593	17.6715
3	-56.9693	3.8438	19.1559
4	-54.0644	6.7486	22.0607
5	-53.8336	6.9795	22.2916
6	-51.4709	9.3421	24.6542
7	-50.2115	10.6016	25.9137
8	-48.4938	12.3192	27.6313
9	-47.9975	12.8156	28.1277
10	-47.6939	13.1191	28.4312

J14o-N2-even

1	-57.5565	0.0000	18.5686
2	-53.2957	4.2609	22.8295
3	-51.3683	6.1882	24.7569
4	-50.2644	7.2921	25.8608
5	-48.8296	8.7269	27.2956
6	-47.8929	9.6637	28.2323
7	-45.9512	11.6053	30.1739
8	-45.0655	12.4910	31.0596
9	-44.6121	12.9444	31.5131
10	-44.0815	13.4750	32.0437

J15e-N2-even

1	-55.4538	0.0000	20.6714
2	-51.2700	4.1838	24.8551
3	-49.2293	6.2245	26.8959
4	-48.1782	7.2756	27.9470
5	-46.8553	8.5985	29.2698
6	-45.9383	9.5155	30.1869
7	-43.8751	11.5787	32.2501
8	-43.1167	12.3371	33.0085
9	-42.5373	12.9165	33.5879
10	-41.8347	13.6190	34.2904

J15o-N2-even

1	-58.6707	0.0000	17.4545
2	-56.4676	2.2031	19.6576
3	-54.9204	3.7502	21.2047
4	-52.1807	6.4899	23.9444
5	-51.9103	6.7603	24.2148
6	-49.3517	9.3190	26.7735
7	-48.1149	10.5557	28.0102
8	-46.5353	12.1353	29.5898
9	-46.0511	12.6196	30.0741
10	-45.6598	13.0109	30.4654

J16e-N2-even

1	-56.4011	0.0000	19.7240
2	-54.3556	2.0455	21.7695
3	-52.7432	3.6579	23.3820
4	-50.1837	6.2175	25.9415
5	-49.8428	6.5584	26.2824
6	-47.1009	9.3003	29.0243
7	-45.8931	10.5080	30.2320
8	-44.4544	11.9467	31.6707
9	-43.9695	12.4317	32.1557
10	-43.5040	12.8971	32.6211

J16o-N2-even

1	-53.2252	0.0000	22.8999
2	-49.1106	4.1146	27.0145
3	-46.9548	6.2704	29.1703
4	-45.9670	7.2582	30.1581
5	-44.7544	8.4709	31.3708
6	-43.8533	9.3720	32.2719
7	-41.6708	11.5544	34.4543
8	-41.0525	12.1728	35.0727
9	-40.3140	12.9113	35.8112
10	-39.4507	13.7746	36.6745

J17e-N2-even

1	-50.8735	0.0000	25.2517
2	-46.8187	4.0547	29.3064
3	-44.5466	6.3269	31.5786

J17o-N2-even

1	-54.0095	0.0000	22.1157
2	-52.1172	1.8923	24.0079
3	-50.4403	3.5692	25.6849

4	-43.6348	7.2387	32.4904
5	-42.5270	8.3465	33.5982
6	-41.6384	9.2350	34.4868
7	-39.3411	11.5324	36.7841
8	-38.8603	12.0132	37.2649
9	-37.9518	12.9217	38.1734
10	-36.9327	13.9407	39.1924

4	-48.0679	5.9416	28.0573
5	-47.6350	6.3744	28.4901
6	-44.7214	9.2881	31.4038
7	-43.5508	10.4587	32.5744
8	-42.2497	11.7597	33.8754
9	-41.7524	12.2570	34.3727
10	-41.2287	12.7808	34.8965

J18e-N2-even

1	-51.5018	0.0000	24.6234
2	-49.7510	1.7508	26.3742
3	-48.0150	3.4868	28.1102
4	-45.8283	5.6735	30.2969
5	-45.2903	6.2115	30.8349
6	-42.2166	9.2852	33.9085
7	-41.0942	10.4076	35.0310
8	-39.9172	11.5846	36.2079
9	-39.4009	12.1009	36.7243
10	-38.8354	12.6664	37.2897

J18o-N2-even

1	-48.4010	0.0000	27.7241
2	-44.3961	4.0050	31.7291
3	-42.0068	6.3942	34.1183
4	-41.1863	7.2147	34.9388
5	-40.1722	8.2289	35.9530
6	-39.2941	9.1069	36.8311
7	-36.8904	11.5107	39.2348
8	-36.5306	11.8705	39.5946
9	-35.4555	12.9455	40.6697
10	-34.2853	14.1157	41.8399

J19e-N2-even

1	-45.8105	0.0000	30.3147
2	-41.8448	3.9657	34.2804
3	-39.3387	6.4717	36.7864
4	-38.6279	7.1826	37.4973
5	-37.6871	8.1234	38.4381
6	-36.8203	8.9902	39.3049
7	-34.3276	11.4828	41.7975
8	-34.0519	11.7585	42.0732
9	-32.8279	12.9825	43.2972
10	-31.5138	14.2967	44.6113

J19o-N2-even

1	-48.8856	0.0000	27.2395
2	-47.2548	1.6308	28.8703
3	-45.4715	3.4142	30.6537
4	-43.4600	5.4256	32.6651
5	-42.8108	6.0748	33.3144
6	-39.5907	9.2949	36.5344
7	-38.5319	10.3538	37.5933
8	-37.4500	11.4357	38.6752
9	-36.9162	11.9695	39.2090
10	-36.3260	12.5596	39.7992

J20e-N2-even

1	-46.1696	0.0000	29.9556
2	-44.6261	1.5434	31.4990
3	-42.8149	3.3547	33.3103
4	-40.9573	5.2123	35.1679
5	-40.1982	5.9714	35.9270
6	-36.8486	9.3210	39.2766
7	-35.8740	10.2956	40.2511
8	-34.8396	11.3300	41.2856
9	-34.2992	11.8704	41.8260
10	-33.7017	12.4679	42.4235

J20o-N2-even

1	-43.1042	0.0000	33.0209
2	-39.1676	3.9366	36.9576
3	-36.5467	6.5575	39.5785
4	-35.9669	7.1373	40.1583
5	-35.0667	8.0376	41.0585
6	-34.2166	8.8876	41.9086
7	-31.6651	11.4392	44.4601
8	-31.4110	11.6932	44.7142
9	-30.0714	13.0328	46.0538
10	-28.6257	14.4785	47.4994

Para N2

	J0e-N2-odd		
1	-73.3887	0.0000	0.0000
2	-68.9682	4.4205	4.4205
3	-61.6793	11.7094	11.7094
4	-54.3771	19.0115	19.0115
5	-53.2918	20.0968	20.0968
6	-51.6156	21.7731	21.7731
7	-46.4161	26.9726	26.9726
8	-43.2192	30.1695	30.1695
9	-42.3804	31.0082	31.0082
10	-40.0013	33.3873	33.3873

	J1e-N2-odd		
1	-73.1907	0.0000	0.1979
2	-69.9490	3.2418	3.4397
3	-66.8415	6.3493	6.5472
4	-65.9355	7.2552	7.4532
5	-61.2892	11.9015	12.0994
6	-60.7241	12.4667	12.6646
7	-58.1296	15.0612	15.2591
8	-54.6795	18.5113	18.7092
9	-51.2599	21.9309	22.1288
10	-50.9467	22.2441	22.4420

	J2e-N2-odd		
1	-73.0687	0.0000	0.3200
2	-72.8136	0.2550	0.5751
3	-69.6844	3.3843	3.7043
4	-68.5421	4.5265	4.8465
5	-67.5622	5.5065	5.8265
6	-65.7009	7.3677	7.6877
7	-63.4127	9.6560	9.9760
8	-61.3094	11.7593	12.0793
9	-61.0149	12.0538	12.3738
10	-60.4194	12.6493	12.9693

	J3e-N2-odd		
1	-72.4433	0.0000	0.9453

	J0o-N2-odd		
1	-66.9777	0.0000	6.4110
2	-58.2833	8.6943	15.1054
3	-50.2959	16.6818	23.0928
4	-48.1317	18.8459	25.2570
5	-41.5857	25.3920	31.8030
6	-38.5474	28.4303	34.8413
7	-33.7363	33.2414	39.6524
8	-31.2693	35.7084	42.1194
9	-29.6463	37.3313	43.7424
10	-26.1684	40.8093	47.2203

	J1o-N2-odd		
1	-73.2999	0.0000	0.0887
2	-73.1467	0.1532	0.2420
3	-69.9489	3.3511	3.4398
4	-68.8262	4.4738	4.5625
5	-65.9595	7.3405	7.4292
6	-61.5567	11.7432	11.8320
7	-61.2830	12.0170	12.1057
8	-60.7088	12.5912	12.6799
9	-54.6915	18.6084	18.6972
10	-54.2293	19.0706	19.1593

	J2o-N2-odd		
1	-72.8917	0.0000	0.4970
2	-69.6847	3.2070	3.7040
3	-67.5623	5.3294	5.8264
4	-66.5696	6.3220	6.8191
5	-65.6288	7.2628	7.7598
6	-63.4127	9.4790	9.9760
7	-61.0329	11.8587	12.3558
8	-60.4623	12.4294	12.9264
9	-58.7169	14.1747	14.6718
10	-57.8221	15.0695	15.5665

	J3o-N2-odd		
1	-72.6955	0.0000	0.6932

2	-69.2876	3.1557	4.1011
3	-67.1039	5.3394	6.2848
4	-66.1629	6.2804	7.2258
5	-65.1686	7.2747	8.2201
6	-63.0144	9.4290	10.3743
7	-60.6507	11.7927	12.7380
8	-60.0645	12.3789	13.3242
9	-58.8082	13.6352	14.5805
10	-58.2545	14.1889	15.1342

2	-72.3411	0.3544	1.0476
3	-69.2871	3.4084	4.1016
4	-68.1163	4.5792	5.2724
5	-67.1033	5.5922	6.2854
6	-65.3135	7.3820	8.0752
7	-63.0144	9.6811	10.3743
8	-60.9345	11.7610	12.4542
9	-60.6159	12.0796	12.7727
10	-59.9868	12.7087	13.4019

J4e-N2-odd

1	-72.1806	0.0000	1.2080
2	-71.7299	0.4507	1.6588
3	-68.7567	3.4240	4.6320
4	-67.5490	4.6316	5.8397
5	-66.4926	5.6880	6.8961
6	-64.7975	7.3831	8.5912
7	-62.4831	9.6976	10.9056
8	-60.4293	11.7513	12.9593
9	-60.0875	12.0931	13.3012
10	-59.4130	12.7676	13.9757

J4o-N2-odd

1	-71.8461	0.0000	1.5426
2	-68.7573	3.0888	4.6314
3	-66.4944	5.3517	6.8943
4	-65.6224	6.2237	7.7662
5	-64.5547	7.2914	8.8340
6	-62.4829	9.3632	10.9058
7	-60.1438	11.7023	13.2449
8	-59.5266	12.3195	13.8621
9	-58.2203	13.6258	15.1684
10	-57.6450	14.2011	15.7437

J5e-N2-odd

1	-71.1004	0.0000	2.2883
2	-68.0931	3.0073	5.2955
3	-65.7351	5.3653	7.6535
4	-64.9492	6.1512	8.4395
5	-63.7873	7.3130	9.6013
6	-61.8181	9.2823	11.5705
7	-59.5125	11.5879	13.8761
8	-58.8456	12.2548	14.5431
9	-57.4857	13.6147	15.9030
10	-56.8912	14.2092	16.4975

J5o-N2-odd

1	-71.5243	0.0000	1.8644
2	-70.9812	0.5430	2.4074
3	-68.0925	3.4318	5.2962
4	-66.8405	4.6838	6.5482
5	-65.7309	5.7934	7.6578
6	-64.1534	7.3709	9.2353
7	-61.8184	9.7058	11.5702
8	-59.7922	11.7320	13.5964
9	-59.4301	12.0942	13.9586
10	-58.7001	12.8242	14.6886

J6e-N2-odd

1	-70.7269	0.0000	2.6618
2	-70.0963	0.6305	3.2924
3	-67.2942	3.4327	6.0945
4	-65.9912	4.7357	7.3975
5	-64.8192	5.9077	8.5695
6	-63.3817	7.3451	10.0070
7	-61.0204	9.7065	12.3683
8	-59.0221	11.7047	14.3665

J6o-N2-odd

1	-70.2069	0.0000	3.1818
2	-67.2945	2.9124	6.0942
3	-64.8279	5.3790	8.5608
4	-64.1439	6.0630	9.2448
5	-62.8670	7.3398	10.5216
6	-61.0198	9.1870	12.3688
7	-58.7554	11.4515	14.6333
8	-58.0203	12.1866	15.3684

9	-58.6434	12.0834	14.7453
10	-57.8503	12.8765	15.5384

9	-56.6059	13.6009	16.7827
10	-55.9947	14.2122	17.3940

J7e-N2-odd

1	-69.1663	0.0000	4.2224
2	-66.3610	2.8053	7.0277
3	-63.7752	5.3911	9.6134
4	-63.2064	5.9599	10.1823
5	-61.7947	7.3716	11.5940
6	-60.0879	9.0784	13.3007
7	-57.8697	11.2966	15.5190
8	-57.0512	12.1151	16.3374
9	-55.5833	13.5830	17.8054
10	-54.9556	14.2107	18.4331

J7o-N2-odd

1	-69.7889	0.0000	3.5997
2	-69.0765	0.7124	4.3121
3	-66.3613	3.4277	7.0274
4	-65.0015	4.7874	8.3872
5	-63.7584	6.0305	9.6302
6	-62.4830	7.3060	10.9057
7	-60.0888	9.7001	13.2998
8	-58.1185	11.6704	15.2702
9	-57.7268	12.0621	15.6619
10	-56.8656	12.9233	16.5230

J8e-N2-odd

1	-68.7113	0.0000	4.6774
2	-67.9235	0.7878	5.4652
3	-65.2936	3.4177	8.0951
4	-63.8720	4.8393	9.5167
5	-62.5499	6.1613	10.8387
6	-61.4575	7.2538	11.9311
7	-59.0237	9.6876	14.3649
8	-57.0812	11.6301	16.3074
9	-56.6796	12.0317	16.7091
10	-55.7477	12.9636	17.6410

J8o-N2-odd

1	-67.9797	0.0000	5.4090
2	-65.2921	2.6875	8.0966
3	-62.5819	5.3977	10.8068
4	-62.1346	5.8450	11.2540
5	-60.5717	7.4079	12.8170
6	-59.0224	8.9572	14.3662
7	-56.8522	11.1275	16.5365
8	-55.9397	12.0400	17.4490
9	-54.4203	13.5594	18.9684
10	-53.7737	14.2060	19.6150

J9e-N2-odd

1	-66.6481	0.0000	6.7406
2	-64.0876	2.5605	9.3011
3	-61.2589	5.3892	12.1298
4	-60.9200	5.7280	12.4686
5	-59.1998	7.4483	14.1889
6	-57.8235	8.8246	15.5652
7	-55.6996	10.9485	17.6891
8	-54.6874	11.9607	18.7013
9	-53.1194	13.5287	20.2693
10	-52.4483	14.1998	20.9404

J9o-N2-odd

1	-67.4948	0.0000	5.8939
2	-66.6387	0.8561	6.7499
3	-64.0911	3.4037	9.2976
4	-62.6032	4.8916	10.7855
5	-61.1952	6.2996	12.1935
6	-60.3056	7.1892	13.0831
7	-57.8252	9.6696	15.5635
8	-55.9104	11.5844	17.4782
9	-55.5011	11.9937	17.8876
10	-54.4977	12.9971	18.8909

J10e-N2-odd

1	-66.1406	0.0000	7.2481
2	-65.2241	0.9164	8.1645
3	-62.7538	3.3868	10.6349

J10o-N2-odd

1	-65.1731	0.0000	8.2156
2	-62.7472	2.4259	10.6415
3	-59.8334	5.3397	13.5553

4	-61.1958	4.9448	12.1929
5	-59.6966	6.4440	13.6921
6	-59.0265	7.1140	14.3622
7	-56.4933	9.6473	16.8954
8	-54.6064	11.5341	18.7822
9	-54.1909	11.9496	19.1977
10	-53.1166	13.0240	20.2721

4	-59.5380	5.6351	13.8507
5	-57.6811	7.4920	15.7076
6	-56.4913	8.6818	16.8974
7	-54.4087	10.7644	18.9800
8	-53.2961	11.8770	20.0926
9	-51.6828	13.4902	21.7058
10	-50.9792	14.1939	22.4095

J11e-N2-odd

1	-63.5564	0.0000	9.8322
2	-61.2707	2.2858	12.1180
3	-58.3342	5.2222	15.0544
4	-57.9623	5.5942	15.4264
5	-56.0184	7.5380	17.3703
6	-55.0258	8.5307	18.3629
7	-52.9765	10.5799	20.4121
8	-51.7676	11.7888	21.6211
9	-50.1125	13.4440	23.2762
10	-49.3668	14.1896	24.0218

J11o-N2-odd

1	-64.6499	0.0000	8.7388
2	-63.6815	0.9684	9.7072
3	-61.2821	3.3678	12.1066
4	-59.6506	4.9993	13.7381
5	-58.0590	6.5909	15.3297
6	-57.6172	7.0326	15.7714
7	-55.0282	9.6217	18.3605
8	-53.1696	11.4802	20.2190
9	-52.7489	11.9009	20.6398
10	-51.6049	13.0450	21.7838

J12e-N2-odd

1	-63.0241	0.0000	10.3646
2	-62.0126	1.0115	11.3760
3	-59.6764	3.3477	13.7123
4	-57.9684	5.0557	15.4202
5	-56.3033	6.7208	17.0853
6	-56.0587	6.9654	17.3300
7	-53.4300	9.5941	19.9587
8	-51.6006	11.4236	21.7881
9	-51.1750	11.8491	22.2136
10	-49.9631	13.0611	23.4256

J12o-N2-odd

1	-61.8005	0.0000	11.5882
2	-59.6577	2.1428	13.7310
3	-56.7476	5.0529	16.6411
4	-56.2096	5.5909	17.1791
5	-54.2155	7.5850	19.1732
6	-53.4266	8.3739	19.9621
7	-51.4003	10.4002	21.9884
8	-50.1035	11.6970	23.2852
9	-48.4095	13.3909	24.9791
10	-47.6124	14.1880	25.7762

J13e-N2-odd

1	-59.9081	0.0000	13.4806
2	-57.9077	2.0004	15.4810
3	-55.0528	4.8552	18.3359
4	-54.3036	5.6044	19.0851
5	-52.2777	7.6304	21.1110
6	-51.6918	8.2162	21.6969
7	-49.6771	10.2309	23.7116
8	-48.3052	11.6028	25.0835
9	-46.5750	13.3331	26.8137
10	-45.7183	14.1898	27.6704

J13o-N2-odd

1	-61.2650	0.0000	12.1237
2	-60.2195	1.0455	13.1692
3	-57.9375	3.3275	15.4512
4	-56.1505	5.1145	17.2382
5	-54.5254	6.7396	18.8632
6	-54.2574	7.0076	19.1313
7	-51.6985	9.5665	21.6902
8	-49.8998	11.3652	23.4889
9	-49.4694	11.7955	23.9192
10	-48.1914	13.0736	25.1973

J14e-N2-odd			
1	-59.3743	0.0000	14.0144
2	-58.3040	1.0703	15.0847
3	-56.0664	3.3079	17.3223
4	-54.1979	5.1764	19.1908
5	-52.7236	6.6507	20.6650
6	-52.2175	7.1568	21.1712
7	-49.8333	9.5410	23.5554
8	-48.0679	11.3064	25.3208
9	-47.6325	11.7418	25.7562
10	-46.2902	13.0841	27.0985

J14o-N2-odd			
1	-57.8829	0.0000	15.5058
2	-56.0198	1.8631	17.3689
3	-53.2416	4.6413	20.1471
4	-52.2560	5.6270	21.1327
5	-50.2153	7.6676	23.1734
6	-49.8150	8.0679	23.5736
7	-47.8043	10.0786	25.5844
8	-46.3743	11.5086	27.0144
9	-44.6094	13.2735	28.7793
10	-43.6873	14.1956	29.7014

J15e-N2-odd			
1	-55.7298	0.0000	17.6588
2	-53.9927	1.7371	19.3959
3	-51.3109	4.4190	22.0778
4	-50.0735	5.6563	23.3152
5	-48.0538	7.6761	25.3349
6	-47.7744	7.9555	25.6143
7	-45.7791	9.9507	27.6095
8	-44.3119	11.4179	29.0768
9	-42.5134	13.2165	30.8753
10	-41.5236	14.2063	31.8651

J15o-N2-odd			
1	-57.3540	0.0000	16.0346
2	-56.2680	1.0860	17.1207
3	-54.0641	3.2899	19.3246
4	-52.1122	5.2419	21.2765
5	-50.8171	6.5369	22.5716
6	-50.0230	7.3311	23.3657
7	-47.8332	9.5209	25.5555
8	-46.1057	11.2484	27.2830
9	-45.6645	11.6896	27.7242
10	-44.2598	13.0943	29.1289

J16e-N2-odd			
1	-55.2064	0.0000	18.1822
2	-54.1135	1.0930	19.2752
3	-51.9322	3.2742	21.4564
4	-49.8951	5.3114	23.4936
5	-48.7897	6.4168	24.5990
6	-47.6940	7.5125	25.6947
7	-45.6961	9.5104	27.6926
8	-44.0138	11.1927	29.3749
9	-43.5659	11.6405	29.8228
10	-42.1004	13.1060	31.2882

J16o-N2-odd			
1	-53.4548	0.0000	19.9339
2	-51.8246	1.6301	21.5640
3	-49.2589	4.1959	24.1298
4	-47.7623	5.6924	25.6264
5	-45.8340	7.6208	27.5547
6	-45.5322	7.9225	27.8564
7	-43.5991	9.8557	29.7896
8	-42.1191	11.3356	31.2695
9	-40.2874	13.1673	33.1012
10	-39.2317	14.2231	34.1570

J17e-N2-odd			
1	-51.0649	0.0000	22.3238
2	-49.5134	1.5515	23.8753
3	-47.0838	3.9811	26.3049
4	-45.3293	5.7356	28.0594
5	-43.5353	7.5295	29.8533

J17o-N2-odd			
1	-52.9339	0.0000	20.4548
2	-51.8422	1.0917	21.5465
3	-49.6726	3.2613	23.7161
4	-47.5486	5.3853	25.8401
5	-46.6371	6.2968	26.7516

6	-43.1116	7.9533	30.2771
7	-41.2619	9.8030	32.1267
8	-39.7969	11.2680	33.5917
9	-37.9323	13.1326	35.4564
10	-36.8172	14.2477	36.5715

6	-45.2400	7.6938	28.1486
7	-43.4185	9.5154	29.9702
8	-41.7929	11.1409	31.5957
9	-41.3373	11.5965	32.0513
10	-39.8125	13.1214	33.5762

J18e-N2-odd

1	-50.5390	0.0000	22.8497
2	-49.4562	1.0827	23.9325
3	-47.2871	3.2518	26.1015
4	-45.0752	5.4638	28.3135
5	-44.3566	6.1824	29.0321
6	-42.6705	7.8684	30.7182
7	-40.9955	9.5435	32.3932
8	-39.4439	11.0951	33.9448
9	-38.9793	11.5596	34.4093
10	-37.3964	13.1426	35.9923

J18o-N2-odd

1	-48.5680	0.0000	24.8207
2	-47.0576	1.5104	26.3311
3	-44.7830	3.7850	28.6057
4	-42.7827	5.7854	30.6060
5	-41.1136	7.4544	32.2751
6	-40.5571	8.0109	32.8315
7	-38.7668	9.8012	34.6219
8	-37.3459	11.2221	36.0428
9	-35.4486	13.1194	37.9401
10	-34.2858	14.2822	39.1028

J19e-N2-odd

1	-45.9714	0.0000	27.4172
2	-44.4581	1.5133	28.9306
3	-42.3524	3.6191	31.0363
4	-40.1317	5.8397	33.2570
5	-38.5487	7.4228	34.8400
6	-37.8874	8.0841	35.5013
7	-36.1146	9.8568	37.2741
8	-34.7663	11.2052	38.6224
9	-32.8370	13.1345	40.5517
10	-31.6426	14.3289	41.7461

J19o-N2-odd

1	-48.0245	0.0000	25.3642
2	-46.9573	1.0672	26.4314
3	-44.7784	3.2461	28.6102
4	-42.4782	5.5463	30.9105
5	-41.9450	6.0795	31.4436
6	-39.9958	8.0287	33.3928
7	-38.4207	9.6038	34.9679
8	-36.9671	11.0574	36.4216
9	-36.4927	11.5318	36.8960
10	-34.8523	13.1722	38.5363

J20e-N2-odd

1	-45.3936	0.0000	27.9951
2	-44.3472	1.0463	29.0414
3	-42.1492	3.2444	31.2395
4	-39.7626	5.6310	33.6261
5	-39.3978	5.9958	33.9909
6	-37.2261	8.1675	36.1626
7	-35.6887	9.7048	37.6999
8	-34.3628	11.0308	39.0259
9	-33.8783	11.5153	39.5104
10	-32.1805	13.2131	41.2082

J20o-N2-odd

1	-43.2806	0.0000	30.1081
2	-41.7203	1.5603	31.6684
3	-39.7854	3.4952	33.6033
4	-37.3852	5.8954	36.0034
5	-35.8309	7.4497	37.5578
6	-35.1093	8.1713	38.2794
7	-33.3094	9.9712	40.0792
8	-32.0579	11.2227	41.3308
9	-30.0980	13.1826	43.2906
10	-28.8907	14.3899	44.4980