ELECTRONIC SUPPLEMENTARY INFORMATION

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Multiconfiguration Pair-Density Functional Theory for Doublet Excitation Energies: The Excited States of CN

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1. Potential energy curves by EOM-CCSD and CR-EOM-CCSD(T)

We calculate the EOM-CCSD potential energy curves in the following way. We first computed the excitation energy using EOM-EE-CCSD[12], where it is defined as:

$$\Delta E_k[\text{EOM-EE-CCSD}] = E_k[\text{EOM-EE-CCSD}] - E(\text{CCSD}) \quad (1)$$

where ΔE_k[EOM-EE-CCSD] is the excitation energy to state k calculated by the EOM-CC method. E_k[EOM-EE-CCSD(T)] is the energy for state k and E(CCSD) is the ground state energy calculated by CCSD.[3] To get the energy of the excited state k, one adds the excitation energy of EOM-EE-CCSD to the ground state energy of CCSD:.

$$E_k[\text{EOM-EE-CCSD}] = \Delta E_k[\text{EOM-EE-CCSD}] + E[\text{CCSD}] \quad (2)$$

One can also use the ground state energy computed from EOM-CCSD for ionization potential (EOM-IP-CCSD)[4] to calculate the energy for state k because EOM-IP-CCSD also provides an accurate ground state potential for CN, at ;least for distances close to the ground-state minimum (as shown in tables and figures below):

$$E_k[\text{EOM-EE-CCSD/EOM-IP-CCSD}] = \Delta E_k[\text{EOM-EE-CCSD}] + E[\text{EOM-IP-CCSD}] \quad (3)$$

The CR-EOM-CCSD(T)[5] potential energy curve can also be calculated in a similar manner to eq. (2):

$$E_k[\text{CR-EOM-CCSD(T)}] = \Delta E_k[\text{CR-EOM-CCSD(T),IA}] + E[\text{CR-CCSD(T)}] \quad (4)$$

where E_k[CR-EOM-CCSD(T)] is the energy used in this paper, and E[CR-CCSD(T)] is the energy for ground state calculated by CR-CCSD(T).[678] The *NWChem*[9] program was used to do CR-EOM-CCSD(T) calculations for open-shell systems, and we used the IA option, which is the only option available for open-shell CR-EOM-CCSD(T).

We can use the notation X/Y where X is the method used to calculate ΔE_k, and Y is the method used to calculate the ground-stat energy. We made four calculations: EOM-EE-CCSD/CCSD, EOM-EE-CCSD/EOM-IP-CCSD, CR-EOM-CCSD(T)/CR-CCSD(T) and EOM-IP-CCSD/ EOM-IP-CCSD for CN, as shown in Table S1 and Table S2, where we compare to experimental results for the equilibrium distance and adiabatic excitation energies. The EOM-IP-CCSD method yields the best agreement of the first three equilibrium distances and the first two adiabatic excitation energies. The results of EOM-EE-CCSD/CCSD and EOM-EE-CCSD/EOM-IP-CCSD are not very different from EOM-IP-CCSD/ EOM-IP-CCSD

The EOM-IP-CCSD calculaltions were applied only to the ground state and the first two excited states. Higher excited states may require a different EOM approach.

The Rydberg-Klein-Rees[101112] method has been applied[13] to obtain the ground-state CN potential energy curve from spectroscopic experiments. This method yields a set of points on the potential energy curve. We fit these points (from 0.9516 Å to 1.6343 Å to the following equation:

$$\begin{aligned}\Delta V(\mathrm{RKR}, r) = &-4988.30071 + 34204.60529r - 98458.37256r^2 \\ &+ 157806.91943r^3 - 155375.32282r^4 + 96715.06336r^5 \\ &- 37275.74939r^6 + 8147.50524r^7 - 774.08757r^8 \end{aligned} \quad (5)$$

where r is the C-N distance in Å, and ΔV(RKR, r) is the energy (in eV). This fit yields a minimum of $V = 0$ at 1.1718 Å, which is consistent with 1.172 Å in Table 5 from Herzberg. The maximum unsigned error of this fit as compared to the fitted experimental data is no more than 0.003 eV, and the mean unsigned error is only 0.001 eV. Using this fit as the benchmark, we calculate the errors of all EOM-CC/CC combinations for the ground state curve using the following equation,

$$\mathrm{Error(X/Y}, r) = \Delta V(\mathrm{X/Y}, r) - \Delta V(\mathrm{RKR}, r) \quad (6)$$

where r is the CN distance, ΔV(X/Y, r) is the relative energy (eV) at distance r with respect to the minimum calculated by parabola fitting for that method. The RKR and X/Y ΔV curves are plotted in Fig. S1(a), and the errors are plotted in Fig. S1(b). The theoretical calculations have similar errors from 1.0 Å to 1.4 Å. But outside this region, the error of EOM-IP-CCSD rises more rapidly than do the errors in the other methods. Therefore, CCSD is more accurate in the region plotted than is EOM-IP-CCSD. This justifies using the CCSD method as the ground state for EOM-CCSD.

Figure 1 also shows CCSD(T),[14] and it is interesting to compare this to CR-CCSD(T). Although CCSD(T) is more accurate than CR-CCSD(T) for r larger than experimental equilibrium distance, it has the largest error in regions smaller than experimental equilibrium distance, so we cannot say which one is better than the other. To apply the available methods consistently, we have uses CR-CCSD(T) energy as the ground state energy for CR-EOM-CCSD(T) excited-state curves.

The above discussion of the validity of CCSD for the ground state and EE-CR-CCSD may also be compared to a discussion provided by Stanton and Gauss.[15] Stanton and Gauss reminded the reader that UHF solutions for open-shell species are always spin-contaminated, and they examined the effect of this spin contamination on ground-state CN. They found that the lowest-energy UHF solution (which is the one used here for CCSD, CCSD(T), and CR-CCSD(T) calculations) is highly spin-contaminated for CN, but they found that a CCSD calculation based on this spin-contaminated UHF reference gave a reasonable bond distance and $<S^2>$ value, as did a CCSD calculation based on an ROHF reference. They concluded that in cases like CN, "CC calculations based on ROHF wave functions actually offer no advantage with regard to a proper treatment of spin."

Table S1. The errors of adiabatic excitation energies (eV) and mean unsigned error over first *n* excitation energies [MUE(*n*)] by several combination of ground-state and excited-state methods

X/Y[a]	$A^2\Pi_i$	$B^2\Sigma^+$	$D^2\Pi_i$	$E^2\Sigma^+$	MUE(2)	MUE(4)
EOM-EE-CCSD/CCSD	0.32	0.30	-0.20	-1.59	0.41	0.60
EOM-EE-CCSD/EOM-IP-CCSD	0.32	0.30	-0.20	-1.60	0.41	0.61
CR-EOM-CCSD(T)/CR-CCSD(T)	-0.07	0.06	-0.62	-2.11	0.38	0.72
EOM-IP-CCSD/IP-EOM-CCSD	0.02	0.03			0.03	

[a]X/Y means excitation energies by method X added on to the ground-state energies by method Y.

Table S2. The errors of equilibrium distances (Å) and mean unsigned error over first *n* equilibrium distances [MUE(*n*)] by several combination of ground-state and excited-state methods

X/Y[a]	$X^2\Sigma^+$	$A^2\Pi_i$	$B^2\Sigma^+$	$D^2\Pi_i$	$E^2\Sigma^+$	MUE(2)	MUE(5)
EOM-EE-CCSD/CCSD	-0.004	-0.024	-0.006	-0.170	-0.046	0.100	0.125
EOM-EE-CCSD/EOM-IP-CCSD	-0.004	-0.024	-0.006	-0.172	-0.047	0.101	0.127
CR-EOM-CCSD(T)/CR-CCSD(T)	-0.007	-0.014	0.000	-0.154	-0.023	0.084	0.099
EOM-IP-CCSD/IP-EOM-CCSD	-0.004	-0.006	-0.006			0.006	

[a]X/Y means excitation energies by method added on to the ground-state energies by method Y.

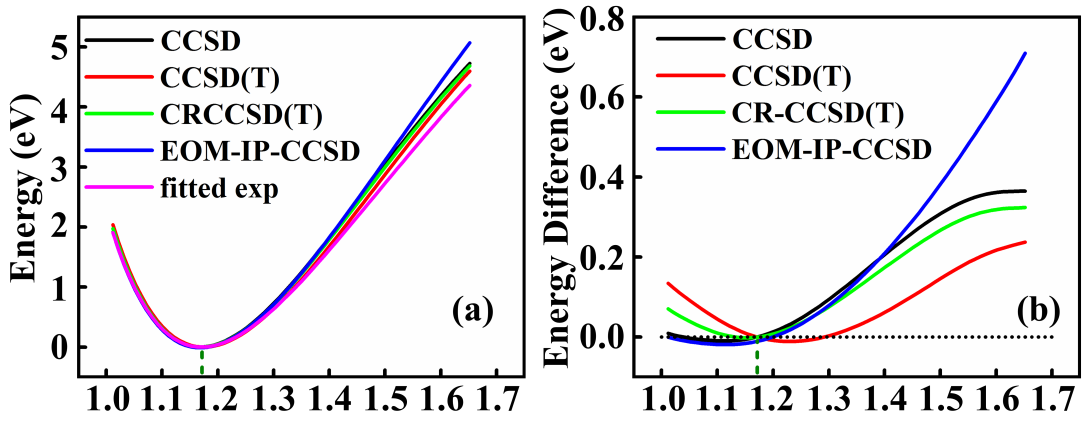

Fig. S1. The energies (a) of computed ground state curves and experimental ground-state curve and (b) signed errors in the potential curves of CN in the ground state by CCSD, CCSD(T), CR-CCSD(T) and EOM-IP-CCSD. The horizontal dotted line denotes zero error; the vertical dark green dashed line marks the location of the experimental equilibrium distance.

2. Absolute energies of some SR and MR methods in this work

TD-MN15L:

r	energy1*	energy2	energy3	energy4	energy5	energy6	energy7
1.1018	-92.655000	-92.562126	-92.562126	-92.515222	-92.366433	-92.329882	-92.329882
1.1118	-92.658140	-92.569165	-92.569165	-92.520093	-92.376144	-92.339317	-92.339317
1.1218	-92.660685	-92.575565	-92.575565	-92.524446	-92.385168	-92.348087	-92.348087
1.1318	-92.662671	-92.581366	-92.581366	-92.528303	-92.393537	-92.356229	-92.356229
1.1418	-92.664132	-92.586598	-92.586598	-92.531682	-92.401283	-92.363765	-92.363765
1.1518	-92.665101	-92.591293	-92.591293	-92.534599	-92.408437	-92.370735	-92.370735
1.1618	-92.665609	-92.595491	-92.595491	-92.537062	-92.415023	-92.377160	-92.377160
1.1718	-92.665685	-92.599212	-92.599212	-92.539082	-92.421064	-92.383072	-92.383072
1.1818	-92.665357	-92.602486	-92.602486	-92.540665	-92.426586	-92.388499	-92.388499
1.1918	-92.664651	-92.605344	-92.605344	-92.541815	-92.431609	-92.393463	-92.393463
1.2018	-92.663592	-92.607805	-92.607805	-92.542527	-92.436147	-92.397990	-92.397990
1.2118	-92.662203	-92.609897	-92.609897	-92.542817	-92.440219	-92.402106	-92.402106
1.2218	-92.660507	-92.611644	-92.611644	-92.542687	-92.443833	-92.405826	-92.405826
1.2318	-92.658525	-92.613069	-92.613069	-92.542153	-92.447004	-92.409177	-92.409177
1.2418	-92.656277	-92.614195	-92.614195	-92.541239	-92.449736	-92.412181	-92.412181
1.2518	-92.653783	-92.615052	-92.615052	-92.539972	-92.452034	-92.414858	-92.414858
1.2618	-92.651061	-92.615667	-92.615667	-92.538389	-92.453905	-92.417221	-92.417221
1.2718	-92.648127	-92.616070	-92.616070	-92.536536	-92.455348	-92.419293	-92.419293
1.2818	-92.644997	-92.616307	-92.616307	-92.534465	-92.456360	-92.421092	-92.421092
1.2918	-92.641688	-92.616422	-92.616422	-92.532232	-92.456943	-92.422629	-92.422629
1.3018	-92.638213	-92.616497	-92.616497	-92.529889	-92.457087	-92.423928	-92.423924
1.3118	-92.634586	-92.616648	-92.616648	-92.527493	-92.456790	-92.424994	-92.424994
1.3218	-92.630820	-92.617123	-92.617123	-92.525101	-92.456056	-92.425847	-92.425847
1.3318	-92.626927	-92.618688	-92.618688	-92.522752	-92.454872	-92.426501	-92.426501
1.3418**	-92.622920			-92.520490	-92.453253	-92.426966	-92.426962
1.3518**	-92.618808			-92.518345	-92.451203	-92.427253	-92.427253
1.3618**	-92.614603			-92.516342	-92.448736	-92.427374	-92.427374
1.3718**	-92.610314			-92.514485	-92.445881	-92.427344	-92.427340
1.3818**	-92.605951			-92.512790	-92.442656	-92.427166	-92.427166
1.3918**	-92.601521			-92.511249	-92.439094	-92.426853	-92.426853
1.4018**	-92.597034			-92.509863	-92.435224	-92.426415	-92.426415
1.4118**	-92.592497			-92.508627	-92.431085	-92.425862	-92.425862
1.4218**	-92.587918			-92.507532	-92.426697	-92.425197	-92.425197
1.4318**	-92.583304			-92.506581	-92.424431	-92.424431	-92.422093
1.4418**	-92.578661			-92.505771	-92.423569	-92.423569	-92.417296
1.4518**	-92.573996			-92.505108	-92.422616	-92.422616	-92.412333
1.4618**	-92.569313			-92.504601	-92.421579	-92.421579	-92.407217
1.4718**	-92.564620			-92.504248	-92.420458	-92.420458	-92.401962
1.4818**	-92.559921			-92.504058	-92.419254	-92.419254	-92.396579
1.4918**	-92.555222			-92.504011	-92.417969	-92.417969	-92.395721

1.5018**	-92.550529	-92.503997	-92.416602	-92.416602	-92.394780
1.5118**	-92.545850	-92.503650	-92.415186	-92.415186	-92.393632

*Energy1, energy2 … mean the lowest energy, the second lowest energy, ... at each C-N distance (*r*). With this ordering, the character of the state is not necessarily the same for all entries in a given column.
**The blank cells indicate that the TD-MN15L calculation does not have the first and the second excitation energy at that point.

CR-CCSD(T)/CR-EOM-CCSD(T):

1.1018	-92.550758	-92.490871	-92.490871	-92.436052	-92.285736	-92.247017	-92.247017
1.1118	-92.553917	-92.496575	-92.496575	-92.438376	-92.295022	-92.256249	-92.256249
1.1218	-92.556487	-92.501607	-92.501607	-92.440104	-92.303601	-92.264783	-92.264783
1.1318	-92.558502	-92.506000	-92.506000	-92.441272	-92.311510	-92.272656	-92.272656
1.1418	-92.559994	-92.509789	-92.509789	-92.441915	-92.318780	-92.279902	-92.279902
1.1518	-92.560996	-92.513007	-92.513007	-92.442068	-92.325446	-92.286553	-92.286553
1.1618	-92.561538	-92.515687	-92.515687	-92.441765	-92.331539	-92.292643	-92.292643
1.1718	-92.561650	-92.517861	-92.517861	-92.441041	-92.337088	-92.298202	-92.298202
1.1818	-92.561359	-92.519559	-92.519559	-92.439928	-92.342123	-92.303262	-92.303262
1.1918	-92.560694	-92.520812	-92.520812	-92.438459	-92.346670	-92.307851	-92.307851
1.2018	-92.559678	-92.521648	-92.521647	-92.436663	-92.350754	-92.311997	-92.311997
1.2118	-92.558338	-92.522093	-92.522093	-92.434570	-92.354397	-92.315727	-92.315727
1.2218	-92.556695	-92.522174	-92.522174	-92.432207	-92.357620	-92.319065	-92.319065
1.2318	-92.554770	-92.521915	-92.521915	-92.429601	-92.360440	-92.322035	-92.322035
1.2418	-92.552585	-92.521339	-92.521339	-92.426779	-92.362872	-92.324659	-92.324659
1.2518	-92.550159	-92.520468	-92.520467	-92.423766	-92.364927	-92.326957	-92.326957
1.2618	-92.547509	-92.519321	-92.519320	-92.420587	-92.366611	-92.328951	-92.328951
1.2718	-92.544653	-92.517917	-92.517917	-92.417269	-92.367928	-92.330657	-92.330657
1.2818	-92.541607	-92.516276	-92.516276	-92.413841	-92.368874	-92.332093	-92.332093
1.2918	-92.538386	-92.514412	-92.514412	-92.410331	-92.369443	-92.333275	-92.333275
1.3018	-92.535005	-92.512344	-92.512344	-92.406773	-92.369625	-92.334221	-92.334221
1.3118	-92.531477	-92.510086	-92.510086	-92.403200	-92.369408	-92.334942	-92.334942
1.3218	-92.527817	-92.507652	-92.507652	-92.399650	-92.368783	-92.335454	-92.335454
1.3318	-92.524035	-92.505056	-92.505056	-92.396158	-92.367748	-92.335770	-92.335770
1.3418	-92.520144	-92.502311	-92.502311	-92.392754	-92.366309	-92.335900	-92.335900
1.3518	-92.516157	-92.499429	-92.499429	-92.389463	-92.364484	-92.335858	-92.335858
1.3618	-92.512082	-92.496422	-92.496422	-92.386300	-92.362301	-92.335654	-92.335654
1.3718	-92.507932	-92.493301	-92.493301	-92.383268	-92.359798	-92.335298	-92.335298
1.3818	-92.503714	-92.490075	-92.490075	-92.380360	-92.357016	-92.334799	-92.334799
1.3918	-92.499439	-92.486756	-92.486756	-92.334168	-92.334168	-92.281824	-92.281824
1.4018	-92.495114	-92.483350	-92.483350	-92.333411	-92.333411	-92.280226	-92.280226
1.4118	-92.490750	-92.479870	-92.479870	-92.332537	-92.332537	-92.278553	-92.278553
1.4518	-92.473050	-92.465348	-92.465348	-92.328023	-92.328023	-92.303259	-92.271287
1.4618	-92.468596	-92.461602	-92.461602	-92.326671	-92.326671	-92.302204	-92.269368
1.4718	-92.464145	-92.457824	-92.457824	-92.325242	-92.325241	-92.301079	-92.267424
1.4818	-92.459701	-92.454019	-92.454019	-92.323740	-92.323740	-92.299887	-92.265464
1.4918	-92.455270	-92.450193	-92.450193	-92.322172	-92.322172	-92.298634	-92.263496
1.5018	-92.460229	-92.455723	-92.455723	-92.329913	-92.329913	-92.306694	-92.270898
1.5118	-92.455807	-92.451838	-92.451838	-92.356332	-92.328194	-92.328194	-92.321092

CASSCF-7m:

1.1018	-92.331108	-92.257886	-92.257886	-92.200511	-91.989585	-91.989585	-91.950997
1.1118	-92.334693	-92.263826	-92.263826	-92.202994	-91.996919	-91.996919	-91.960870
1.1218	-92.337704	-92.269135	-92.269135	-92.204918	-92.003633	-92.003633	-91.970035
1.1318	-92.340174	-92.273851	-92.273851	-92.206324	-92.009762	-92.009762	-91.978525
1.1418	-92.342139	-92.278010	-92.278010	-92.207248	-92.015339	-92.015338	-91.986375
1.1518	-92.343630	-92.281647	-92.281647	-92.207726	-92.020394	-92.020394	-91.993614
1.1618	-92.344677	-92.284793	-92.284793	-92.207791	-92.024958	-92.024958	-92.000271
1.1718	-92.345310	-92.287481	-92.287481	-92.207477	-92.029060	-92.029060	-92.006372
1.1818	-92.345555	-92.289739	-92.289739	-92.206815	-92.032728	-92.032728	-92.011942
1.1918	-92.345438	-92.291596	-92.291596	-92.205833	-92.035987	-92.035987	-92.017006
1.2018	-92.344983	-92.293077	-92.293077	-92.204562	-92.038863	-92.038862	-92.021583
1.2118	-92.344213	-92.294210	-92.294210	-92.203029	-92.041380	-92.041380	-92.025696
1.2218	-92.343147	-92.295017	-92.295016	-92.201261	-92.043574	-92.043557	-92.029359
1.2318	-92.341811	-92.295527	-92.295527	-92.199278	-92.045432	-92.045432	-92.032603
1.2418	-92.340216	-92.295760	-92.295760	-92.197110	-92.047012	-92.047012	-92.035434
1.2518	-92.338382	-92.295748	-92.295748	-92.194775	-92.048320	-92.048320	-92.037878
1.2618	-92.336319	-92.295523	-92.295523	-92.192294	-92.049379	-92.049378	-92.039960
1.2718	-92.334029	-92.295149	-92.295149	-92.189673	-92.050200	-92.050198	-92.041716
1.2818	-92.331460	-92.294811	-92.294811	-92.186847	-92.050754	-92.050754	-92.043265
1.2918	-92.327475	-92.296433	-92.296433	-92.180545	-92.051746	-92.051746	-92.045786
1.3018	-92.324504	-92.295759	-92.295759	-92.176252	-92.055313	-92.055313	-92.046645
1.3118	-92.321583	-92.294656	-92.294653	-92.172731	-92.058731	-92.058720	-92.046981
1.3218	-92.318579	-92.293329	-92.293329	-92.169464	-92.061935	-92.061935	-92.046939
1.3318	-92.315471	-92.291838	-92.291837	-92.166313	-92.064944	-92.064942	-92.046569
1.3418	-92.311919	-92.290475	-92.290444	-92.161008	-92.069271	-92.069265	-92.051234
1.3518	-92.308008	-92.287460	-92.286412	-92.163558	-92.070597	-92.069522	-92.046530
1.3618	-92.304689	-92.285567	-92.284552	-92.160451	-92.073032	-92.071925	-92.045648
1.3718	-92.301884	-92.285342	-92.284972	-92.150996	-92.076943	-92.076855	-92.052991
1.3818	-92.298361	-92.283402	-92.282928	-92.147944	-92.079125	-92.079009	-92.053240
1.3918	-92.294750	-92.281038	-92.281038	-92.145176	-92.081086	-92.081086	-92.053201
1.4018	-92.291097	-92.279191	-92.278547	-92.142340	-92.082944	-92.082774	-92.053285
1.4118	-92.287372	-92.276926	-92.276214	-92.139802	-92.084585	-92.084391	-92.053099
1.4218	-92.281903	-92.275617	-92.275617	-92.131490	-92.088562	-92.088562	-92.053489
1.4318	-92.278040	-92.273133	-92.273133	-92.129408	-92.089851	-92.089851	-92.054839
1.4418	-92.274149	-92.270562	-92.270562	-92.127474	-92.090975	-92.090975	-92.056029
1.4518	-92.270239	-92.267914	-92.267914	-92.125670	-92.091940	-92.091940	-92.057069
1.4618	-92.266314	-92.265199	-92.265199	-92.123960	-92.092761	-92.092761	-92.057970
1.4718	-92.262425	-92.262425	-92.262382	-92.122329	-92.093445	-92.093445	-92.058742
1.4818	-92.259602	-92.259602	-92.258446	-92.120751	-92.094004	-92.094004	-92.059393
1.4918	-92.256738	-92.256738	-92.254513	-92.119219	-92.094446	-92.094445	-92.059932
1.5018	-92.253840	-92.253840	-92.250584	-92.117714	-92.094779	-92.094779	-92.060367
1.5118	-92.250912	-92.250912	-92.246667	-92.116237	-92.095010	-92.095010	-92.060703

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1.1018	-92.544149	-92.479330	-92.479330	-92.429850	-92.226467	-92.226467	-92.193145
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1.1218	-92.550508	-92.490598	-92.490598	-92.434385	-92.240018	-92.240018	-92.211733
1.1318	-92.552868	-92.495322	-92.495322	-92.435854	-92.245916	-92.245916	-92.220031
1.1418	-92.554725	-92.499487	-92.499487	-92.436838	-92.251271	-92.251271	-92.227708
1.1518	-92.556112	-92.503124	-92.503124	-92.437371	-92.256116	-92.256116	-92.234795
1.1618	-92.557058	-92.506267	-92.506267	-92.437484	-92.260479	-92.260479	-92.241319
1.1718	-92.557592	-92.508944	-92.508944	-92.437210	-92.264388	-92.264388	-92.247307
1.1818	-92.557740	-92.511184	-92.511184	-92.436575	-92.267871	-92.267871	-92.252785
1.1918	-92.557527	-92.513013	-92.513013	-92.435608	-92.270953	-92.270953	-92.257776
1.2018	-92.556978	-92.514456	-92.514456	-92.434334	-92.273657	-92.273657	-92.262302
1.2118	-92.556113	-92.515536	-92.515536	-92.432778	-92.276009	-92.276009	-92.266385
1.2218	-92.554954	-92.516276	-92.516276	-92.430966	-92.278032	-92.278032	-92.270045
1.2318	-92.553520	-92.516699	-92.516699	-92.428920	-92.279746	-92.279746	-92.273300
1.2418	-92.551831	-92.516823	-92.516823	-92.426665	-92.281172	-92.281172	-92.276168
1.2518	-92.549904	-92.516669	-92.516669	-92.424220	-92.282325	-92.282325	-92.278668
1.2618	-92.547756	-92.516255	-92.516255	-92.421607	-92.283217	-92.283217	-92.280816
1.2718	-92.545364	-92.515639	-92.515639	-92.418954	-92.284210	-92.284210	-92.282670
1.2818	-92.542834	-92.514753	-92.514753	-92.416066	-92.285011	-92.285011	-92.284147
1.2918	-92.540131	-92.513656	-92.513656	-92.413067	-92.285952	-92.285952	-92.285314
1.3018	-92.537270	-92.512362	-92.512362	-92.409974	-92.287339	-92.287339	-92.286182
1.3118	-92.534220	-92.510889	-92.510832	-92.406469	-92.289339	-92.289068	-92.284782
1.3218	-92.531075	-92.509249	-92.509193	-92.403227	-92.291671	-92.291539	-92.285839
1.3318	-92.527810	-92.507451	-92.507396	-92.399942	-92.294068	-92.293997	-92.286703
1.3418	-92.524436	-92.505507	-92.505454	-92.396628	-92.296384	-92.296339	-92.287386
1.3518	-92.520961	-92.503430	-92.503377	-92.393300	-92.298557	-92.298527	-92.287898
1.3618	-92.517397	-92.501229	-92.501177	-92.389971	-92.300566	-92.300544	-92.288250
1.3718	-92.513753	-92.498915	-92.498865	-92.386654	-92.302405	-92.302388	-92.288452
1.3818	-92.510036	-92.496498	-92.496449	-92.383359	-92.304075	-92.304061	-92.288513
1.3918	-92.506212	-92.493965	-92.493965	-92.379987	-92.305641	-92.305641	-92.288466
1.4018	-92.502376	-92.491368	-92.491368	-92.376766	-92.306988	-92.306988	-92.288274
1.4118	-92.498492	-92.488693	-92.488693	-92.373593	-92.308183	-92.308183	-92.287967
1.4218	-92.494566	-92.485949	-92.485949	-92.370473	-92.309234	-92.309234	-92.287554
1.4318	-92.490606	-92.483142	-92.483142	-92.367409	-92.310146	-92.310146	-92.287041
1.4418	-92.486616	-92.480279	-92.480279	-92.364404	-92.310927	-92.310927	-92.286435
1.4518	-92.482575	-92.477343	-92.477343	-92.361399	-92.311571	-92.311571	-92.285704
1.4618	-92.478546	-92.474387	-92.474387	-92.358516	-92.312110	-92.312110	-92.284932
1.4718	-92.474505	-92.471392	-92.471392	-92.355694	-92.312537	-92.312537	-92.284085
1.4818	-92.470456	-92.468365	-92.468365	-92.352932	-92.312858	-92.312858	-92.283170
1.4918	-92.466405	-92.465310	-92.465310	-92.350229	-92.313079	-92.313079	-92.282192
1.5018	-92.462356	-92.462231	-92.462231	-92.347583	-92.313205	-92.313205	-92.281597
1.5118	-92.459134	-92.459134	-92.458313	-92.344991	-92.313241	-92.313241	-92.281758

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1.1018	-92.593220	-92.528274	-92.528274	-92.484773	-92.280223	-92.280223	-92.265077
1.1118	-92.596477	-92.534013	-92.534013	-92.486960	-92.287244	-92.287244	-92.274810
1.1218	-92.599171	-92.539129	-92.539130	-92.488571	-92.293656	-92.293656	-92.283861
1.1318	-92.601336	-92.543658	-92.543659	-92.489642	-92.299494	-92.299494	-92.292265
1.1418	-92.603005	-92.547637	-92.547637	-92.490210	-92.304790	-92.304790	-92.300059
1.1518	-92.604210	-92.551097	-92.551097	-92.490307	-92.309575	-92.309575	-92.307274
1.1618	-92.604979	-92.554070	-92.554070	-92.489965	-92.313880	-92.313880	-92.313939
1.1718	-92.605341	-92.556587	-92.556587	-92.489215	-92.317732	-92.317732	-92.320081
1.1818	-92.605321	-92.558675	-92.558675	-92.488086	-92.321160	-92.321160	-92.325725
1.1918	-92.604945	-92.560362	-92.560362	-92.486606	-92.324187	-92.324187	-92.330898
1.2018	-92.604235	-92.561674	-92.561674	-92.484801	-92.326839	-92.326839	-92.335622
1.2118	-92.603215	-92.562635	-92.562635	-92.482699	-92.329141	-92.329141	-92.339916
1.2218	-92.601903	-92.563270	-92.563271	-92.480327	-92.331123	-92.331111	-92.343795
1.2318	-92.600320	-92.563603	-92.563603	-92.477700	-92.332787	-92.332786	-92.347283
1.2418	-92.598482	-92.563657	-92.563657	-92.474848	-92.334178	-92.334178	-92.350392
1.2518	-92.596403	-92.563455	-92.563455	-92.471784	-92.335319	-92.335319	-92.353141
1.2618	-92.594093	-92.563027	-92.563027	-92.468526	-92.336243	-92.336242	-92.355545
1.2718	-92.591543	-92.562416	-92.562417	-92.465056	-92.337008	-92.337007	-92.357622
1.2818	-92.588670	-92.561734	-92.561734	-92.461230	-92.337765	-92.337765	-92.359398
1.2918	-92.583432	-92.561548	-92.561548	-92.452388	-92.330029	-92.330030	-92.360154
1.3018	-92.579788	-92.560197	-92.560197	-92.446638	-92.329197	-92.329197	-92.360697
1.3118	-92.576389	-92.558655	-92.558656	-92.441829	-92.331031	-92.331032	-92.361028
1.3218	-92.572962	-92.556954	-92.556954	-92.437297	-92.333412	-92.333412	-92.361005
1.3318	-92.569453	-92.555104	-92.555105	-92.432876	-92.335882	-92.335881	-92.360582
1.3418	-92.565745	-92.553059	-92.553056	-92.424270	-92.338135	-92.338134	-92.340731
1.3518	-92.563350	-92.551009	-92.550973	-92.428729	-92.340414	-92.339951	-92.332383
1.3618	-92.559629	-92.548747	-92.548714	-92.424451	-92.342527	-92.341851	-92.331463
1.3718	-92.554082	-92.546308	-92.546264	-92.410149	-92.344472	-92.344369	-92.340567
1.3818	-92.550030	-92.543855	-92.543795	-92.405893	-92.346293	-92.346144	-92.340140
1.3918	-92.545978	-92.541289	-92.541289	-92.402095	-92.347886	-92.347886	-92.339891
1.4018	-92.541776	-92.538700	-92.538613	-92.398212	-92.349469	-92.349234	-92.338903
1.4118	-92.537602	-92.536013	-92.535913	-92.394808	-92.350830	-92.350557	-92.338164
1.4218	-92.530216	-92.533034	-92.533034	-92.384216	-92.352561	-92.352561	-92.322282
1.4318	-92.525955	-92.530231	-92.530231	-92.381613	-92.353599	-92.353599	-92.323379
1.4418	-92.521712	-92.527377	-92.527377	-92.379234	-92.354507	-92.354507	-92.324342
1.4518	-92.517494	-92.524480	-92.524480	-92.377044	-92.355291	-92.355291	-92.325179
1.4618	-92.513297	-92.521542	-92.521542	-92.374993	-92.355955	-92.355955	-92.325898
1.4718	-92.518571	-92.518570	-92.509124	-92.373053	-92.356507	-92.356507	-92.326502
1.4818	-92.515572	-92.515572	-92.504977	-92.371192	-92.356953	-92.356953	-92.327001
1.4918	-92.512547	-92.512547	-92.500854	-92.369392	-92.357298	-92.357298	-92.327399
1.5018	-92.509503	-92.509503	-92.496759	-92.367633	-92.357545	-92.357545	-92.327700
1.5118	-92.506441	-92.506442	-92.492692	-92.365909	-92.357700	-92.357700	-92.327910

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