

Table 1 Comparisons of the spectroscopic constants for CN.

State	R_e (Å)	$\omega_e(\text{cm}^{-1})$	$\omega_e x_e(\text{cm}^{-1})$	$B_e(\text{cm}^{-1})$	$\alpha_e(\text{cm}^{-1})$
A $^2\Pi$ ^a	1.24	1781.8313	12.766	1.6914	0.01691
A $^2\Pi$ ^b	1.24	1781.3268	12.7775	1.6911	0.01673
D $^2\Pi$ ^a	1.51	986.2968	9.211	1.1452	0.01737
D $^2\Pi$ ^b	1.51	986.10298	9.20309	1.14482	0.01734
H $^2\Pi$ ^a	1.325	2070.8921	119.917	1.4715	0.05594
H $^2\Pi$ ^b	1.325	2070.1574	119.853	1.47126	0.05592
4 $^2\Pi$ ^a	1.475	1368.7963	23.273	1.2349	0.00057
4 $^2\Pi$ ^b	1.475	1368.9268	23.34271	1.20318	0.00058

Notes: ^a spectroscopic constants fitted based on those data calculated using d-aug-cc-pVTZ basis set.

^b spectroscopic constants fitted based on those data calculated using aug-cc-pVTZ basis set.

Table 2 PECs of the A $^2\Pi$, D $^2\Pi$, H $^2\Pi$, 4 $^2\Pi$ states of CN calculated using aug-cc-pVTZ basis set.

R	A $^2\Pi$	D $^2\Pi$	H $^2\Pi$	4 $^2\Pi$
0.8	189583.68778	236260.52524	238033.47643	250447.53221
0.85	132253.2686	185087.56999	189236.97054	200106.40996
0.9	90709.39847	146538.23149	154640.75423	163887.69671
0.95	61069.65677	117684.30334	129595.36936	138272.6786
0.98	47734.34305	104285.69972	118648.31493	127083.11787
1	40355.82322	96740.55256	112753.96157	121192.4056
1.02	34035.70664	90171.97094	107824.84886	116450.86908
1.04	28660.55563	84479.49254	103732.6017	112742.16481
1.06	24195.20818	79551.90079	100346.64146	105261.84387
1.08	20409.65926	75350.37502	97585.99298	100148.15519
1.1	17291.27152	71782.99705	92618.49635	97923.35183
1.12	14766.3761	68781.71877	86914.75891	96091.0525
1.14	12768.31418	66285.64916	82076.66672	94810.5146
1.16	11247.01699	64224.54533	77801.88909	91541.11295
1.18	10133.8263	62679.59317	74091.79116	88308.54572
1.2	9376.98778	61391.65239	70776.79804	85291.80327
1.22	8941.47988	60412.11955	67877.50305	82572.51917
1.24	8788.31073	59699.14524	65358.04402	80157.10648
1.26	8882.4017	59207.7569	63193.2099	78031.70756
1.28	9192.30208	58869.58161	61387.14218	76177.93923
1.3	9689.794	58498.72435	60068.08868	74575.44521
1.32	10349.52596	57707.66096	59567.73261	73204.1743
1.34	11148.77137	56695.50761	59639.30767	72045.29557
1.36	12067.11687	55773.13475	59926.94674	71081.84583
1.38	13086.28683	54996.00141	60335.3166	70298.62427
1.4	14189.89745	54362.52081	60825.94555	69683.05719
1.42	15363.29443	53863.03606	61220.55655	69225.04875
1.44	16593.3817	53485.49579	61851.08741	68917.15876
1.46	17868.4503	53217.96939	62489.10017	68754.91434
1.48	19178.0664	53049.12097	63113.69205	68735.38329
1.5	20512.94403	52968.6067	63681.34782	68855.93851
1.55	23908.72795	53094.07157	64888.23881	69716.71143
1.6	27307.83911	53590.3081	65880.1171	71144.15688
1.65	30632.83368	54362.16307	66813.55368	72789.86765
1.68	32568.17854	54926.76814	67388.32921	73774.69641
1.73	35664.56834	55997.15031	68391.51263	75302.41103
1.75	36851.73296	56461.97343	68808.43103	75853.91566
1.8	39677.03867	57694.57808	69881.84853	77052.12863
1.85	42284.34022	59004.39829	70983.94039	77996.42043
1.9	44661.96158	60366.59612	72093.65242	78740.45918
1.95	46804.85262	61760.38294	73190.09719	79362.24398
2	48714.07341	63166.91684	74252.87895	79917.92961

2.05	50396.37499	64568.15262	75261.71824	80439.02603
2.1	51863.48389	65946.5806	76195.96468	80940.06467
2.15	53131.02671	67285.61069	77034.86915	81432.25408
2.2	54217.32956	68570.323	77759.04984	81927.54249
2.25	55141.60088	69788.27991	78354.37697	82438.24239
2.3	55923.60216	70929.65334	78818.38804	82968.92547
2.35	56587.75874	71992.31	79172.67058	83517.29161
2.4	57142.33601	72965.44735	79418.78723	84060.50669
2.45	57606.87602	73851.85491	79588.37528	84581.03028
2.5	57995.80482	74653.5694	79694.34641	85055.69904
2.55	58321.60613	75373.93781	79755.75541	85450.17177
2.6	58594.94422	76016.35103	79795.4474	85693.30577
2.7	59018.74315	77082.85947	79839.22381	85022.09309
2.8	59321.97589	77891.51156	79858.30274	81918.42112
2.9	59540.20829	78502.37749	79892.36301	80500.26165
3	59703.68178	78952.24562	79913.25919	80271.17403
3.2	59921.42256	79529.22028	79940.35772	80006.15183
3.3	59994.82585	79712.82618	79953.04774	79925.84167
3.35	60025.40305	79786.99543	79958.81334	79895.07132
3.45	60076.87863	79908.57121	79967.27409	79846.69253
3.5	60098.5759	79958.86163	79968.75774	79828.21935
3.6	60135.5859	80044.73547	79962.57294	79799.92688
3.7	60165.32033	80118.75987	79941.0754	79781.0367
3.8	60189.39669	80187.93169	79926.60325	79768.75051
4	60224.80015	80297.70632	79948.20833	79756.91643
4.1	60237.71184	80326.80865	79963.1765	79754.95214
4.2	60248.23784	80345.23355	79976.34059	79754.53733
4.3	60256.85442	80358.09257	79987.39991	79755.14527
4.4	60263.94564	80367.85699	79996.66613	79756.39408
4.5	60269.82317	80375.90732	80004.20728	79758.0182
4.6	60274.73282	80382.6408	80010.44914	79759.84203
4.7	60278.8765	80388.26155	80015.65069	79761.73829
4.8	60282.40126	80393.34897	80020.02043	79763.62577
4.9	60285.42782	80398.00403	80023.72077	79765.4518
5	60288.04835	80402.05772	80026.87901	79767.18785

Table 3 PECs of the A $^2\Pi$, D $^2\Pi$, H $^2\Pi$, 4 $^2\Pi$ states of CN calculated using d-aug-cc-pVTZ basis set.

R	A $^2\Pi$	D $^2\Pi$	H $^2\Pi$	4 $^2\Pi$
0.8	189494.37039	235688.95843	236747.5197	245632.3422
0.85	132167.17089	185084.60708	188000.64799	195925.18559
0.9	90619.35022	146802.38896	152430.17062	160366.80566
0.95	60969.76508	117760.17133	127388.87676	135181.95564
0.98	47672.67068	104247.735	116519.69193	123954.3402
1.02	34017.16103	90112.85545	105798.91805	113162.75283
1.04	28650.52345	84426.10534	101790.81965	109475.06325
1.06	24192.70178	79502.67263	98529.76243	105185.45792
1.08	20408.25682	75306.74785	95950.3561	100261.59943
1.1	17290.97523	71744.62849	92754.28311	97848.06764
1.12	14767.24961	68749.12899	87039.85506	95638.59238
1.14	12770.46064	66259.32098	82041.63418	93794.55556
1.16	11252.82209	64204.40854	77777.58447	90641.45132
1.18	10132.7399	62560.58086	74007.07834	90282.36229
1.2	9380.52352	61390.13582	70770.9666	85277.5462
1.22	8946.31271	60413.44079	67874.14289	82561.71663
1.24	8794.33751	59702.99263	65356.65474	80148.51843
1.26	8889.58511	59213.24377	63194.08341	78026.3041
1.28	9200.53676	58876.44019	61390.31579	76174.96974
1.3	9699.01413	58505.66194	60074.46441	74574.68802
1.32	10359.67447	57713.93355	59577.63969	73205.44506
1.34	11159.79777	56702.80514	59650.82351	72048.42967
1.36	12078.98167	55782.0103	59939.64334	71086.61502
1.38	13098.94832	55005.84046	60348.67602	70305.02196
1.4	14203.32711	54373.58014	60839.96559	69691.08777
1.42	15377.45932	53875.19056	61235.31622	69234.44007
1.44	16608.25111	53498.72134	61866.31017	68928.05349
1.46	17883.9891	53232.14964	62504.48973	68767.14127
1.48	19194.25046	53064.22082	63129.51178	68748.96877
1.5	20529.74261	52984.5669	63696.7681	68870.85181
1.55	23926.93776	53111.6866	64903.68544	69734.61837
1.6	27327.33284	53609.58675	65895.89074	71163.87228
1.65	30653.56745	54382.68175	66829.95722	72810.97233
1.68	32589.67389	54947.94525	67405.1695	73796.47487
1.73	35687.43321	56019.2097	68409.1979	75325.19469
1.75	36875.20796	56484.45642	68826.4894	75877.17778
1.8	39702.23874	57718.33182	69901.01525	77076.7888
1.85	42311.5858	59029.42279	71004.50956	78021.99581
1.9	44691.63235	60393.11963	72116.0103	78767.91546
1.95	46837.33267	61788.67102	73214.68494	79391.27609
2	48749.73146	63197.25701	74280.17721	79949.11695
2.05	50435.52707	64600.83459	75292.2296	80472.91072

2.1	51906.3846	65981.87871	76230.2115	80976.853
2.15	53177.84723	67323.76416	77073.30355	81471.80341
2.2	54268.16867	68611.53156	77802.06248	81970.03497
2.25	55196.46954	69832.6928	78402.20488	82483.84922
2.3	55982.4477	70977.36713	78870.93905	83017.38547
2.35	56644.98236	72039.06907	79219.52183	83564.98126
2.4	57201.68634	73014.36386	79468.92841	84111.19655
2.45	57668.70861	73902.77522	79641.89417	84635.69483
2.5	58060.00554	74706.35744	79753.05149	85116.39256
2.55	58388.12889	75428.62211	79816.62012	85521.98607
2.6	58663.7144	76073.13132	79858.35541	85790.66033
2.7	59091.77114	77144.40235	79905.9024	85259.79728
2.75	59282.31024	77522.86441	80281.70442	81031.1225
2.85	59544.79312	78193.53499	80355.89782	80724.24209
2.9	59648.3193	78460.00792	80387.03249	80606.35129
3	59814.60426	78884.50477	80432.07527	80426.08142
3.2	60036.4141	79430.98124	80247.04499	80455.21448
3.3	60111.43272	79599.86917	80159.65458	80503.47476
3.4	60170.65137	79723.58263	80097.02969	80545.04984
3.5	60217.93937	79815.65882	80052.033	80580.9515
3.55	60209.24817	80088.04439	80047.25942	79908.50317
3.6	60227.19242	80130.07598	80042.29491	79896.47596
3.7	60257.98032	80206.99306	80021.26485	79878.88288
3.8	60283.15406	80279.38457	80009.29251	79867.90475
4	60321.06172	80388.20229	80034.97323	79858.46076
4.1	60335.23759	80416.27748	80051.616	79857.81112
4.2	60347.04971	80434.43462	80066.24617	79858.68682
4.3	60356.93046	80447.38582	80078.69697	79860.52163
