SUPPORTING INFORMATION

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Title: Towards Hartree-Fock and Density Functional Complete Basis Set Predicted NMR Parameters.
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SUPPLEMENTARY MATERIAL

Tab. 1. DFT, RHF and MP2 optimized ammonia geometry (in Å and deg), nonscaled harmonic vibrations (in cm^{-1}), dipole moment (in D) and energy (in au).

Method	DFT		RHF		MP2	Exp.
Parameter	6-31G*	6-311++G**	6-31G*	6-311++G**	6-311++G**	
Bond and Angle						
NH	1.0176	1.0137	1.0025	1.0003	1.0135	1.0124[a]
HNH	105.97	107.66	107.18	108.35	107.29	106.68[a]
Vibration						
1	1123.6	1009.57	1208.88	1094.47	1069.19	1022[b]
2, 3	1726.94	1667.40	1849.50	1792.95	1665.29	1691[b]
4	3465.80	3500.42	3689.42	3697.21	3530.04	3485[c]
5,6	3605.9	3633.61	3822.46	3826.36	3681.54	3624[c]
Dipole Moment	1.9423	1.7103	1.9199	1.7192	1.7821	1.472[d]
Energy	-56.5277243	-56.5602715	-56.1843563	-56.2147544	-56.4155236	
ZPVE	0.034754	0.034428	0.037002	0.036520	0.034840	

a) From ref. 80; b) from ref. 81; c) from ref. 82; d) ref. 66.

Tab. 2A. DFT, RHF and MP2 optimized dinitrogen geometry, harmonic vibrations and energy.

Method	DFT		RHF		MP2	Exp.[a]
Parameter	6-31G*	6-311++G**	6-31G*	6-311++G**	6-311++G**	
NN [Å]	1.1045	1.0951	1.0784	1.0706	1.1203	1.0977
Vibration [cm^{-1}]	2471.3	2459.3	2758.0	2734.5	2175.71	2358.6
Energy [a.u.]	-109.4771044	-109.5100123	-108.9439495	-108.9740882	-109.3015563	
ZPVE [a.u.]	0.005630	0.005603	0.006283	0.006230	0.004957	

a) from ref. 83

Tab. 2B. DFT, RHF and MP2 optimized methane geometry (in Å and deg) and energy (in au).

Method	DFT		RHF		MP2	Exp.
Parameter	6-31G*	6-311++G**	6-31G*		6-311++G**	
CH	1.0930	1.0911	1.0837	1.0843	1.0903	1.0858[a]; 1.0870[b]
HCH	109.72	109.47	109.47	109.47	109.47	
Energy	-40.5033635	-40.517381	-40.1951719	-40.2091498	-40.379638	

a) from ref. 17; b) from ref. 77

Tab. 2C. DFT and RHF optimized ethene geometry and energy.

Method	DFT		RHF		
Parameter	6-31G*	6-311++G**	6-31G*	6-311++G**	Exp.[a,b]
Bond and angle (Å and deg)					
CH	1.0877	1.0859	1.076	1.0767	1.0809
C=C	1.3301	1.3277	1.3169	1.3184	1.3307
CCH	121.8	121.7	121.81	121.66	121.44
Energy [a.u.]	- 78.5553806	-78.5804697	-78.0317182	-78.0561082	

a) From ref. 78. Best estimate from CCSD(T), no experimental r_e geometry available; b) From ref. 79.

Tab. 2D. DFT, RHF and MP2 optimized HCN geometry, dipole moment and energy.

Method	DFT		RHF		MP2	Exp.
Parameter	6-31G*	6-311++G**	6-31G*	6-311++G**	6-311++G**	
Bond (Å)						
NC	1.1569	1.1494	1.1325	1.1271	1.1713	1.156[a]; 1.1530[a]; 1.15324[b]
HC	1.0711	1.0681	1.0590	1.0583	1.0680	1.064[a]; 1.0657[a]; 1.06501[b]
Dipole Moment [D]	2.9316	3.0485	3.2088	3.2745	3.3194	2.9847[a]; 2.985[c]
Energy [a.u.]	-93.3809205	-93.4097687	-92.8751975	-92.9014695	-93.2032245	
ZPVE [a.u.]	0.016510	0.016397				

a) quoted from ref. 88; b) from ref. 89; c) from ref. 70.

Tab. 2E. DFT and RHF optimized CH_3CN geometry, dipole moment and energy.

Method	DFT		RHF		Exp.
Parameter	6-31G*	6-311++G**	6-31G*	6-311++G**	
Bond and Angle (Å and deg)					
NC	1.1604	1.1530	1.1347	1.1295	1.157[a];1.157[b]
CC	1.4568	1.4517	1.4678	1.4654	1.458[a];1.460[b]
HC	1.0944	1.0922	1.0821	1.0823	1.102[a];1.094[b]
HCC	110.3	110.1	109.8	109.7	109.5[a]
HCH	108.6	108.8	109.1	109.3	109.4[c];109.0[b]
Dipole Moment [D]	3.8554	4.0553	4.0424	4.2032	3.92[a,d];3.9252[d]
Energy [a.u.]	-132.6999629	-132.7374788	-131.9275339	-131.9627858	
ZPVE [a.u.]	0.045720	0.045236			

a) from ref. 90; b – from ref. 91; c) from ref. 92; d) from ref. 75.

Tab. 3A. The aug-cc-pVxZ basis set dependence of GIAO predicted ammonia isotropic shieldings (in ppm), dipole moment (in D) and energy (in au).

	6-31G*	6-311++G**	aug-cc-pVDZ	aug-cc-pVTZ	aug-cc-pVQZ	aug-cc-pV5Z	aug-cc-pV6Z	CBS(2-6)	CBS(2-6) +Rovibr[a].	ΔY_i	Exp.
DFT											
N	257.6421	260.6928	269.4267	261.8599	260.3896	259.3501	259.2221	259.2691	252.47	10.1576	264.54±0.05[b]
H	32.6945	32.0123	31.8349	31.6668	31.5424	31.5012	31.4790	31.4398	30.83	0.3951	31.2±1.0[b]; 30.68±0.6[c]
Dipole Moment	1.9423	1.7103	1.4805	1.4731	1.4733	1.4744	1.4744	1.4773		0.0042	1.472[d]
Energy	-56.5277243	-56.5602715	-56.5495128	-56.5662526	-56.5704352	-56.5716203	-56.5718159	-56.57193		0.02242	
RHF											
N	266.7159	266.5939	274.9459	267.0030	266.0487	265.5066	265.4056	265.5268	258.73	9.4191	264.54±0.05[b]
H	33.2065	32.3421	32.2179	31.9959	31.8557	31.8084	31.7878	31.7536	31.14	0.4643	31.2±1.0[b]; 30.68±0.6[c]
Dipole Moment	1.9199	1.7192	1.5394	1.5314	1.5319	1.5329	1.5329	1.5339		0.0026	1.472[d]
Energy	-56.1843563	-56.2147544	-56.20553947	-56.22079356	-56.22448262	-56.2253736	-56.22548013	-56.2256		0.02006	
MP2											
N	278.5041	276.3072	283.3920	276.4336				273.5038	266.70	9.89	264.54±0.05[b]
H	32.6849	31.8175	31.6654	31.3786				31.2578	30.65	0.41	31.2±1.0[b]; 30.68±0.6[c]
Dipole Moment	1.9710	1.7821	1.5929	1.5847				1.5813		0.012	1.472[d]
Energy	-56.3573775	-56.4155236	-56.4075814	-56.4774424				-56.50686		0.099279	

a) after adding MCSCF rovibrational corrections (N –6.80, H –0.61 ppm , respectively) from ref. 50; b) ref. 64; c) ref. 65; d) ref.66;

B3PW91/ 6-311++G** geometry: NH = 1.0137 HNH =107.6579; RHF/ 6-311++G** geometry: NH = 1.0003 HNH =108.3526; MP2/6-311++G** NH 1.0135, HNH 107.29

Tab. 3B. The cc-pVxZ basis set dependence of GIAO predicted ammonia isotropic shieldings (in ppm), dipole moment (in D) and energy (in au).

	6-311++G**	cc-pVDZ	cc-pVTZ	cc-pVQZ	cc-pV5Z	cc-pV6Z	CBS(2-6)	CBS(2-6) +Rovibr [a].	ΔY_i	Exp.
DFT										
N	260.6928	272.4447	265.9393	262.6849	260.0376	259.2470	257.5486	250.75	14.90	264.54±0.05 [b]
H	32.0123	32.0822	31.8687	31.6596	31.5290	31.4905	31.2939	30.68	0.79	31.2±1.0 [b]; 30.68±0.6 [c]
Dipole Moment	1.7103	1.5684	1.5291	1.5026	1.4857	1.4798	1.4640		0.0651	1.472 [d]
Energy	-56.5602715	-56.5350627	-56.56273676	-56.56896820	-56.5713301	-56.57174172	-56.57175		0.03669	
RHF										
N	266.5939	281.2591	272.0162	268.3485	265.8920	265.4629	264.6698	257.87	16.59	264.54±0.05 [b]
H	32.3421	32.4686	32.1619	31.9458	31.8265	31.7922	31.6870	31.08	0.78	31.2±1.0 [b]; 30.68±0.6 [c]
Dipole Moment	1.7192	1.6012	1.5611	1.5438	1.5379	1.5361	1.5340		0.0271	1.472 [d]
Energy	-56.2147544	-56.19530985	-56.21824652	-56.22356351	-56.2252276	-56.22545135	-56.22555		0.03024	

a) after adding MCSCF rovibrational corrections (N –6.80, H –0.61 ppm , respectively) from ref. 50; b) ref. 64; c) ref. 65; d) ref.66.

B3PW91/ 6-311++G** geometry: NH = 1.0137 HNH =107.6579; RHF/ 6-311++G** geometry: NH = 1.0003 HNH =108.3526.

Tab. 3C. The aug-cc-pCVxZ basis set dependence of GIAO predicted ammonia isotropic shieldings (in ppm), dipole moment (in D) and energy (in au).

	aug-cc-pCVDZ	aug-cc-pCVTZ	aug-cc-pCVQZ	aug-cc-pCV5Z	CBS(2-5)	CBS(2-5) +Rovibr[a].	ΔY_i	Exp.	Lit.[c]
DFT									
N	266.5434	260.6841	259.7566	259.3911	259.42	252.69	7.12	264.54±0.05[b]	266.99
H	31.8357	31.6638	31.5412	31.5014	31.42	30.81	0.42	31.2±1.0[b]; 30.68±0.6[d];	30.78
Dipole Moment	1.4825	1.4732	1.4731	1.4743	1.473		0.0095	1.472[e]	
Energy	-56.550891066	-56.5672740904	-56.5709432182	-56.5717777318	-56.57202		0.002112894		
RHF									
N	272.9703	266.6530	265.8397	265.5087	265.57	258.77	7.40	264.54±0.05[b]	266.99
H	32.2185	31.9920	31.8564	31.8082	31.74	31.13	0.48	31.2±1.0[b]; 30.68±0.6[d];	30.78
Dipole Moment	1.5407	1.5309	1.5317	1.5328	1.529		0.0117	1.472[e]	
Energy	-56.2059713298	-56.2210193584	-56.2245599722	-56.2253871715	-56.22564		0.01967		

a) after adding MCSCF rovibrational corrections (N –6.80, H –0.61 ppm , respectively) from ref. 50; b) ref. 64; c) ref. 65; d) ref.66.

B3PW91/ 6-311++G** geometry: NH = 1.0137 HNH =107.6579; RHF/ 6-311++G** geometry: NH = 1.0003 HNH =108.3526.

Tab. 3D. The cc-pCVxZ basis set dependence of GIAO predicted ammonia isotropic shieldings (in ppm), dipole moment (in D) and energy (in au).

	cc-pCVDZ	cc-pCVTZ	cc-pCVQZ	cc-pCV5Z	CBS(2-5)	CBS(2-5) +Rovibr[a].	ΔY_i	Exp.
DFT								
N	269.8778	264.7901	261.9221	259.9923	259.42	252.69	10.46	264.54±0.05[b]
H	32.0842	31.8709	31.6587	31.5282	31.42	30.81	0.66	31.2±1.0[b]; 30.68±0.6[c]
Dipole Moment	1.5720	1.5300	1.5023	1.4850	1.464		0.108	1.472[d]
Total SP Energy	-56.5366869688	-56.5637485416	-56.5695620519	-56.5715056613	-56.57175		0.03506	
RHF								
N	279.5567	271.4915	268.0022	265.9402	264.67	257.87	14.89	264.54±0.05[b]
H	32.4699	32.1598	31.9467	31.8259	31.69	31.08	0.78	31.2±1.0[b]; 30.68±0.6[c]
Dipole Moment	1.6036	1.5607	1.5436	1.5376	1.534		0.07	1.472[d]
Total SP Energy	-56.1958822911	-56.2184825508	-56.2236603525	-56.2252450990	-56.2256		0.02972	

a) after adding MCSCF rovibrational corrections (N –6.80, H –0.61 ppm , respectively) from ref. 50; b) ref. 64; c) ref. 65; d) ref.66.

B3PW91/ 6-311++G** geometry: NH = 1.0137 HNH =107.6579; RHF/ 6-311++G** geometry: NH = 1.0003 HNH =108.3526.

Tab. 4A. Basis set dependence of GIAO predicted dinitrogen NMR parameters (in ppm) and energy (in au).

	6-31G*	6-311++G**	aug-cc-pVDZ	aug-cc-pVTZ	aug-cc-pVQZ	aug-cc-pV5Z	aug-cc-pV6Z	CBS(2-6)	CBS(2-6) +Rovibr[a].	ΔY_i	Exp.
DFT											
Isotropic shieldings	-55.9716	-78.1575	-49.9416	-77.9695	-85.8964	-90.3495	-91.7182	-91.9648	-96.23	-42.0232	-101.3±25[b]; -61.6[a,b]
Energy	-109.4771044	-109.5100123	-109.4949216	-109.5210688	-109.5285495	-109.5306043	-109.5309709	-109.53132		0.036398	
RHF											
Isotropic shieldings	-55.5822	-75.8456	-50.8804	-75.3250	-79.9766	-83.0850	-83.5669	-83.3535	87.62	32.4731	-101.3±25[b]; -61.6[a,b]
Energy	-108.9439495	-108.9740882	-108.9617102	-108.9877506	-108.9948475	-108.9962845	-108.996465331	-108.99682		0.035110	
MP2											
Isotropic shieldings	-8.8000	-35.3271	-5.2484	-41.0801	-48.1530			-49.89	-54.16[c]	44.64	-101.3±25[b]; -61.6[a,b]
Energy	-109.261573	-109.3388867	-109.2850127	-109.394284	-109.4511652			-109.51292		0.227907	

a) with rovibrational correction (-4.27 ppm) from refs. 63 and 67; b) from ref. 68.

Tab. 4B. Basis set dependence of GIAO predicted ethene isotropic shieldings (in ppm) and energy (in au).

	6-31G*	6-311++G**	aug-cc-pVDZ	aug-cc-pVTZ	aug-cc-pVQZ	aug-cc-pV5Z	aug-cc-pV6Z	CBS(2-6)	CBS(2-5) +Rovibr[a].	ΔY_i	Exp.
DFT											
C	74.7767	56.8057	71.9465	57.3479	51.8948	49.0778	48.1969	47.5367	42.7467	24.4098	64.5[b]; 57.5[b]; 60.89[c]
H	26.5545	26.0629	25.7885	25.7593	25.7162	25.6872	25.6729	25.5592	25.0392	0.2293	25.43[d]; 26.28[c]
Energy	- 78.5553806	-78.5804697	-78.5656799	-78.5884471	-78.5938765	-78.5955113	-78.5958234	-78.59591		0.03023	
RHF											
C	81.6018	66.4557	79.3390	66.7423	63.4797	61.7326		61.45	56.66	17.89	64.5[b]; 57.5[b]; 60.89[c]
H	27.2943	26.7071	26.4964	26.4680	26.4200	26.3881		26.37	25.85	0.098	25.43[d]; 26.28[c]
Energy	-78.03171815	-78.05610816	-78.0435962	-78.0652181	-78.06995	-78.0710614		-78.07134		0.02774	

a) with rovibrational correction (C = -4.79 ppm; H = - 0.52 ppm) from ref. 51 (Supplement); b) both values from ref. 16; c) calculated in ref. 51; d) from refs. 15 and 44.

Tab. 4C. Basis set dependence of GIAO predicted acetonitrile isotropic shieldings (in ppm), dipole moment (in D) and energy (in au).

	6-31G*	6-311++G**	aug-cc-pVDZ	aug-cc-pVTZ	aug-cc-pVQZ	aug-cc-pV5Z	CBS(2-5)	ΔY_i	Exp.
DFT									
N	-1.3825	-25.5977	0.7462	-23.8653	-32.1252	-36.0837	-37.7167	38.4629	-2.1[a]; -9.1[b]
C1	87.1180	67.4644	82.5525	67.9697	63.1149	60.6943	59.7301	22.8224	73.8[a]; 67.5[b]
C2	190.1183	185.8298	193.1845	185.9459	183.3472	182.0386	181.4063	11.7782	187.7[a];
H	30.5202	30.1475	29.8381	29.7749	29.7251	29.6965	29.6220	0.2161	29.06[c]
Dipole Moment	3.8554	4.0553	4.0433	4.0443	4.0429	4.0424	4.04212	0.0022	3.92[d]; 3.9252[e]
Energy	-132.6999629	-132.7374788	-132.715378	-132.7496821	-132.7585295	-132.761065	-132.76184	0.046462	
RHF									
N	1.9285	-19.7720	3.5114	-17.7455	-23.2529	-26.0007	-26.4641	29.9755	-2.1[a]; -9.1[b]
C1	91.6680	73.7918	87.6628	74.4630	71.1382	69.5118	69.2681	18.3947	73.8[a]; 67.5[b]
C2	198.6615	194.7231	201.5830	194.4139	192.7297	192.0506	191.9604	9.6226	187.7[a];
H	31.2165	30.7366	30.4762	30.3990	30.3442	30.3110	30.2396	0.2366	29.06[c]
Dipole Moment	4.0424	4.2032	4.2154	4.2110	4.2095	4.2090	4.2087	0.0067	3.92[d]; 3.9252[e]
Energy	-131.9275339	-131.9627858	-131.9440697	-131.9769162	-131.9846864	-131.986407137	-131.98699	0.04292	

a) Assumed approximate rovibrational correction taken from HCN and CH_4: –4, –3, –3 and –0.6 ppm for N, C1, C2 and H, respectively; b) from ref. 16; c) from refs. 54 and 73 ; d) from ref. 74; e) from ref. 75.

Tab. 5. Basis set dependence of GIAO predicted methane isotropic shieldings (in ppm) and energy (aug- and cc-pVxZ basis sets).

	6-31G*	6-311++G**	X = 2	X = 3	X = 4	X = 5	CBS(2-6)	CBS(2-6) +Rovibr[a].	ΔY_i	Exp.[b]
DFT/aug-cc-pVxZ										
C	195.3587	192.6054	199.0622	191.7475	189.9837	189.3589	189.2451	186.0451	9.8171	194.8±0.9; 198.7
H	31.8591	31.6615	31.4578	31.3790	31.3267	31.2898	31.2133	30.6133	0.2445	30.611±0.024
Energy	-40.5033635	-40.517381	-40.5058798	-40.5214542	-40.5245356	-40.5254703	-40.52561		0.01973	
RHF/aug-cc-pVxZ										
C	201.0320	197.5194	204.4542	197.5466	195.6912	195.0859	194.9082	191.71	9.54	194.8±0.9; 198.7
H	32.3803	31.9335	31.7836	31.6836	31.6359	31.6042	31.5739	30.97	0.21	30.611±0.024
Energy	-40.1951719	-40.2091498	-40.1995636482	-40.2136889938	-40.2163250772	-40.2170337341	-40.2171		0.0175	
MP2/aug-cc-pVxZ										
C	208.4581	202.1598	209.0240	202.5565			200.36	197.16	8.66	194.8±0.9; 198.7
H	31.7551	31.6266	31.4615	31.2726			31.10	30.49	0.17	30.611±0.024
Energy	-40.3370422	-40.379638	-40.3706967	-40.4328985			-40.46401		0.093313	
DFT/cc-pVxZ										
C	195.3587	192.6054	200.1786	192.1153	190.2307	189.5116	189.2451	186.05	10.9335	194.8±0.9; 198.7
H	31.8591	31.6615	31.3368	31.3807	31.3303	31.2972	31.2330	30.62	0.1477	30.611±0.024
Energy	-40.5033635	-40.517381	-40.5030792802	-40.5212733586	-40.5244187796	-40.5254498023	-40.52554		0.02246	
RHF/cc-pVxZ										
C	201.0320	197.5194	205.5961	197.0544	195.8710	195.1160	195.2550	192.06	10.3411	194.8±0.9; 198.7
H	32.3803	31.9335	31.7046	31.6873	31.6368	31.6047	31.5487	30.94	0.1386	30.611±0.024
Energy	-40.1951719	-40.2091498	-40.1985975538	-40.2134526846	-40.2162804758	-40.2170243275	-40.2171		0.0185	

a) after adding MCSCF rovibrational corrections (C – 3.2, H – 0.61 ppm , respectively) from ref. 50; b) experimental values taken from ref. 11 and references therein; CH = 1.0911Å (DFT/6-311++G** geometry); CH = 1.0843Å (RHF/6-311++G** geometry) and CH = 1.0903Å (MP2/6-311++G** geometry)

Tab. 6A. Basis set dependence of GIAO predicted HCN isotropic shieldings (in ppm), dipole moment and energy (aug-cc-pVxZ basis set).

	6-31G*	6-311++G**	aug-cc-pVDZ	aug-cc-pVTZ	aug-cc-pVQZ	aug-cc-pV5Z	aug-cc-pV6Z	CBS(2-6)	CBS(2-6)+Rov [a].	ΔY	Exp.
DFT											
N	-7.1630	-35.5791	-8.7514	-34.0958	-42.8388	-46.7616	-48.0147	-48.6897	-58.69	39.9383	-31.4±10[b]; -37[c]; -20.4
C	94.6489	75.8992	89.8654	76.9134	72.3141	69.9826	69.3051	68.8372	66.54	21.0282	82.1[e]
H	29.4757 (27.79[d])	29.4386 (27.76[d])	28.9598	29.0726	29.0574	29.0375	29.0282	28.9608	28.24	0.0010	28.32[f]
Dipole Moment	2.9316	3.0485	3.0287	3.0320	3.0305	3.0307	3.0308	3.0309		0.0022	2.98519[g]
Energy	-93.3809205	-93.4097687	-93.3943462	-93.4180366	-93.4242283	-93.425961	-93.4262884	-93.42648		0.03213	
RHF											
N	-3.0820	-28.3881	-5.2124	-26.3547	-32.1834	-34.8982	-35.3141	-35.5189	-45.52	30.31	-31.4±10[b]; -37[c]; -20.4
C	98.0863	80.2543	94.3713	81.7470	78.8150	77.2523	76.9999	77.1234	74.82	17.25	82.1[e]
H	29.6640	29.8597	29.4052	29.5137	29.4741	29.4483	29.4356	29.4001	28.68	0.17	28.32[f]
Dipole Moment	3.2088	3.2745	3.2689	3.2669	3.2659	3.2658	3.2659	3.2655		0.0034	2.98519[g]
Energy	-92.8751975	-92.9014695	-92.8882594672	-92.9112920553	-92.9168757404	-92.9180439898	-92.9181919594	-92.9185		0.03024	
MP2											
N	39.0794	8.0317	35.7274	6.3401				-6.0335	-16.03	41.7609	-31.4±10[b]; -37[c]; -20.4
C	109.8299	91.3880	106.3838	90.6745				84.0601	81.76	22.3237	82.1[e]
H	28.9531	29.1706	28.6731	28.7819				-		-	28.32[f]
Dipole Moment	3.2552	3.3191	3.3112	3.3086				3.3075		0.0037	2.98519[g]
Energy	-93.1669374	-93.2032245	-93.1885009	-93.2918267				-93.33533		0.146829	

a) K. Ruud, *private commun.*: -10.0, -2.3 and –0.72 ppm for N, C and H, respectively; b) from ref. 93; c) from ref. 68; d) from ref. 77-79; e) from ref. 94; f) from ref. 70.;
HCN oriented along z axis (x, y = 0);
RHF/6-311++G** structure: HC = 1.0583; CN = 1.1271;
B3PW91/6-311++G** structure: HC = 1.0681; CN = 1.1494;
MP2/6-311++G** structure: HC = 1.0680; CN = 1.1713.

Tab. 6B. The cc-pVxZ Basis set dependence of the calculated HCN isotropic shieldings (in ppm), dipole moment and energy.

	6-31G*	6-311++G**	aug-cc-pVDZ	aug-cc-pVTZ	aug-cc-pVQZ	aug-cc-pV5Z	aug-cc-pV6Z	CBS(2-6)	CBS(2-6) +Rov[a].	ΔY_i(T-CBS)	Exp.
DFT											
N	-35.5791	-11.0259	-37.3945	-43.3216	-46.9280	-47.9863	-47.7775	-47.78	36.75	-31.4±10[b]; -37[c]; -20.4[d]	-31.4±10[b]; -37[c]; -20.4
C	75.8992	95.2339	77.4316	72.5275	70.1194	69.3191	69.2526	66.95	25.91	82.1[e]	82.1[e]
H	29.4386 (27.76[d])	29.2813	29.1585	29.0831	29.0444	29.0303	29.0025	28.28	0.28	28.32[f]	28.32[f]
Dipole Moment	3.0485	2.8244	2.9865	3.0123	3.0284	3.0300	3.0283		0.2058	2.98519[g]	2.98519[g]
Energy	-93.4097687	-93.3888791	-93.4168380498	-93.4238892506	-93.4259107662	-93.4262755834	-93.42646		0.03758		
RHF											
N	-28.3881	-7.3677	-29.0854	-32.6018	-34.9830	-35.3081	-35.0339	-45.03	27.66	-31.4±10[b]; -37[c]; -20.4[d]	-31.4±10[b]; -37[c]; -20.4
C	80.2543	98.9600	81.8883	78.8869	77.3262	77.0330	77.2104	74.91	21.75	82.1[e]	82.1[e]
H	29.8597	29.6745	29.5712	29.4990	29.4548	29.4373	29.3929	28.67	0.28	28.32[f]	28.32[f]
Dipole Moment	3.2745	3.1126	3.2305	3.2557	3.2652	3.2657	3.2661		0.1535	2.98519[g]	2.98519[g]
Energy	-92.9014695	-92.8840148	-92.9102112942	-92.9166957715	-92.9180154433	-92.9181874740	-92.91844		0.034425		

a) K. Ruud, *private commun.*: -10.0, -2.3 and –0.72 ppm for N, C and H, respectively; b) from ref. 93; c) from ref. 68; d) from ref. 77-79; e) from ref. 94; f) from ref. 70.;
HCN oriented along z axis (x, y = 0);
RHF/6-311++G** structure: HC = 1.0583; CN = 1.1271;
B3PW91/6-311++G** structure: HC = 1.0681; CN = 1.1494.