Electronic Supplementary Material (ESI) for RSC Advances.

Dipole moments of conjugated donor – acceptor substituted systems: calculations vs. experiments

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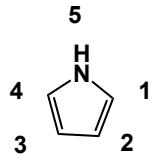
Pyrrole, hf/aug-cc-pvdz



Electric dipole

Property at reference geometry, Unit: Debye

X= 1.8615 Y= -0.0000 Z= 0.0000

Temperature: 0K, Unit: Debye

X= 1.7990 Y= -0.0000 Z= 0.0000

Temperature: 298K, Unit: Debye

X= 1.7848 Y= -0.0000 Z= -0.0002

Internal coordinates for the Equilibrium structure (Se)

	1	2	3	4	5	6	7	8	9	10
1 C	0.000000									
2 C	1.363229	0.000000								
3 C	2.246784	1.430228	0.000000							
4 C	2.230166	2.246784	1.363229	0.000000						
5 N	1.364705	2.208961	2.208961	1.364705	0.000000					
6 H	2.100377	3.165016	3.165016	2.100377	0.993165	0.000000				
7 H	1.075189	2.217941	3.306072	3.244812	2.131750	2.498627	0.000000			
8 H	2.176395	1.076314	2.249310	3.289296	3.248984	4.171306	2.693236	0.000000		
9 H	3.289296	2.249310	1.076314	2.176395	3.248984	4.171306	4.326250	2.727498	0.000000	
10 H	3.244812	3.306072	2.217941	1.075189	2.131750	2.498627	4.202725	4.326250	2.693236	0.000000

Internal coordinates for the vibrationally average structure at 0K (Sz)

	1	2	3	4	5	6	7	8	9	10
1 C	0.000000									
2 C	1.367165	0.000000								
3 C	2.255140	1.436658	0.000000							
4 C	2.238887	2.255140	1.367165	0.000000						
5 N	1.371867	2.219469	2.219469	1.371867	0.000000					
6 H	2.103420	3.170245	3.170245	2.103420	0.987781	0.000000				
7 H	1.077960	2.223067	3.316946	3.256694	2.140569	2.506039	0.000000			
8 H	2.182138	1.078899	2.257576	3.300049	3.261903	4.179127	2.698718	0.000000		
9 H	3.300049	2.257576	1.078899	2.182138	3.261903	4.179127	4.339322	2.737342	0.000000	
10 H	3.256694	3.316946	2.223067	1.077960	2.140569	2.506039	4.218194	4.339322	2.698718	0.000000

Internal coordinates for the vibr. average structure at 298.15K (Sa)

	1	2	3	4	5	6	7	8	9	10
1 C	0.000000									
2 C	1.366953	0.000000								
3 C	2.255160	1.436937	0.000000							
4 C	2.238918	2.255160	1.366953	0.000000						
5 N	1.372212	2.219883	2.219883	1.372212	0.000000					
6 H	2.101590	3.167984	3.167984	2.101590	0.985037	0.000000				
7 H	1.077647	2.222507	3.316653	3.256460	2.140493	2.504816	0.000000			
8 H	2.181750	1.078608	2.257551	3.299748	3.262044	4.176690	2.698079	0.000000		
9 H	3.299748	2.257551	1.078608	2.181750	3.262044	4.176690	4.338704	2.737172	0.000000	
10 H	3.256460	3.316653	2.222507	1.077647	2.140493	2.504816	4.217755	4.338704	2.698079	0.000000

Pyrrole, hf/aug-cc-pvtz

Electric dipole

Property at reference geometry, Unit: Debye

X= 1.8549 Y= -0.0000 Z= 0.0000

Temperature: 0K, Unit: Debye

X= 1.7948 Y= -0.0000 Z= 0.0000

Temperature: 298K, Unit: Debye

X= 1.7815 Y= -0.0000 Z= -0.0002

Internal coordinates for the Equilibrium structure (Se)

		1	2	3	4	5	6	7	8	9	10
1	C	0.000000									
2	C	1.355594	0.000000								
3	C	2.236637	1.425135	0.000000							
4	C	2.220780	2.236637	1.355594	0.000000						
5	N	1.359759	2.199379	2.199379	1.359759	0.000000					
6	H	2.092245	3.150818	3.150818	2.092245	0.988437	0.000000				
7	H	1.067834	2.204379	3.288787	3.228431	2.120639	2.486985	0.000000			
8	H	2.163058	1.068510	2.237458	3.271216	3.232065	4.150092	2.676903	0.000000		
9	H	3.271216	2.237458	1.068510	2.163059	3.232064	4.150092	4.301182	2.711674	0.000000	
10	H	3.228431	3.288787	2.204379	1.067834	2.120639	2.486985	4.179839	4.301182	2.676903	0.000000

Internal coordinates for the vibrationally average structure at 0K (Sz)

		1	2	3	4	5	6	7	8	9	10
1	C	0.000000									
2	C	1.359498	0.000000								
3	C	2.245040	1.431567	0.000000							
4	C	2.229704	2.245040	1.359498	0.000000						
5	N	1.366955	2.209742	2.209742	1.366955	0.000000					
6	H	2.095446	3.156107	3.156107	2.095446	0.983267	0.000000				
7	H	1.070851	2.209746	3.299962	3.240746	2.129743	2.494664	0.000000			
8	H	2.169333	1.071551	2.245904	3.282364	3.245379	4.158533	2.683136	0.000000		
9	H	3.282363	2.245903	1.071551	2.169332	3.245378	4.158532	4.314862	2.721395	0.000000	
10	H	3.240744	3.299961	2.209744	1.070849	2.129741	2.494663	4.195941	4.314861	2.683134	0.000000

Internal coordinates for the vibr. average structure at 298.15K (Sa)

		1	2	3	4	5	6	7	8	9	10
1	C	0.000000									
2	C	1.359293	0.000000								
3	C	2.245066	1.431836	0.000000							
4	C	2.229756	2.245066	1.359293	0.000000						
5	N	1.367287	2.210122	2.210122	1.367287	0.000000					
6	H	2.093734	3.153975	3.153975	2.093734	0.980691	0.000000				
7	H	1.070555	2.209215	3.299693	3.240548	2.129685	2.493526	0.000000			
8	H	2.168988	1.071297	2.245892	3.282100	3.245527	4.156263	2.682556	0.000000		
9	H	3.282099	2.245891	1.071296	2.168987	3.245526	4.156262	4.314297	2.721227	0.000000	
10	H	3.240546	3.299691	2.209213	1.070553	2.129684	2.493525	4.195554	4.314296	2.682554	0.000000

Pyrrole, b3lyp/aug-cc-pvdz

Electric dipole

Property at reference geometry, Unit: Debye			
X= -1.8412	Y= -0.0000	Z= 0.0000	
Temperature: 0K, Unit: Debye			
X= -1.7815	Y= -0.0000	Z= 0.0000	
Temperature: 298K, Unit: Debye			
X= -1.7695	Y= -0.0000	Z= -0.0001	

Internal coordinates for the Equilibrium structure (Se)

		1	2	3	4	5	6	7	8	9	10
1	C	0.000000									
2	C	1.382597	0.000000								
3	C	2.265382	1.428297	0.000000							
4	C	2.254700	2.265382	1.382597	0.000000						
5	N	1.376463	2.226799	2.226799	1.376463	0.000000					
6	H	2.122126	3.198081	3.198081	2.122126	1.008148	0.000000				
7	H	1.084325	2.249013	3.333861	3.276677	2.149535	2.519998	0.000000			
8	H	2.200608	1.085636	2.253980	3.316935	3.275766	4.213115	2.729813	0.000000		
9	H	3.316936	2.253980	1.085636	2.200608	3.275766	4.213115	4.363007	2.731799	0.000000	
10	H	3.276677	3.333861	2.249013	1.084325	2.149535	2.519998	4.240411	4.363006	2.729812	0.000000

Internal coordinates for the vibrationally average structure at 0K (Sz)

		1	2	3	4	5	6	7	8	9	10
1	C	0.000000									
2	C	1.387460	0.000000								
3	C	2.274676	1.434776	0.000000							
4	C	2.264538	2.274675	1.387459	0.000000						
5	N	1.384025	2.237995	2.237995	1.384024	0.000000					
6	H	2.126718	3.205534	3.205534	2.126718	1.004328	0.000000				
7	H	1.086404	2.254328	3.344914	3.289107	2.158498	2.528603	0.000000			
8	H	2.206769	1.087970	2.262179	3.328451	3.289058	4.222791	2.735181	0.000000		
9	H	3.328452	2.262180	1.087972	2.206770	3.289059	4.222792	4.376087	2.741734	0.000000	
10	H	3.289110	3.344917	2.254330	1.086407	2.158500	2.528604	4.256038	4.376089	2.735183	0.000000

Internal coordinates for the vibr. average structure at 298.15K (Sa)

		1	2	3	4	5	6	7	8	9	10
1	C	0.000000									
2	C	1.387342	0.000000								
3	C	2.274709	1.434966	0.000000							
4	C	2.264572	2.274709	1.387341	0.000000						
5	N	1.384317	2.238390	2.238390	1.384317	0.000000					
6	H	2.124960	3.203422	3.203422	2.124960	1.001755	0.000000				
7	H	1.085788	2.253578	3.344323	3.288594	2.158171	2.527285	0.000000			
8	H	2.206274	1.087478	2.261911	3.327980	3.288975	4.220296	2.734276	0.000000		
9	H	3.327982	2.261912	1.087479	2.206275	3.288976	4.220297	4.374996	2.741273	0.000000	
10	H	3.288597	3.344326	2.253581	1.085791	2.158173	2.527287	4.255075	4.374997	2.734279	0.000000

Pyrrole, b3lyp/aug-cc-pvtz

Electric dipole

Property at reference geometry, Unit: Debye			
X= 1.8327	Y= -0.0000	Z= 0.0000	
Temperature: 0K, Unit: Debye			
X= 1.7723	Y= -0.0000	Z= 0.0000	
Temperature: 298K, Unit: Debye			
X= 1.7589	Y= -0.0000	Z= 0.0003	

Internal coordinates for the Equilibrium structure (Se)

		1	2	3	4	5	6	7	8	9	10
1	C	0.000000									
2	C	1.373536	0.000000								
3	C	2.253051	1.421420	0.000000							
4	C	2.243980	2.253051	1.373536	0.000000						
5	N	1.371263	2.215933	2.215933	1.371263	0.000000					
6	H	2.113865	3.182415	3.182415	2.113865	1.003171	0.000000				
7	H	1.075495	2.232513	3.312795	3.257886	2.137261	2.508115	0.000000			
8	H	2.184421	1.076437	2.239350	3.295311	3.256122	4.189008	2.709218	0.000000		
9	H	3.295311	2.239350	1.076437	2.184421	3.256122	4.189008	4.332741	2.712761	0.000000	
10	H	3.257886	3.312795	2.232513	1.075495	2.13726	2.508115	4.214445	4.332741	2.709218	0.000000

Internal coordinates for the vibrationally average structure at 0K (Sz)

		1	2	3	4	5	6	7	8	9	10
1	C	0.000000									
2	C	1.378332	0.000000								
3	C	2.262376	1.427926	0.000000							
4	C	2.254000	2.262376	1.378332	0.000000						
5	N	1.378887	2.227020	2.227020	1.378887	0.000000					
6	H	2.117936	3.189125	3.189125	2.117936	0.998706	0.000000				
7	H	1.077771	2.238116	3.324125	3.270601	2.146319	2.516284	0.000000			
8	H	2.191214	1.079310	2.247769	3.307261	3.269950	4.198639	2.715624	0.000000		
9	H	3.307260	2.247769	1.079309	2.191213	3.269950	4.198638	4.346476	2.722519	0.000000	
10	H	3.270599	3.324124	2.238114	1.077769	2.14631	2.516284	4.230363	4.346475	2.715622	0.000000

Internal coordinates for the vibr. average structure at 298.15K (Sa)

		1	2	3	4	5	6	7	8	9	10
1	C	0.000000									
2	C	1.378186	0.000000								
3	C	2.262408	1.428134	0.000000							
4	C	2.254055	2.262408	1.378186	0.000000						
5	N	1.379217	2.227436	2.227436	1.379217	0.000000					
6	H	2.115949	3.186718	3.186718	2.115949	0.995808	0.000000				
7	H	1.077183	2.237368	3.323564	3.270136	2.146037	2.514841	0.000000			
8	H	2.190768	1.078887	2.247560	3.306846	3.269964	4.195934	2.714779	0.000000		
9	H	3.306845	2.247559	1.078887	2.190768	3.269963	4.195934	4.345466	2.722100	0.000000	
10	H	3.270134	3.323562	2.237367	1.077181	2.14603	2.514840	4.229473	4.345465	2.714777	0.000000

Pyrrole, apfd/aug-cc-pvdz

Electric dipole

Property at reference geometry, Unit: Debye			
X= 1.8767	Y= -0.0000	Z= 0.0000	
Temperature: 0K, Unit: Debye			
X= 1.8204	Y= -0.0000	Z= 0.0000	
Temperature: 298K, Unit: Debye			
X= 1.8093	Y= -0.0000	Z= 0.0003	

Internal coordinates for the Equilibrium structure (Se)

	1	2	3	4	5	6	7	8	9	10
1 C	0.000000									
2 C	1.379804	0.000000								
3 C	2.258481	1.423809	0.000000							
4 C	2.245301	2.258481	1.379804	0.000000						
5 N	1.370045	2.219793	2.219793	1.370045	0.000000					
6 H	2.115290	3.190482	3.190482	2.115290	1.007503	0.000000				
7 H	1.084734	2.246709	3.327394	3.267424	2.143856	2.512508	0.000000			
8 H	2.198603	1.086204	2.250941	3.311097	3.269096	4.205666	2.727617	0.000000		
9 H	3.311097	2.250941	1.086204	2.198603	3.269096	4.205666	4.357714	2.729928	0.000000	
10 H	3.267424	3.327394	2.246709	1.084734	2.143856	2.512508	4.230799	4.357714	2.727617	0.000000

Internal coordinates for the vibrationally average structure at 0K (Sz)

	1	2	3	4	5	6	7	8	9	10
1 C	0.000000									
2 C	1.384536	0.000000								
3 C	2.267394	1.430020	0.000000							
4 C	2.254610	2.267395	1.384536	0.000000						
5 N	1.377212	2.230563	2.230563	1.377212	0.000000					
6 H	2.119415	3.197438	3.197438	2.119415	1.003608	0.000000				
7 H	1.086675	2.251677	3.337901	3.279239	2.152460	2.520732	0.000000			
8 H	2.204410	1.088326	2.258795	3.322075	3.281720	4.214590	2.732391	0.000000		
9 H	3.322074	2.258795	1.088326	2.204410	3.281720	4.214590	4.370092	2.739611	0.000000	
10 H	3.279239	3.337901	2.251677	1.086675	2.152460	2.520731	4.245765	4.370092	2.732391	0.000000

Internal coordinates for the vibr. average structure at 298.15K (Sa)

	1	2	3	4	5	6	7	8	9	10
1 C	0.000000									
2 C	1.384427	0.000000								
3 C	2.267415	1.430187	0.000000							
4 C	2.254622	2.267415	1.384427	0.000000						
5 N	1.377470	2.230922	2.230922	1.377470	0.000000					
6 H	2.117732	3.195427	3.195426	2.117732	1.001175	0.000000				
7 H	1.086078	2.250957	3.337316	3.278720	2.152124	2.519460	0.000000			
8 H	2.203933	1.087849	2.258524	3.321610	3.281614	4.212203	2.731517	0.000000		
9 H	3.321610	2.258523	1.087849	2.203933	3.281614	4.212203	4.369027	2.739161	0.000000	
10 H	3.278719	3.337316	2.250958	1.086078	2.152124	2.519460	4.244808	4.369027	2.731517	0.000000

Pyrrole, apfd/aug-cc-pvtz

Electric dipole

Property at reference geometry, Unit: Debye
X= -1.8701 Y= -0.0000 Z= -0.0000
Temperature: 0K, Unit: Debye
X= -1.8137 Y= -0.0000 Z= -0.0000
Temperature: 298K, Unit: Debye
X= -1.8021 Y= 0.0000 Z= -0.0001

Internal coordinates for the Equilibrium structure (Se)

	1	2	3	4	5	6	7	8	9	10
1 C	0.000000									
2 C	1.371858	0.000000								
3 C	2.247595	1.417815	0.000000							
4 C	2.235617	2.247595	1.371858	0.000000						
5 N	1.365233	2.210096	2.210096	1.365233	0.000000					
6 H	2.107808	3.176610	3.176610	2.107808	1.003182	0.000000				
7 H	1.077298	2.232608	3.309193	3.250867	2.132977	2.501747	0.000000			
8 H	2.184689	1.078386	2.238356	3.292315	3.251954	4.184636	2.710171	0.000000		
9 H	3.292315	2.238356	1.078386	2.184689	3.251954	4.184636	4.331719	2.713558	0.000000	
10 H	3.250867	3.309193	2.232608	1.077298	2.132977	2.501747	4.208040	4.331719	2.710171	0.000000

Internal coordinates for the vibrationally average structure at 0K (Sz)

	1	2	3	4	5	6	7	8	9	10
1 C	0.000000									
2 C	1.376537	0.000000								
3 C	2.256536	1.424029	0.000000							
4 C	2.245110	2.256536	1.376537	0.000000						
5 N	1.372446	2.220736	2.220736	1.372446	0.000000					
6 H	2.111590	3.183035	3.183035	2.111590	0.998879	0.000000				
7 H	1.079401	2.237808	3.319925	3.262960	2.141691	2.509709	0.000000			
8 H	2.191046	1.080953	2.246341	3.303642	3.264998	4.193625	2.715828	0.000000		
9 H	3.303642	2.246341	1.080953	2.191046	3.264998	4.193625	4.344615	2.722970	0.000000	
10 H	3.262960	3.319925	2.237808	1.079401	2.141691	2.509709	4.223312	4.344615	2.715828	0.000000

Internal coordinates for the vibr. average structure at 298.15K (Sa)

	1	2	3	4	5	6	7	8	9	10
1 C	0.000000									
2 C	1.376413	0.000000								
3 C	2.256559	1.424206	0.000000							
4 C	2.245142	2.256559	1.376413	0.000000						
5 N	1.372723	2.221098	2.221098	1.372723	0.000000					
6 H	2.109797	3.180877	3.180877	2.109797	0.996293	0.000000				
7 H	1.078829	2.237100	3.319369	3.262485	2.141391	2.508387	0.000000			
8 H	2.190617	1.080534	2.246112	3.303227	3.264957	4.191160	2.715015	0.000000		
9 H	3.303227	2.246112	1.080534	2.190617	3.264957	4.191160	4.343621	2.722546	0.000000	
10 H	3.262485	3.319369	2.237100	1.078829	2.141391	2.508387	4.222421	4.343621	2.715015	0.000000

Pyrrole, m062x/aug-cc-pvdz

Electric dipole

Property at reference geometry, Unit: Debye			
X= -1.8853	Y= -0.0000	Z= 0.0000	
Temperature: 0K, Unit: Debye			
X= -1.8332	Y= -0.0000	Z= 0.0000	
Temperature: 298K, Unit: Debye			
X= -1.8237	Y= 0.0000	Z= -0.0001	

Internal coordinates for the Equilibrium structure (Se)

	1	2	3	4	5	6	7	8	9	10
1 C	0.000000									
2 C	1.377785	0.000000								
3 C	2.257727	1.425072	0.000000							
4 C	2.244827	2.257727	1.377785	0.000000						
5 N	1.370123	2.218699	2.218699	1.370123	0.000000					
6 H	2.115430	3.189131	3.189131	2.115430	1.007342	0.000000				
7 H	1.083106	2.243406	3.325183	3.265318	2.142193	2.511359	0.000000			
8 H	2.194681	1.084084	2.250634	3.308244	3.265893	4.202188	2.722926	0.000000		
9 H	3.308244	2.250634	1.084084	2.194681	3.265893	4.202188	4.353553	2.729768	0.000000	
10 H	3.265318	3.325183	2.243406	1.083106	2.142193	2.511359	4.227135	4.353553	2.722926	0.000000

Internal coordinates for the vibrationally average structure at 0K (Sz)

	1	2	3	4	5	6	7	8	9	10
1 C	0.000000									
2 C	1.382628	0.000000								
3 C	2.266568	1.431278	0.000000							
4 C	2.253699	2.266568	1.382628	0.000000						
5 N	1.377130	2.229671	2.229671	1.377130	0.000000					
6 H	2.119387	3.196205	3.196205	2.119387	1.003354	0.000000				
7 H	1.085761	2.248988	3.336298	3.277401	2.151218	2.519807	0.000000			
8 H	2.200038	1.086376	2.259427	3.319666	3.278541	4.210902	2.727074	0.000000		
9 H	3.319666	2.259427	1.086376	2.200038	3.278541	4.210902	4.367147	2.742163	0.000000	
10 H	3.277401	3.336298	2.248988	1.085761	2.151218	2.519807	4.243016	4.367147	2.727074	0.000000

Internal coordinates for the vibr. average structure at 298.15K (Sa)

	1	2	3	4	5	6	7	8	9	10
1 C	0.000000									
2 C	1.382517	0.000000								
3 C	2.266589	1.431451	0.000000							
4 C	2.253707	2.266589	1.382517	0.000000						
5 N	1.377359	2.229987	2.229987	1.377359	0.000000					
6 H	2.117901	3.194425	3.194425	2.117901	1.001204	0.000000				
7 H	1.085248	2.248349	3.335800	3.276953	2.150932	2.518691	0.000000			
8 H	2.199577	1.085928	2.259196	3.319233	3.278417	4.208760	2.726271	0.000000		
9 H	3.319233	2.259196	1.085928	2.199577	3.278417	4.208760	4.366201	2.741780	0.000000	
10 H	3.276953	3.335800	2.248349	1.085248	2.150932	2.518691	4.242193	4.366201	2.726271	0.000000

Pyrrole,m062x/aug-cc-pvtz

Electric dipole

Property at reference geometry, Unit: Debye

X= 1.8571 Y= -0.0000 Z= 0.0000

Temperature: 0K, Unit: Debye

X= 1.8039 Y= -0.0000 Z= 0.0000

Temperature: 298K, Unit: Debye

X= 1.7932 Y= 0.0000 Z= -0.0001

Internal coordinates for the Equilibrium structure (Se)

		1	2	3	4	5	6	7	8	9	10
1	C	0.000000									
2	C	1.369716	0.000000								
3	C	2.247853	1.420288	0.000000							
4	C	2.236675	2.247853	1.369716	0.000000						
5	N	1.366823	2.210484	2.210484	1.366823	0.000000					
6	H	2.109905	3.177003	3.177003	2.109905	1.003312	0.000000				
7	H	1.075460	2.229102	3.307853	3.250062	2.132121	2.502077	0.000000			
8	H	2.180408	1.076110	2.239064	3.290238	3.250075	4.182750	2.705116	0.000000		
9	H	3.290238	2.239064	1.076110	2.180408	3.250075	4.182750	4.328221	2.714516	0.000000	
10	H	3.250062	3.307853	2.229102	1.075460	2.132121	2.502077	4.205480	4.328221	2.705116	0.000000

Internal coordinates for the vibrationally average structure at 0K (Sz)

		1	2	3	4	5	6	7	8	9	10
1	C	0.000000									
2	C	1.374369	0.000000								
3	C	2.256705	1.426528	0.000000							
4	C	2.245891	2.256705	1.374369	0.000000						
5	N	1.373968	2.221219	2.221219	1.373968	0.000000					
6	H	2.113700	3.183551	3.183551	2.113700	0.999036	0.000000				
7	H	1.078423	2.235016	3.319352	3.262691	2.141403	2.510399	0.000000			
8	H	2.186980	1.079193	2.247781	3.302096	3.263604	4.192190	2.711247	0.000000		
9	H	3.302096	2.247781	1.079193	2.186980	3.263604	4.192190	4.342524	2.725402	0.000000	
10	H	3.262691	3.319352	2.235016	1.078423	2.141403	2.510399	4.222001	4.342524	2.711247	0.000000

Internal coordinates for the vibr. average structure at 298.15K (Sa)

		1	2	3	4	5	6	7	8	9	10
1	C	0.000000									
2	C	1.374233	0.000000								
3	C	2.256726	1.426718	0.000000							
4	C	2.245921	2.256726	1.374233	0.000000						
5	N	1.374231	2.221551	2.221551	1.374231	0.000000					
6	H	2.112052	3.181553	3.181553	2.112052	0.996646	0.000000				
7	H	1.077940	2.234385	3.318887	3.262292	2.141159	2.509196	0.000000			
8	H	2.186577	1.078810	2.247593	3.301713	3.263573	4.189918	2.710524	0.000000		
9	H	3.301713	2.247593	1.078810	2.186577	3.263573	4.189918	4.341654	2.725026	0.000000	
10	H	3.262292	3.318887	2.234385	1.077940	2.141159	2.509196	4.221251	4.341654	2.710524	0.000000

Pyrrole, mp2fc/aug-cc-pvdz

Electric dipole

Property at reference geometry, Unit: Debye
X= -1.9085 Y= -0.0000 Z= 0.0000

Temperature: 0K, Unit: Debye
X= -1.8503 Y= -0.0000 Z= 0.0000

Temperature: 298K, Unit: Debye
X= -1.8389 Y= -0.0000 Z= -0.0001

Internal coordinates for the Equilibrium structure (Se)

		1	2	3	4	5	6	7	8	9	10
1	C	0.000000									
2	C	1.397500	0.000000								
3	C	2.278646	1.429375	0.000000							
4	C	2.266181	2.278646	1.397500	0.000000						
5	N	1.379545	2.237529	2.237529	1.379545	0.000000					
6	H	2.126159	3.212964	3.212964	2.126159	1.012148	0.000000				
7	H	1.087802	2.268160	3.350595	3.290262	2.155417	2.523979	0.000000			
8	H	2.215096	1.089018	2.259633	3.334895	3.288687	4.229763	2.749339	0.000000		
9	H	3.334895	2.259633	1.089018	2.215096	3.288687	4.229763	4.384958	2.742445	0.000000	
10	H	3.290262	3.350595	2.268160	1.087802	2.155417	2.523979	4.254962	4.384959	2.749339	0.000000

Internal coordinates for the vibrationally average structure at 0K (Sz)

		1	2	3	4	5	6	7	8	9	10
1	C	0.000000									
2	C	1.403123	0.000000								
3	C	2.288445	1.435625	0.000000							
4	C	2.276519	2.288445	1.403123	0.000000						
5	N	1.387231	2.249218	2.249218	1.387231	0.000000					
6	H	2.131190	3.221400	3.221400	2.131190	1.008806	0.000000				
7	H	1.089114	2.273747	3.361419	3.302342	2.163721	2.532228	0.000000			
8	H	2.220898	1.090796	2.267650	3.346617	3.301677	4.239537	2.754147	0.000000		
9	H	3.346617	2.267650	1.090796	2.220898	3.301677	4.239537	4.397644	2.753087	0.000000	
10	H	3.302342	3.361419	2.273747	1.089114	2.163721	2.532228	4.269369	4.397644	2.754147	0.000000

Internal coordinates for the vibr. average structure at 298.15K (Sa)

		1	2	3	4	5	6	7	8	9	10
1	C	0.000000									
2	C	1.403070	0.000000								
3	C	2.288481	1.435746	0.000000							
4	C	2.276545	2.288481	1.403070	0.000000						
5	N	1.387481	2.249595	2.249594	1.387481	0.000000					
6	H	2.129539	3.219461	3.219461	2.129539	1.006426	0.000000				
7	H	1.088388	2.272970	3.360719	3.301715	2.163281	2.530912	0.000000			
8	H	2.220397	1.090270	2.267323	3.346136	3.301524	4.237154	2.753171	0.000000		
9	H	3.346136	2.267323	1.090270	2.220397	3.301524	4.237154	4.396438	2.752620	0.000000	
10	H	3.301715	3.360719	2.272970	1.088388	2.163281	2.530912	4.268194	4.396438	2.753171	0.000000

Pyrrole, mp2fc/aug-cc-pvtz

Electric dipole

Property at reference geometry, Unit: Debye
X= -1.8783 Y= -0.0000 Z= 0.0000

Temperature: 0K, Unit: Debye
X= -1.8222 Y= -0.0000 Z= 0.0000

Temperature: 298K, Unit: Debye
X= -1.8111 Y= -0.0000 Z= -0.0001

Internal coordinates for the Equilibrium structure (Se)

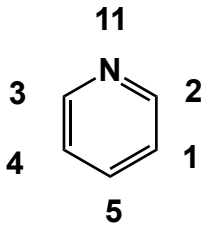
	1	2	3	4	5	6	7	8	9	10
1 C	0.000000									
2 C	1.382929	0.000000								
3 C	2.257392	1.416804	0.000000							
4 C	2.246836	2.257392	1.382929	0.000000						
5 N	1.369256	2.218160	2.218160	1.369256	0.000000					
6 H	2.111530	3.186794	3.186795	2.111530	1.005062	0.000000				
7 H	1.076097	2.244362	3.317886	3.259970	2.135644	2.503692	0.000000			
8 H	2.191041	1.076818	2.237325	3.301510	3.257573	4.192204	2.719856	0.000000		
9 H	3.301510	2.237325	1.076818	2.191041	3.257574	4.192205	4.340339	2.714621	0.000000	
10 H	3.259969	3.317886	2.244362	1.076097	2.135644	2.503692	4.214557	4.340339	2.719856	0.000000

Internal coordinates for the vibrationally average structure at 0K (Sz)

	1	2	3	4	5	6	7	8	9	10
1 C	0.000000									
2 C	1.388450	0.000000								
3 C	2.267106	1.423080	0.000000							
4 C	2.257060	2.267107	1.388451	0.000000						
5 N	1.376885	2.229749	2.229749	1.376885	0.000000					
6 H	2.116152	3.194718	3.194718	2.116152	1.001300	0.000000				
7 H	1.077726	2.249984	3.328901	3.272325	2.144327	2.512073	0.000000			
8 H	2.197613	1.079187	2.245544	3.313591	3.271188	4.202249	2.725421	0.000000		
9 H	3.313591	2.245545	1.079188	2.197614	3.271189	4.202250	4.353570	2.724952	0.000000	
10 H	3.272322	3.328898	2.249981	1.077723	2.144325	2.512072	4.229666	4.353566	2.725420	0.000000

Internal coordinates for the vibr. average structure at 298.15K (Sa)

	1	2	3	4	5	6	7	8	9	10
1 C	0.000000									
2 C	1.388389	0.000000								
3 C	2.267145	1.423206	0.000000							
4 C	2.257102	2.267145	1.388390	0.000000						
5 N	1.377133	2.230103	2.230103	1.377133	0.000000					
6 H	2.114472	3.192733	3.192734	2.114472	0.998898	0.000000				
7 H	1.077069	2.249262	3.328272	3.271779	2.143952	2.510780	0.000000			
8 H	2.197201	1.078750	2.245274	3.313189	3.271112	4.199920	2.724570	0.000000		
9 H	3.313189	2.245275	1.078750	2.197202	3.271112	4.199921	4.352505	2.724523	0.000000	
10 H	3.271776	3.328270	2.249260	1.077066	2.143950	2.510779	4.228632	4.352501	2.724569	0.000000



Pyridine, hf/aug-cc-pvdz

Electric dipole

Property at reference geometry, Unit: Debye

X= -2.2915 Y= 0.0000 Z= 0.0000

Temperature: 0K, Unit: Debye

X= -2.2445 Y= 0.0000 Z= 0.0000

Temperature: 298K, Unit: Debye

X= -2.2430 Y= 0.0000 Z= 0.0001

Internal coordinates for the Equilibrium structure (Se)

		1	2	3	4	5	6	7	8	9	10	11
1	C	0.000000										
2	C	1.388705	0.000000									
3	C	2.707545	2.265408	0.000000								
4	C	2.384692	2.707545	1.388705	0.000000							
5	C	1.386706	2.381979	2.381979	1.386706	0.000000						
6	H	1.079636	2.146289	3.786126	3.377283	2.156786	0.000000					
7	H	2.146397	1.081633	3.229607	3.788806	3.369051	2.476420	0.000000				
8	H	3.788806	3.229607	1.081633	2.146397	3.369051	4.866871	4.087754	0.000000			
9	H	3.377283	3.786126	2.146289	1.079636	2.156786	4.294235	4.866871	2.476420	0.000000		
10	H	2.149932	3.372341	3.372341	2.149932	1.080998	2.502261	4.278953	4.278953	2.502261	0.000000	
11	N	2.390443	1.323422	1.323422	2.390443	2.779843	3.353375	2.046400	2.046400	3.353375	3.860841	0.000000

Internal coordinates for the vibrationally average structure at 0K (Sz)

		1	2	3	4	5	6	7	8	9	10	11
1	C	0.000000										
2	C	1.393895	0.000000									
3	C	2.717368	2.273098	0.000000								
4	C	2.393714	2.717368	1.393895	0.000000							
5	C	1.391661	2.390206	2.390206	1.391661	0.000000						
6	H	1.083493	2.154402	3.799803	3.389818	2.164655	0.000000					
7	H	2.155629	1.086873	3.241743	3.803852	3.382339	2.486896	0.000000				
8	H	3.803852	3.241743	1.086873	2.155629	3.382339	4.885759	4.103478	0.000000			
9	H	3.389818	3.799803	2.154402	1.083493	2.164655	4.310000	4.885759	2.486896	0.000000		
10	H	2.157703	3.384463	3.384463	2.157703	1.085223	2.511314	4.295836	4.295836	2.511314	0.000000	
11	N	2.398326	1.327403	1.327403	2.398326	2.788450	3.364855	2.054149	2.054149	3.364855	3.873673	0.000000

Internal coordinates for the vibr. average structure at 298.15K (Sa)

		1	2	3	4	5	6	7	8	9	10	11
1	C	0.000000										
2	C	1.393774	0.000000									
3	C	2.717172	2.272906	0.000000								
4	C	2.393594	2.717172	1.393774	0.000000							
5	C	1.391544	2.389939	2.389939	1.391544	0.000000						
6	H	1.083170	2.154055	3.799284	3.389387	2.164301	0.000000					
7	H	2.155231	1.086521	3.241215	3.803302	3.381764	2.486487	0.000000				
8	H	3.803302	3.241215	1.086521	2.155231	3.381764	4.884888	4.102653	0.000000			
9	H	3.389387	3.799284	2.154055	1.083170	2.164301	4.309287	4.884888	2.486487	0.000000		
10	H	2.157270	3.383863	3.383863	2.157270	1.084871	2.510829	4.294970	4.294970	2.510829	0.000000	
11	N	2.398112	1.327274	1.327274	2.398112	2.788108	3.364363	2.053740	2.053740	3.364363	3.872980	0.000000

Pyridine, hf/aug-cc-pvtz

Electric dipole

Property at reference geometry, Unit: Debye

X= 2.2720 Y= 0.0000 Z= 0.0000

Temperature: 0K, Unit: Debye

X= 2.2259 Y= 0.0000 Z= 0.0000

Temperature: 298K, Unit: Debye

X= 2.2246 Y= 0.0000 Z= -0.0000

Internal coordinates for the Equilibrium structure (Se)

		1	2	3	4	5	6	7	8	9	10	11
1	C	0.000000										
2	C	1.382092	0.000000									
3	C	2.695833	2.256651	0.000000								
4	C	2.374021	2.695833	1.382092	0.000000							
5	C	1.380058	2.370559	2.370559	1.380058	0.000000						
6	H	1.072076	2.134266	3.766902	3.359300	2.144283	0.000000					
7	H	2.134996	1.074430	3.214170	3.769877	3.351328	2.463498	0.000000				
8	H	3.769877	3.214170	1.074430	2.134996	3.351328	4.840437	4.066419	0.000000			
9	H	3.359300	3.766902	2.134266	1.072076	2.144283	4.269361	4.840437	2.463498	0.000000		
10	H	2.137293	3.353717	3.353717	2.137293	1.073401	2.487025	4.254750	4.254750	2.487025	0.000000	
11	N	2.378072	1.317284	1.317284	2.378072	2.764603	3.334699	2.035692	2.035692	3.334699	3.838005	0.000000

Internal coordinates for the vibrationally average structure at 0K (Sz)

		1	2	3	4	5	6	7	8	9	10	11
1	C	0.000000										
2	C	1.387286	0.000000									
3	C	2.705644	2.264384	0.000000								
4	C	2.382964	2.705644	1.387286	0.000000							
5	C	1.384969	2.378785	2.378785	1.384969	0.000000						
6	H	1.076164	2.142498	3.780794	3.372005	2.152354	0.000000					
7	H	2.144176	1.079813	3.226618	3.785062	3.364631	2.473778	0.000000				
8	H	3.785062	3.226618	1.079813	2.144176	3.364631	4.859697	4.082816	0.000000			
9	H	3.372005	3.780794	2.142498	1.076164	2.152354	4.285541	4.859697	2.473778	0.000000		
10	H	2.145245	3.366081	3.366081	2.145245	1.077889	2.496366	4.271814	4.271815	2.496366	0.000000	
11	N	2.385885	1.321251	1.321251	2.385885	2.773132	3.346288	2.043786	2.043786	3.346288	3.851021	0.000000

Internal coordinates for the vibr. average structure at 298.15K (Sa)

		1	2	3	4	5	6	7	8	9	10	11
1	C	0.000000										
2	C	1.387171	0.000000									
3	C	2.705459	2.264205	0.000000								
4	C	2.382852	2.705459	1.387171	0.000000							
5	C	1.384858	2.378531	2.378531	1.384858	0.000000						
6	H	1.075859	2.142172	3.780306	3.371598	2.152018	0.000000					
7	H	2.143793	1.079470	3.226109	3.784533	3.364077	2.473391	0.000000				
8	H	3.784533	3.226109	1.079470	2.143793	3.364077	4.858865	4.082018	0.000000			
9	H	3.371598	3.780306	2.142172	1.075859	2.152018	4.284866	4.858865	2.473391	0.000000		
10	H	2.144830	3.365506	3.365506	2.144830	1.077551	2.495901	4.270981	4.270982	2.495901	0.000000	
11	N	2.385678	1.321127	1.321127	2.385678	2.772801	3.345820	2.043390	2.043390	3.345820	3.850352	0.000000

Pyridine, b3lyp/aug-cc-pvdz

Electric dipole

Property at reference geometry, Unit: Debye

X= 2.2767 Y= 0.0000 Z= 0.0000

Temperature: 0K, Unit: Debye

X= 2.2222 Y= 0.0000 Z= 0.0000

Temperature: 298K, Unit: Debye

X= 2.2196 Y= 0.0000 Z= 0.0001

Internal coordinates for the Equilibrium structure (Se)

		1	2	3	4	5	6	7	8	9	10	11
1	C	0.000000										
2	C	1.398727	0.000000									
3	C	2.729539	2.289267	0.000000								
4	C	2.399871	2.729539	1.398727	0.000000							
5	C	1.396341	2.401991	2.401991	1.396342	0.000000						
6	H	1.090245	2.163399	3.818825	3.401503	2.172450	0.000000					
7	H	2.165852	1.092806	3.264033	3.821994	3.399184	2.498111	0.000000				
8	H	3.821994	3.264033	1.092806	2.165852	3.399185	4.910802	4.132189	0.000000			
9	H	3.401503	3.818825	2.163399	1.090245	2.172450	4.325895	4.910802	2.498112	0.000000		
10	H	2.167425	3.401000	3.401000	2.167425	1.090872	2.520392	4.316646	4.316646	2.520391	0.000000	
11	N	2.414265	1.340313	1.340314	2.414265	2.809043	3.386731	2.069012	2.069012	3.386732	3.899915	0.000000

Internal coordinates for the vibrationally average structure at 0K (Sz)

		1	2	3	4	5	6	7	8	9	10	11
1	C	0.000000										
2	C	1.404268	0.000000									
3	C	2.740308	2.297987	0.000000								
4	C	2.409639	2.740307	1.404267	0.000000							
5	C	1.401655	2.410845	2.410845	1.401656	0.000000						
6	H	1.094322	2.172063	3.833678	3.414913	2.180766	0.000000					
7	H	2.175874	1.098227	3.277177	3.838155	3.413458	2.509722	0.000000				
8	H	3.838150	3.277172	1.098221	2.175869	3.413453	4.931027	4.148752	0.000000			
9	H	3.414914	3.833678	2.172064	1.094324	2.180767	4.342597	4.931034	2.509721	0.000000		
10	H	2.175469	3.413707	3.413707	2.175469	1.095100	2.529737	4.334538	4.334533	2.529737	0.000000	
11	N	2.422521	1.344658	1.344659	2.422521	2.817944	3.398900	2.077142	2.077137	3.398901	3.913043	0.000000

Internal coordinates for the vibr. average structure at 298.15K (Sa)

		1	2	3	4	5	6	7	8	9	10	11
1	C	0.000000										
2	C	1.404090	0.000000									
3	C	2.740059	2.297769	0.000000								
4	C	2.409489	2.740057	1.404090	0.000000							
5	C	1.401498	2.410476	2.410477	1.401498	0.000000						
6	H	1.093815	2.171525	3.832924	3.414271	2.180226	0.000000					
7	H	2.175273	1.097665	3.276414	3.837341	3.412604	2.509111	0.000000				
8	H	3.837335	3.276408	1.097658	2.175268	3.412599	4.929708	4.147504	0.000000			
9	H	3.414272	3.832924	2.171526	1.093817	2.180227	4.341509	4.929715	2.509109	0.000000		
10	H	2.174827	3.412823	3.412823	2.174827	1.094560	2.529002	4.333241	4.333236	2.529002	0.000000	
11	N	2.422180	1.344476	1.344477	2.422179	2.817412	3.398130	2.076522	2.076517	3.398132	3.911972	0.000000

Pyridine b3lyp/aug-cc-pvtz

Electric dipole

Property at reference geometry, Unit: Debye

X= 2.2639 Y= 0.0000 Z= 0.0000

Temperature: 0K, Unit: Debye

X= 2.2098 Y= 0.0000 Z= 0.0000

Temperature: 298K, Unit: Debye

X= 2.2072 Y= -0.0000 Z= 0.0001

Internal coordinates for the Equilibrium structure (Se)

		1	2	3	4	5	6	7	8	9	10	11
1	C	0.000000										
2	C	1.390469	0.000000									
3	C	2.715673	2.279583	0.000000								
4	C	2.387048	2.715673	1.390469	0.000000							
5	C	1.388331	2.388172	2.388172	1.388331	0.000000						
6	H	1.081220	2.148567	3.795998	3.379937	2.157452	0.000000					
7	H	2.152052	1.084112	3.246246	3.799412	3.377864	2.482376	0.000000				
8	H	3.799412	3.246246	1.084112	2.152052	3.377864	4.879267	4.107250	0.000000			
9	H	3.379937	3.795998	2.148567	1.081220	2.157452	4.296076	4.879267	2.482376	0.000000		
10	H	2.152276	3.378528	3.378528	2.152276	1.081832	2.502109	4.287547	4.287547	2.502109	0.000000	
11	N	2.399779	1.333673	1.333673	2.399779	2.791130	3.364696	2.056528	2.056528	3.364696	3.872962	0.000000

Internal coordinates for the vibrationally average structure at 0K (Sz)

		1	2	3	4	5	6	7	8	9	10	11
1	C	0.000000										
2	C	1.396042	0.000000									
3	C	2.726436	2.288284	0.000000								
4	C	2.396784	2.726436	1.396042	0.000000							
5	C	1.393598	2.396994	2.396994	1.393598	0.000000						
6	H	1.085530	2.157332	3.811069	3.393603	2.166054	0.000000					
7	H	2.161891	1.089642	3.259682	3.815690	3.392021	2.493536	0.000000				
8	H	3.815690	3.259682	1.089642	2.161891	3.392021	4.899844	4.124578	0.000000			
9	H	3.393603	3.811069	2.157332	1.085530	2.166054	4.313351	4.899844	2.493536	0.000000		
10	H	2.160559	3.391544	3.391544	2.160559	1.086424	2.511893	4.305556	4.305556	2.511893	0.000000	
11	N	2.408046	1.338004	1.338005	2.408046	2.799987	3.377006	2.065057	2.065057	3.377006	3.886411	0.000000

Internal coordinates for the vibr. average structure at 298.15K (Sa)

		1	2	3	4	5	6	7	8	9	10	11
1	C	0.000000										
2	C	1.395869	0.000000									
3	C	2.726191	2.288071	0.000000								
4	C	2.396634	2.726191	1.395869	0.000000							
5	C	1.393443	2.396634	2.396634	1.393443	0.000000						
6	H	1.085055	2.156824	3.810352	3.392993	2.165542	0.000000					
7	H	2.161304	1.089094	3.258937	3.814895	3.391187	2.492948	0.000000				
8	H	3.814895	3.258937	1.089094	2.161304	3.391187	4.898577	4.123363	0.000000			
9	H	3.392993	3.810352	2.156824	1.085055	2.165542	4.312321	4.898576	2.492948	0.000000		
10	H	2.159949	3.390700	3.390700	2.159949	1.085917	2.511194	4.304307	4.304307	2.511194	0.000000	
11	N	2.407709	1.337825	1.337825	2.407709	2.799465	3.376270	2.064454	2.064454	3.376270	3.885382	0.000000

Pyridine, apfd/aug-cc-pvdz

Electric dipole

Property at reference geometry, Unit: Debye

X= 2.2593 Y= 0.0000 Z= 0.0000

Temperature: 0K, Unit: Debye

X= 2.2019 Y= 0.0000 Z= 0.0000

Temperature: 298K, Unit: Debye

X= 2.1989 Y= -0.0000 Z= 0.0001

Internal coordinates for the Equilibrium structure (Se)

		1	2	3	4	5	6	7	8	9	10	11
1	C	0.000000										
2	C	1.396122	0.000000									
3	C	2.722750	2.281182	0.000000								
4	C	2.395343	2.722750	1.396122	0.000000							
5	C	1.393690	2.396498	2.396498	1.393690	0.000000						
6	H	1.090906	2.162147	3.812667	3.397815	2.170894	0.000000					
7	H	2.164295	1.093301	3.255727	3.815661	3.394706	2.497513	0.000000				
8	H	3.815661	3.255727	1.093301	2.164295	3.394706	4.905067	4.122624	0.000000			
9	H	3.397815	3.812667	2.162147	1.090906	2.170894	4.323002	4.905067	2.497513	0.000000		
10	H	2.165692	3.396575	3.396575	2.165692	1.091674	2.518921	4.313324	4.313324	2.518921	0.000000	
11	N	2.409677	1.336179	1.336179	2.409677	2.803673	3.382638	2.064059	2.064059	3.382638	3.895348	0.000000

Internal coordinates for the vibrationally average structure at 0K (Sz)

		1	2	3	4	5	6	7	8	9	10	11
1	C	0.000000										
2	C	1.402171	0.000000									
3	C	2.736431	2.292810	0.000000								
4	C	2.408386	2.736431	1.402171	0.000000							
5	C	1.399565	2.405024	2.405024	1.399565	0.000000						
6	H	1.094663	2.171868	3.830177	3.413687	2.179635	0.000000					
7	H	2.175214	1.098426	3.270941	3.834393	3.409125	2.511729	0.000000				
8	H	3.834393	3.270941	1.098426	2.175214	3.409125	4.927611	4.140123	0.000000			
9	H	3.413687	3.830177	2.171868	1.094663	2.179635	4.341069	4.927611	2.511729	0.000000		
10	H	2.173112	3.408512	3.408512	2.173112	1.095726	2.527341	4.331132	4.331132	2.527341	0.000000	
11	N	2.417897	1.340996	1.340996	2.417897	2.809933	3.395344	2.072536	2.072536	3.395344	3.905659	0.000000

Internal coordinates for the vibr. average structure at 298.15K (Sa)

		1	2	3	4	5	6	7	8	9	10	11
1	C	0.000000										
2	C	1.402009	0.000000									
3	C	2.736313	2.292725	0.000000								
4	C	2.408391	2.736313	1.402009	0.000000							
5	C	1.399432	2.404627	2.404627	1.399432	0.000000						
6	H	1.094151	2.171383	3.829553	3.413171	2.179123	0.000000					
7	H	2.174652	1.097850	3.270267	3.833695	3.408268	2.511246	0.000000				
8	H	3.833695	3.270267	1.097850	2.174652	3.408268	4.926405	4.138906	0.000000			
9	H	3.413171	3.829553	2.171383	1.094151	2.179123	4.340064	4.926405	2.511246	0.000000		
10	H	2.172439	3.407580	3.407580	2.172439	1.095181	2.526566	4.329824	4.329824	2.526565	0.000000	
11	N	2.417543	1.340832	1.340832	2.417543	2.809257	3.394600	2.071925	2.071925	3.394600	3.904438	0.000000

Pyridine, apfd/aug-cc-pvtz

Electric dipole

Property at reference geometry, Unit: Debye

X= 2.2447 Y= 0.0000 Z= -0.0000

Temperature: 0K, Unit: Debye

X= 2.1845 Y= 0.0000 Z= -0.0000

Temperature: 298K, Unit: Debye

X= 2.1814 Y= 0.0000 Z= 0.0001

Internal coordinates for the Equilibrium structure (Se)

		1	2	3	4	5	6	7	8	9	10	11
1	C	0.000000										
2	C	1.388623	0.000000									
3	C	2.709205	2.271168	0.000000								
4	C	2.382702	2.709205	1.388623	0.000000							
5	C	1.386299	2.384191	2.384191	1.386299	0.000000						
6	H	1.083295	2.148881	3.791540	3.377991	2.157643	0.000000					
7	H	2.151913	1.086022	3.239160	3.794835	3.375842	2.482836	0.000000				
8	H	3.794835	3.239160	1.086022	2.151913	3.375842	4.876668	4.100405	0.000000			
9	H	3.377990	3.791540	2.148881	1.083295	2.157643	4.296506	4.876668	2.482836	0.000000		
10	H	2.152612	3.377038	3.377038	2.152611	1.084002	2.503280	4.287878	4.287878	2.503280	0.000000	
11	N	2.396606	1.329827	1.329827	2.396606	2.788399	3.362922	2.052963	2.052963	3.362922	3.872401	0.000000

Internal coordinates for the vibrationally average structure at 0K (Sz)

		1	2	3	4	5	6	7	8	9	10	11
1	C	0.000000										
2	C	1.395421	0.000000									
3	C	2.726050	2.285902	0.000000								
4	C	2.399118	2.726050	1.395421	0.000000							
5	C	1.392895	2.392853	2.392853	1.392895	0.000000						
6	H	1.087163	2.160073	3.812379	3.396910	2.167378	0.000000					
7	H	2.164032	1.091155	3.257050	3.816704	3.391007	2.499751	0.000000				
8	H	3.816702	3.257048	1.091154	2.164031	3.391005	4.902510	4.119927	0.000000			
9	H	3.396910	3.812379	2.160074	1.087163	2.167378	4.317033	4.902512	2.499751	0.000000		
10	H	2.160048	3.389158	3.389158	2.160047	1.088381	2.511632	4.306602	4.306601	2.511631	0.000000	
11	N	2.405044	1.335216	1.335216	2.405044	2.792503	3.376701	2.062337	2.062336	3.376701	3.880884	0.000000

Internal coordinates for the vibr. average structure at 298.15K (Sa)

		1	2	3	4	5	6	7	8	9	10	11
1	C	0.000000										
2	C	1.395321	0.000000									
3	C	2.726183	2.286062	0.000000								
4	C	2.399389	2.726183	1.395321	0.000000							
5	C	1.392823	2.392474	2.392474	1.392823	0.000000						
6	H	1.086673	2.159727	3.812032	3.396641	2.166947	0.000000					
7	H	2.163588	1.090585	3.256579	3.816257	3.390231	2.499534	0.000000				
8	H	3.816256	3.256577	1.090583	2.163587	3.390229	4.901584	4.118842	0.000000			
9	H	3.396641	3.812032	2.159727	1.086673	2.166947	4.316229	4.901586	2.499534	0.000000		
10	H	2.159385	3.388253	3.388253	2.159384	1.087866	2.510849	4.305397	4.305395	2.510848	0.000000	
11	N	2.404710	1.335098	1.335098	2.404710	2.791667	3.376062	2.061782	2.061781	3.376062	3.879533	0.000000

Pyridine, m062x/aug-cc-pvdz

Electric dipole

Property at reference geometry, Unit: Debye

X= 2.2469 Y= 0.0000 Z= 0.0000

Temperature: 0K, Unit: Debye

X= 2.2000 Y= 0.0000 Z= 0.0000

Temperature: 298K, Unit: Debye

X= 2.1976 Y= -0.0000 Z= 0.0001

Internal coordinates for the Equilibrium structure (Se)

		1	2	3	4	5	6	7	8	9	10	11
1	C	0.000000										
2	C	1.395208	0.000000									
3	C	2.720887	2.280644	0.000000								
4	C	2.392579	2.720887	1.395208	0.000000							
5	C	1.392139	2.394979	2.394979	1.392139	0.000000						
6	H	1.088509	2.158281	3.808369	3.393165	2.168021	0.000000					
7	H	2.161252	1.091214	3.253913	3.811750	3.390737	2.491954	0.000000				
8	H	3.811750	3.253913	1.091214	2.161252	3.390737	4.898734	4.120417	0.000000			
9	H	3.393165	3.808369	2.158281	1.088509	2.168021	4.316981	4.898734	2.491954	0.000000		
10	H	2.162554	3.392982	3.392982	2.162554	1.089537	2.515925	4.307272	4.307272	2.515925	0.000000	
11	N	2.407900	1.335748	1.335748	2.407900	2.801704	3.378172	2.063071	2.063071	3.378172	3.891241	0.000000

Internal coordinates for the vibrationally average structure at 0K (Sz)

		1	2	3	4	5	6	7	8	9	10	11
1	C	0.000000										
2	C	1.400650	0.000000									
3	C	2.731352	2.288741	0.000000								
4	C	2.402397	2.731352	1.400650	0.000000							
5	C	1.397670	2.403923	2.403923	1.397670	0.000000						
6	H	1.092972	2.167537	3.823316	3.406863	2.176510	0.000000					
7	H	2.170338	1.097005	3.267469	3.828017	3.404767	2.502618	0.000000				
8	H	3.828017	3.267469	1.097005	2.170338	3.404767	4.919497	4.138928	0.000000			
9	H	3.406863	3.823316	2.167537	1.092972	2.176510	4.334057	4.919497	2.502618	0.000000		
10	H	2.170506	3.405359	3.405359	2.170506	1.093255	2.525101	4.324259	4.324259	2.525101	0.000000	
11	N	2.416043	1.339810	1.339810	2.416043	2.810846	3.390749	2.072238	2.072238	3.390749	3.904100	0.000000

Internal coordinates for the vibr. average structure at 298.15K (Sa)

		1	2	3	4	5	6	7	8	9	10	11
1	C	0.000000										
2	C	1.400459	0.000000									
3	C	2.731083	2.288500	0.000000								
4	C	2.402241	2.731083	1.400459	0.000000							
5	C	1.397513	2.403540	2.403540	1.397513	0.000000						
6	H	1.092482	2.167021	3.822561	3.406222	2.175966	0.000000					
7	H	2.169724	1.096470	3.266722	3.827212	3.403913	2.502011	0.000000				
8	H	3.827213	3.266722	1.096470	2.169724	3.403913	4.918207	4.137742	0.000000			
9	H	3.406222	3.822561	2.167021	1.092482	2.175966	4.332966	4.918207	2.502011	0.000000		
10	H	2.169875	3.404473	3.404473	2.169875	1.092727	2.524356	4.322966	4.322966	2.524356	0.000000	
11	N	2.415687	1.339617	1.339617	2.415687	2.810303	3.389993	2.071650	2.071650	3.389993	3.903030	0.000000

Pyridine, m062x/aug-cc-pvtz

Electric dipole

Property at reference geometry, Unit: Debye

X= 2.2535 Y= 0.0000 Z= 0.0000

Temperature: 0K, Unit: Debye

X= 2.2063 Y= 0.0000 Z= -0.0000

Temperature: 298K, Unit: Debye

X= 2.2041 Y= 0.0000 Z= 0.0001

Internal coordinates for the Equilibrium structure (Se)

		1	2	3	4	5	6	7	8	9	10	11
1	C	0.000000										
2	C	1.388122	0.000000									
3	C	2.709582	2.273050	0.000000								
4	C	2.382241	2.709582	1.388121	0.000000							
5	C	1.385408	2.383047	2.383047	1.385409	0.000000						
6	H	1.080673	2.145703	3.789305	3.375091	2.155146	0.000000					
7	H	2.149211	1.083703	3.239423	3.792919	3.372289	2.478487	0.000000				
8	H	3.792920	3.239423	1.083703	2.149211	3.372289	4.872160	4.099975	0.000000			
9	H	3.375091	3.789305	2.145703	1.080673	2.155146	4.291499	4.872160	2.478488	0.000000		
10	H	2.149419	3.373460	3.373460	2.149419	1.081677	2.499914	4.281949	4.281949	2.499914	0.000000	
11	N	2.395430	1.330231	1.330231	2.395430	2.785820	3.359374	2.052839	2.052839	3.359374	3.867496	0.000000

Internal coordinates for the vibrationally average structure at 0K (Sz)

		1	2	3	4	5	6	7	8	9	10	11
1	C	0.000000										
2	C	1.393650	0.000000									
3	C	2.720123	2.281237	0.000000								
4	C	2.392040	2.720123	1.393649	0.000000							
5	C	1.390860	2.391967	2.391967	1.390860	0.000000						
6	H	1.085126	2.154971	3.804315	3.388779	2.163636	0.000000					
7	H	2.158383	1.089511	3.253104	3.809282	3.386302	2.489144	0.000000				
8	H	3.809283	3.253104	1.089511	2.158383	3.386303	4.893004	4.118666	0.000000			
9	H	3.388778	3.804315	2.154970	1.085126	2.163636	4.308591	4.893003	2.489144	0.000000		
10	H	2.157676	3.386286	3.386286	2.157676	1.085907	2.509317	4.299350	4.299351	2.509316	0.000000	
11	N	2.403654	1.334336	1.334337	2.403654	2.794917	3.371987	2.062098	2.062099	3.371987	3.880824	0.000000

Internal coordinates for the vibr. average structure at 298.15K (Sa)

		1	2	3	4	5	6	7	8	9	10	11
1	C	0.000000										
2	C	1.393464	0.000000									
3	C	2.719856	2.280997	0.000000								
4	C	2.391881	2.719856	1.393463	0.000000							
5	C	1.390699	2.391586	2.391586	1.390700	0.000000						
6	H	1.084660	2.154483	3.803586	3.388155	2.163106	0.000000					
7	H	2.157776	1.088986	3.252371	3.808488	3.385453	2.488554	0.000000				
8	H	3.808489	3.252371	1.088986	2.157776	3.385454	4.891750	4.117509	0.000000			
9	H	3.388154	3.803585	2.154482	1.084660	2.163106	4.307533	4.891748	2.488555	0.000000		
10	H	2.157058	3.385421	3.385421	2.157059	1.085400	2.508585	4.298078	4.298079	2.508584	0.000000	
11	N	2.403310	1.334149	1.334150	2.403310	2.794385	3.371266	2.061525	2.061526	3.371266	3.879784	0.000000

Pyridine, mp2fc/aug-cc-pvdz

Electric dipole

Property at reference geometry, Unit: Debye

X= 2.3508 Y= 0.0000 Z= -0.0000

Temperature: 0K, Unit: Debye

X= 2.2981 Y= 0.0000 Z= -0.0000

Temperature: 298K, Unit: Debye

X= 2.2955 Y= 0.0000 Z= -0.0000

Internal coordinates for the Equilibrium structure (Se)

		1	2	3	4	5	6	7	8	9	10	11
1	C	0.000000										
2	C	1.406703	0.000000									
3	C	2.744738	2.304254	0.000000								
4	C	2.410660	2.744738	1.406703	0.000000							
5	C	1.404895	2.419378	2.419378	1.404895	0.000000						
6	H	1.093584	2.171495	3.837303	3.415794	2.182122	0.000000					
7	H	2.175963	1.094986	3.280745	3.839371	3.418311	2.507739	0.000000				
8	H	3.839371	3.280745	1.094986	2.175963	3.418311	4.931443	4.150712	0.000000			
9	H	3.415794	3.837303	2.171495	1.093584	2.182122	4.343925	4.931443	2.507739	0.000000		
10	H	2.179350	3.421222	3.421222	2.179350	1.093953	2.533488	4.338707	4.338707	2.533488	0.000000	
11	N	2.433923	1.352707	1.352707	2.433923	2.836253	3.407774	2.078825	2.078825	3.407774	3.930207	0.000000

Internal coordinates for the vibrationally average structure at 0K (Sz)

		1	2	3	4	5	6	7	8	9	10	11
1	C	0.000000										
2	C	1.412493	0.000000									
3	C	2.756052	2.313504	0.000000								
4	C	2.420866	2.756052	1.412493	0.000000							
5	C	1.410356	2.428512	2.428512	1.410356	0.000000						
6	H	1.097248	2.179966	3.852285	3.429277	2.190351	0.000000					
7	H	2.185837	1.099834	3.293827	3.855502	3.432396	2.519146	0.000000				
8	H	3.855502	3.293827	1.099834	2.185838	3.432396	4.951224	4.166694	0.000000			
9	H	3.429277	3.852285	2.179966	1.097248	2.190351	4.360418	4.951224	2.519146	0.000000		
10	H	2.186983	3.433654	3.433654	2.186983	1.097620	2.542556	4.355954	4.355954	2.542556	0.000000	
11	N	2.443003	1.357572	1.357572	2.443003	2.845902	3.420301	2.086691	2.086691	3.420301	3.943523	0.000000

Internal coordinates for the vibr. average structure at 298.15K (Sa)

		1	2	3	4	5	6	7	8	9	10	11
1	C	0.000000										
2	C	1.412290	0.000000									
3	C	2.755768	2.313279	0.000000								
4	C	2.420674	2.755768	1.412290	0.000000							
5	C	1.410162	2.428088	2.428088	1.410162	0.000000						
6	H	1.096732	2.179399	3.851489	3.428581	2.189772	0.000000					
7	H	2.185209	1.099252	3.293034	3.854634	3.431476	2.518515	0.000000				
8	H	3.854634	3.293034	1.099252	2.185209	3.431476	4.949844	4.165395	0.000000			
9	H	3.428581	3.851489	2.179399	1.096732	2.189772	4.359260	4.949844	2.518515	0.000000		
10	H	2.186284	3.432695	3.432695	2.186284	1.097062	2.541758	4.354572	4.354572	2.541758	0.000000	
11	N	2.442623	1.357383	1.357383	2.442623	2.845303	3.419491	2.086046	2.086046	3.419491	3.942365	0.000000

Pyridine mp2fc/aug-cc-pvtz

Electric dipole

Property at reference geometry, Unit: Debye

X= -0.0000 Y= 0.0000 Z= -2.3347

Temperature: 0K, Unit: Debye

X= 0.0000 Y= 0.0000 Z= -2.2849

Temperature: 298K, Unit: Debye

X= 0.0001 Y= -0.0000 Z= -2.2826

Internal coordinates for the Equilibrium structure (Se)

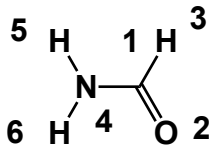
		1	2	3	4	5	6	7	8	9	10	11
1	C	0.000000										
2	C	1.392930	0.000000									
3	C	2.720233	2.285276	0.000000								
4	C	2.388952	2.720233	1.392930	0.000000							
5	C	1.391253	2.395371	2.395371	1.391253	0.000000						
6	H	1.081509	2.149229	3.800785	3.382640	2.159940	0.000000					
7	H	2.154576	1.083587	3.251444	3.803455	3.384305	2.483098	0.000000				
8	H	3.803455	3.251444	1.083587	2.154576	3.384305	4.883525	4.112294	0.000000			
9	H	3.382640	3.800785	2.149229	1.081509	2.159940	4.300042	4.883525	2.483098	0.000000		
10	H	2.156284	3.385811	3.385811	2.156284	1.081902	2.506638	4.294242	4.294242	2.506638	0.000000	
11	N	2.409983	1.340623	1.340623	2.409983	2.806452	3.373574	2.059551	2.059551	3.373574	3.888354	0.000000

Internal coordinates for the vibrationally average structure at 0K (Sz)

		1	2	3	4	5	6	7	8	9	10	11
1	C	0.000000										
2	C	1.398680	0.000000									
3	C	2.731257	2.294452	0.000000								
4	C	2.398593	2.731257	1.398680	0.000000							
5	C	1.396637	2.404745	2.404745	1.396637	0.000000						
6	H	1.085408	2.157718	3.815708	3.395807	2.168149	0.000000					
7	H	2.164160	1.088601	3.264944	3.819482	3.398449	2.493843	0.000000				
8	H	3.819482	3.264944	1.088601	2.164160	3.398449	4.903444	4.129443	0.000000			
9	H	3.395807	3.815708	2.157718	1.085408	2.168149	4.316444	4.903444	2.493843	0.000000		
10	H	2.164313	3.398828	3.398828	2.164313	1.085909	2.515981	4.311741	4.311741	2.515981	0.000000	
11	N	2.418895	1.345457	1.345457	2.418895	2.816392	3.386088	2.068037	2.068037	3.386088	3.902301	0.000000

Internal coordinates for the vibr. average structure at 298.15K (Sa)

		1	2	3	4	5	6	7	8	9	10	11
1	C	0.000000										
2	C	1.398488	0.000000									
3	C	2.730981	2.294233	0.000000								
4	C	2.398400	2.730981	1.398488	0.000000							
5	C	1.396460	2.404361	2.404361	1.396460	0.000000						
6	H	1.084922	2.157180	3.814949	3.395141	2.167603	0.000000					
7	H	2.163549	1.088039	3.264183	3.818642	3.397577	2.493223	0.000000				
8	H	3.818642	3.264183	1.088039	2.163549	3.397577	4.902121	4.128205	0.000000			
9	H	3.395141	3.814949	2.157180	1.084922	2.167603	4.315347	4.902121	2.493223	0.000000		
10	H	2.163661	3.397932	3.397932	2.163661	1.085375	2.515235	4.310427	4.310427	2.515235	0.000000	
11	N	2.418536	1.345277	1.345277	2.418536	2.815849	3.385321	2.067424	2.067424	3.385321	3.901224	0.000000



Formamide, hf/aug-cc-pvdz

Electric dipole

Property at reference geometry, Unit: Debye

X= 4.0088 Y= 1.1076 Z= 0.0000

Temperature: 0K, Unit: Debye

X= 3.7374 Y= 1.1133 Z= 0.0000

Temperature: 298K, Unit: Debye

X= 3.3772 Y= 1.1553 Z= -0.0632

Internal coordinates for the Equilibrium structure (Se)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.194457	0.000000				
3	H	1.097081	2.006361	0.000000			
4	N	1.350324	2.256367	2.046040	0.000000		
5	H	2.033800	2.523593	2.944736	0.996143	0.000000	
6	H	2.048957	3.135943	2.299187	0.993285	1.717963	0.000000

Internal coordinates for the vibrationally average structure at 0K (Sz)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.195320	0.000000				
3	H	1.106732	2.014887	0.000000			
4	N	1.364430	2.268412	2.068293	0.000000		
5	H	2.022637	2.508605	2.946024	0.984554	0.000000	
6	H	2.032023	3.117182	2.297048	0.966323	1.703396	0.000000

Internal coordinates for the vibr. average structure at 298.15K (Sa)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.192923	0.000000				
3	H	1.106828	2.012057	0.000000			
4	N	1.375394	2.275448	2.079751	0.000000		
5	H	1.990070	2.469831	2.919781	0.963352	0.000000	
6	H	1.987778	3.068020	2.268378	0.916286	1.671599	0.000000

Formamide, hf/aug-cc-pvtz

Electric dipole

Property at reference geometry, Unit: Debye

X= 3.9731 Y= 1.0861 Z= 0.0000

Temperature: 0K, Unit: Debye

X= 3.7328 Y= 1.0890 Z= 0.0000

Temperature: 298K, Unit: Debye

X= 3.4810 Y= 1.1197 Z= -0.0474

Internal coordinates for the Equilibrium structure (Se)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.187913	0.000000				
3	H	1.091022	1.995413	0.000000			
4	N	1.346079	2.248060	2.036049	0.000000		
5	H	2.027513	2.517140	2.931547	0.991718	0.000000	
6	H	2.041520	3.123114	2.288187	0.988791	1.709123	0.000000

Internal coordinates for the vibrationally average structure at 0K (Sz)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.188901	0.000000				
3	H	1.100664	2.004230	0.000000			
4	N	1.359494	2.259605	2.057453	0.000000		
5	H	2.018804	2.504872	2.934786	0.981806	0.000000	
6	H	2.028840	3.108814	2.289013	0.966125	1.697245	0.000000

Internal coordinates for the vibr. average structure at 298.15K (Sa)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.187195	0.000000				
3	H	1.100669	2.002333	0.000000			
4	N	1.367532	2.264755	2.065637	0.000000		
5	H	1.995912	2.477539	2.916192	0.966396	0.000000	
6	H	1.998324	3.074721	2.269243	0.931016	1.674860	0.000000

Formamide, b3lyp/aug-cc-pvdz

Electric dipole

Property at reference geometry, Unit: Debye

X= -3.8863 Y= 0.8291 Z= 0.0000

Temperature: 0K, Unit: Debye

X= -3.7093 Y= 0.8179 Z= 0.0000

Temperature: 298K, Unit: Debye

X= -3.6114 Y= 0.8319 Z= -0.0221

Internal coordinates for the Equilibrium structure (Se)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.217970	0.000000				
3	H	1.111146	2.044299	0.000000			
4	N	1.362052	2.286342	2.062668	0.000000		
5	H	2.057085	2.555219	2.976985	1.011233	0.000000	
6	H	2.073693	3.181989	2.319505	1.008639	1.742688	0.000000

Internal coordinates for the vibrationally average structure at 0K (Sz)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.220033	0.000000				
3	H	1.121832	2.055309	0.000000			
4	N	1.373217	2.296995	2.082267	0.000000		
5	H	2.054927	2.550929	2.986378	1.006182	0.000000	
6	H	2.068124	3.176607	2.324152	0.995237	1.737863	0.000000

Internal coordinates for the vibr. average structure at 298.15K (Sa)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.219413	0.000000				
3	H	1.121754	2.054252	0.000000			
4	N	1.376203	2.299109	2.085368	0.000000		
5	H	2.044484	2.539321	2.977676	0.998813	0.000000	
6	H	2.053911	3.161178	2.314683	0.979495	1.727191	0.000000

Formamide, b3lyp/aug-cc-pvdz temp = 423 K

Electric dipole

Property at reference geometry, Unit: Debye

X= -3.8863 Y= 0.8291 Z= 0.0000

Temperature: 0K, Unit: Debye

X= -3.7093 Y= 0.8179 Z= 0.0000

Temperature: 423K, Unit: Debye

X= -3.5311 Y= 0.8410 Z= -0.0314

Internal coordinates for the Equilibrium structure (Se)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.217970	0.000000				
3	H	1.111146	2.044300	0.000000			
4	N	1.362052	2.286342	2.062668	0.000000		
5	H	2.057086	2.555219	2.976985	1.011233	0.000000	
6	H	2.073693	3.181989	2.319505	1.008640	1.742689	0.000000

Internal coordinates for the vibrationally average structure at 0K (Sz)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.220033	0.000000				
3	H	1.121832	2.055309	0.000000			
4	N	1.373218	2.296995	2.082267	0.000000		
5	H	2.054928	2.550930	2.986378	1.006183	0.000000	
6	H	2.068125	3.176608	2.324152	0.995238	1.737864	0.000000

Internal coordinates for the vibr. average structure at 423.00K (Sa)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.218884	0.000000				
3	H	1.121466	2.053126	0.000000			
4	N	1.378819	2.300985	2.087925	0.000000		
5	H	2.036071	2.530474	2.970235	0.992232	0.000000	
6	H	2.042518	3.148718	2.307245	0.966618	1.717369	0.000000

Formamide, b3lyp/aug-cc-pvtz

Electric dipole

Property at reference geometry, Unit: Debye

X= -3.8643 Y= 0.8163 Z= 0.0000

Temperature: 0K, Unit: Debye

X= -3.6714 Y= 0.8086 Z= 0.0000

Temperature: 298K, Unit: Debye

X= -3.5404 Y= 0.8263 Z= -0.0274

Internal coordinates for the Equilibrium structure (Se)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.210790	0.000000				
3	H	1.103808	2.031484	0.000000			
4	N	1.356946	2.277346	2.050412	0.000000		
5	H	2.049626	2.548117	2.961285	1.006623	0.000000	
6	H	2.064636	3.167632	2.305232	1.003899	1.734255	0.000000

Internal coordinates for the vibrationally average structure at 0K (Sz)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.212687	0.000000				
3	H	1.114322	2.042141	0.000000			
4	N	1.368850	2.288395	2.070726	0.000000		
5	H	2.045382	2.541310	2.968866	0.999965	0.000000	
6	H	2.057314	3.160022	2.309224	0.987903	1.727279	0.000000

Internal coordinates for the vibr. average structure at 298.15K (Sa)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.211852	0.000000				
3	H	1.114219	2.040866	0.000000			
4	N	1.373047	2.291305	2.074992	0.000000		
5	H	2.031467	2.525626	2.957258	0.990153	0.000000	
6	H	2.038798	3.139817	2.296857	0.967236	1.713410	0.000000

Formamide, b3lyp/aug-cc-pvtz temp = 423 K

Electric dipole

Property at reference geometry, Unit: Debye

X= -3.8643 Y= 0.8163 Z= 0.0000

Temperature: 0K, Unit: Debye

X= -3.6714 Y= 0.8086 Z= 0.0000

Temperature: 423K, Unit: Debye

X= -3.4403 Y= 0.8405 Z= -0.0388

Internal coordinates for the Equilibrium structure (Se)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.210790	0.000000				
3	H	1.103808	2.031484	0.000000			
4	N	1.356946	2.277346	2.050411	0.000000		
5	H	2.049626	2.548118	2.961285	1.006623	0.000000	
6	H	2.064637	3.167632	2.305231	1.003899	1.734255	0.000000

Internal coordinates for the vibrationally average structure at 0K (Sz)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.212687	0.000000				
3	H	1.114322	2.042142	0.000000			
4	N	1.368850	2.288395	2.070726	0.000000		
5	H	2.045382	2.541310	2.968866	0.999965	0.000000	
6	H	2.057314	3.160022	2.309222	0.987903	1.727279	0.000000

Internal coordinates for the vibr. average structure at 423.00K (Sa)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.211186	0.000000				
3	H	1.113913	2.039620	0.000000			
4	N	1.376444	2.293683	2.078294	0.000000		
5	H	2.020933	2.514265	2.948035	0.982123	0.000000	
6	H	2.024859	3.124493	2.287747	0.951402	1.701621	0.000000

Formamide, b3lyp/aug-cc-pvqz

Electric dipole

Property at reference geometry, Unit: Debye

X= -3.8534 Y= 0.8137 Z= 0.0000

Temperature: 0K, Unit: Debye

X= -3.6653 Y= 0.8049 Z= 0.0000

Temperature: 298K, Unit: Debye

X= -3.5461 Y= 0.8208 Z= -0.0253

Internal coordinates for the Equilibrium structure (Se)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.209151	0.000000				
3	H	1.103671	2.030001	0.000000			
4	N	1.356453	2.275428	2.049815	0.000000		
5	H	2.048916	2.546548	2.960361	1.006126	0.000000	
6	H	2.063949	3.165325	2.304615	1.003425	1.733154	0.000000

Internal coordinates for the vibrationally average structure at 0K (Sz)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.211048	0.000000				
3	H	1.114227	2.040787	0.000000			
4	N	1.368187	2.286351	2.069873	0.000000		
5	H	2.045199	2.540362	2.968322	0.999833	0.000000	
6	H	2.057193	3.158351	2.308760	0.988163	1.726716	0.000000

Internal coordinates for the vibr. average structure at 298.15K (Sa)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.210273	0.000000				
3	H	1.114122	2.039611	0.000000			
4	N	1.372005	2.288983	2.073739	0.000000		
5	H	2.032601	2.526157	2.957798	0.990909	0.000000	
6	H	2.040412	3.140003	2.297588	0.969361	1.714047	0.000000

Formamide, apfd/aug-cc-pvdz

Electric dipole

Property at reference geometry, Unit: Debye

X= -3.9005 Y= 0.8047 Z= 0.0000

Temperature: 0K, Unit: Debye

X= -3.7125 Y= 0.8008 Z= 0.0000

Temperature: 298K, Unit: Debye

X= -3.6024 Y= 0.8151 Z= -0.0242

Internal coordinates for the Equilibrium structure (Se)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.215559	0.000000				
3	H	1.111637	2.041029	0.000000			
4	N	1.359266	2.285043	2.058751	0.000000		
5	H	2.053702	2.555884	2.972847	1.010155	0.000000	
6	H	2.070622	3.178934	2.314299	1.007501	1.740395	0.000000

Internal coordinates for the vibrationally average structure at 0K (Sz)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.216359	0.000000				
3	H	1.121913	2.052830	0.000000			
4	N	1.367095	2.286002	2.078751	0.000000		
5	H	2.045835	2.534766	2.980127	1.004510	0.000000	
6	H	2.062135	3.165485	2.322030	0.992810	1.734776	0.000000

Internal coordinates for the vibr. average structure at 298.15K (Sa)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.215611	0.000000				
3	H	1.121835	2.051779	0.000000			
4	N	1.370072	2.287482	2.082275	0.000000		
5	H	2.033794	2.520286	2.970488	0.996595	0.000000	
6	H	2.046202	3.147739	2.312075	0.975197	1.723056	0.000000

Formamide, apfd/aug-cc-pvtz

Electric dipole

Property at reference geometry, Unit: Debye

X= -3.8734 Y= 0.7906 Z= 0.0000

Temperature: 0K, Unit: Debye

X= -3.6653 Y= 0.7971 Z= 0.0000

Temperature: 298K, Unit: Debye

X= -3.5327 Y= 0.8155 Z= -0.0277

Internal coordinates for the Equilibrium structure (Se)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.208802	0.000000				
3	H	1.105626	2.029585	0.000000			
4	N	1.354909	2.277141	2.048304	0.000000		
5	H	2.047331	2.550096	2.959449	1.006053	0.000000	
6	H	2.062584	3.166013	2.301648	1.003244	1.732880	0.000000

Internal coordinates for the vibrationally average structure at 0K (Sz)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.207926	0.000000				
3	H	1.115642	2.042830	0.000000			
4	N	1.359229	2.265721	2.069996	0.000000		
5	H	2.032304	2.506572	2.964629	0.999429	0.000000	
6	H	2.051750	3.142819	2.315747	0.986891	1.725720	0.000000

Internal coordinates for the vibr. average structure at 298.15K (Sa)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.206931	0.000000				
3	H	1.115538	2.041783	0.000000			
4	N	1.362790	2.266881	2.074403	0.000000		
5	H	2.017512	2.487803	2.952948	0.989994	0.000000	
6	H	2.032886	3.121278	2.304368	0.965862	1.711870	0.000000

Formamide, m062x/aug-cc-pvdz

Electric dipole

Property at reference geometry, Unit: Debye

X= -3.8638 Y= 0.8867 Z= 0.0000

Temperature: 0K, Unit: Debye

X= -3.6689 Y= 0.8798 Z= 0.0000

Temperature: 298K, Unit: Debye

X= -3.5245 Y= 0.8982 Z= -0.0286

Internal coordinates for the Equilibrium structure (Se)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.211644	0.000000				
3	H	1.108224	2.036297	0.000000			
4	N	1.359045	2.275202	2.060867	0.000000		
5	H	2.048941	2.536321	2.970527	1.009916	0.000000	
6	H	2.070018	3.170290	2.319890	1.006764	1.743171	0.000000

Internal coordinates for the vibrationally average structure at 0K (Sz)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.213248	0.000000				
3	H	1.118272	2.045814	0.000000			
4	N	1.370969	2.287183	2.080097	0.000000		
5	H	2.046453	2.534742	2.977798	1.002354	0.000000	
6	H	2.058679	3.160021	2.317218	0.989640	1.734902	0.000000

Internal coordinates for the vibr. average structure at 298.15K (Sa)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.212289	0.000000				
3	H	1.118254	2.044204	0.000000			
4	N	1.375277	2.290498	2.084422	0.000000		
5	H	2.032390	2.519896	2.965825	0.991961	0.000000	
6	H	2.037493	3.137740	2.301492	0.967874	1.720782	0.000000

Formamide, m062x/aug-cc-pvtz

Electric dipole

Property at reference geometry, Unit: Debye

X= -3.8697 Y= 0.8955 Z= 0.0000

Temperature: 0K, Unit: Debye

X= -3.6646 Y= 0.8947 Z= 0.0000

Temperature: 298K, Unit: Debye

X= -3.4936 Y= 0.9171 Z= -0.0331

Internal coordinates for the Equilibrium structure (Se)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.205613	0.000000				
3	H	1.101420	2.024645	0.000000			
4	N	1.354900	2.268171	2.050158	0.000000		
5	H	2.043447	2.531956	2.957359	1.006258	0.000000	
6	H	2.063254	3.159158	2.308725	1.002904	1.735428	0.000000

Internal coordinates for the vibrationally average structure at 0K (Sz)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.207152	0.000000				
3	H	1.110787	2.033720	0.000000			
4	N	1.367395	2.280281	2.069461	0.000000		
5	H	2.038937	2.527193	2.962586	0.997789	0.000000	
6	H	2.050868	3.147390	2.305432	0.984099	1.726617	0.000000

Internal coordinates for the vibr. average structure at 298.15K (Sa)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.205986	0.000000				
3	H	1.110774	2.031951	0.000000			
4	N	1.372797	2.284490	2.074621	0.000000		
5	H	2.022533	2.509928	2.948456	0.985513	0.000000	
6	H	2.025776	3.121089	2.286233	0.958479	1.710326	0.000000

Formamide, m062x/aug-cc-pvqz

Electric dipole

Property at reference geometry, Unit: Debye

X= -3.8465 Y= 0.8770 Z= 0.0000

Temperature: 0K, Unit: Debye

X= -3.6426 Y= 0.8754 Z= 0.0000

Temperature: 298K, Unit: Debye

X= -3.4822 Y= 0.8965 Z= -0.0311

Internal coordinates for the Equilibrium structure (Se)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.204042	0.000000				
3	H	1.101075	2.022882	0.000000			
4	N	1.354304	2.266531	2.049149	0.000000		
5	H	2.042995	2.531560	2.956175	1.005535	0.000000	
6	H	2.062242	3.156839	2.307430	1.002299	1.733664	0.000000

Internal coordinates for the vibrationally average structure at 0K (Sz)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.205525	0.000000				
3	H	1.110203	2.032124	0.000000			
4	N	1.366728	2.278235	2.068022	0.000000		
5	H	2.038423	2.525922	2.961157	0.997419	0.000000	
6	H	2.051383	3.146154	2.305491	0.984319	1.725354	0.000000

Internal coordinates for the vibr. average structure at 298.15K (Sa)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.204430	0.000000				
3	H	1.110169	2.030505	0.000000			
4	N	1.371769	2.281940	2.072998	0.000000		
5	H	2.022786	2.508915	2.947901	0.986001	0.000000	
6	H	2.028725	3.122066	2.288806	0.960602	1.710219	0.000000

Formamide, mp2fc/aug-cc-pvdz

Electric dipole

Property at reference geometry, Unit: Debye

X= 3.8139 Y= 0.8287 Z= 0.0000

Temperature: 0K, Unit: Debye

X= 3.5416 Y= 0.8303 Z= 0.0000

Temperature: 298K, Unit: Debye

X= 3.1943 Y= 0.8802 Z= -0.0559

Internal coordinates for the Equilibrium structure (Se)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.228348	0.000000				
3	H	1.110501	2.054538	0.000000			
4	N	1.367904	2.299260	2.066910	0.000000		
5	H	2.061560	2.562860	2.980689	1.012459	0.000000	
6	H	2.078034	3.195319	2.321985	1.009862	1.748171	0.000000

Internal coordinates for the vibrationally average structure at 0K (Sz)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.230390	0.000000				
3	H	1.120318	2.064274	0.000000			
4	N	1.381802	2.311994	2.089180	0.000000		
5	H	2.050607	2.548487	2.982463	1.001282	0.000000	
6	H	2.061099	3.177921	2.319181	0.984036	1.735422	0.000000

Internal coordinates for the vibr. average structure at 298.15K (Sa)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.228807	0.000000				
3	H	1.120322	2.061284	0.000000			
4	N	1.391562	2.319043	2.099996	0.000000		
5	H	2.014797	2.507785	2.953536	0.978409	0.000000	
6	H	2.013416	3.126786	2.287388	0.932891	1.702705	0.000000

Formamide, mp2fc/aug-cc-pvtz

Electric dipole

Property at reference geometry, Unit: Debye

X= 3.7908 Y= 0.8205 Z= 0.0000

Temperature: 0K, Unit: Debye

X= 3.4550 Y= 0.8344 Z= 0.0000

Temperature: 298K, Unit: Debye

X= 2.8170 Y= 0.9312 Z= -0.0937

Internal coordinates for the Equilibrium structure (Se)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.217687	0.000000				
3	H	1.099854	2.035445	0.000000			
4	N	1.357831	2.281993	2.048997	0.000000		
5	H	2.047193	2.545543	2.956738	1.005568	0.000000	
6	H	2.062690	3.171125	2.302251	1.002882	1.736250	0.000000

Internal coordinates for the vibrationally average structure at 0K (Sz)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.219350	0.000000				
3	H	1.109664	2.044689	0.000000			
4	N	1.373884	2.296192	2.073480	0.000000		
5	H	2.027598	2.521139	2.951421	0.988927	0.000000	
6	H	2.036710	3.143882	2.293289	0.967084	1.717358	0.000000

Internal coordinates for the vibr. average structure at 298.15K (Sa)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.216366	0.000000				
3	H	1.109778	2.039846	0.000000			
4	N	1.392822	2.309719	2.093899	0.000000		
5	H	1.959458	2.443039	2.896120	0.947841	0.000000	
6	H	1.949443	3.050127	2.234497	0.874409	1.658345	0.000000

Formamide, mp2fc/aug-cc-pvqz

Electric dipole

Property at reference geometry, Unit: Debye

X= 3.7908 Y= 0.8208 Z= 0.0000

Temperature: 0K, Unit: Debye

X= 3.5586 Y= 0.8191 Z= 0.0000

Temperature: 298K, Unit: Debye

X= 3.3430 Y= 0.8504 Z= 0.0386

Internal coordinates for the Equilibrium structure (Se)

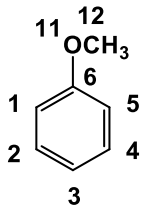
		1	2	3	4	5	6
1	C	0.000000					
2	O	1.214617	0.000000				
3	H	1.099183	2.032115	0.000000			
4	N	1.355195	2.276403	2.046809	0.000000		
5	H	2.043303	2.538875	2.953115	1.004287	0.000000	
6	H	2.059468	3.164692	2.300067	1.001557	1.734157	0.000000

Internal coordinates for the vibrationally average structure at 0K (Sz)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.216695	0.000000				
3	H	1.108925	2.042134	0.000000			
4	N	1.368102	2.288282	2.067776	0.000000		
5	H	2.034755	2.527067	2.956634	0.994970	0.000000	
6	H	2.047090	3.152082	2.299965	0.980774	1.724809	0.000000

Internal coordinates for the vibr. average structure at 298.15K (Sa)

		1	2	3	4	5	6
1	C	0.000000					
2	O	1.215592	0.000000				
3	H	1.108858	2.040282	0.000000			
4	N	1.374485	2.292809	2.074553	0.000000		
5	H	2.011833	2.501072	2.937820	0.979792	0.000000	
6	H	2.017247	3.119990	2.279647	0.948595	1.704151	0.000000



Anisole, b3lyp/aug-cc-pvtz

Electric dipole

Property at reference geometry, Unit: Debye					
X=	0.7964	Y=	1.0370	Z=	0.0000	**Total**	**1.308**
Temperature: 0K, Unit: Debye					
X=	0.7901	Y=	1.0037	Z=	0.0000	**Total**	**1.277**
Temperature: 298K, Unit: Debye					
X=	0.7680	Y=	0.9942	Z=	0.0004	**Total**	**1.256**

Internal coordinates for the Equilibrium structure (Se)

	1	2	3	4	5
1 C	0.000000				
2 C	1.393863	0.000000			
3 C	2.419400	1.386532	0.000000		
4 C	2.782622	2.397698	1.394080	0.000000	
5 C	2.414819	2.774216	2.413454	1.384370	0.000000
6 C	1.394080	2.408193	2.793410	2.409524	1.397475
7 H	1.079122	2.141892	3.389664	3.861620	3.400341
8 H	2.139223	1.081987	2.143597	3.381994	3.856175
9 H	3.864490	3.380667	2.150260	1.081890	2.134482
10 H	3.385586	3.855145	3.400531	2.154380	1.081079
11 O	2.439991	3.687461	4.154498	3.618055	2.339156
12 C	2.832643	4.225215	5.044209	4.800298	3.646194
13 H	3.893970	5.280110	6.014090	5.615701	4.348416
14 H	2.824470	4.157315	5.103283	5.036147	4.019274
15 H	2.824470	4.157314	5.103282	5.036146	4.019273
16 H	3.399053	2.146940	1.080919	2.153490	3.392873

	6	7	8	9	10
6 C	0.000000				
7 H	2.158486	0.000000			
8 H	3.383706	2.449598	0.000000		
9 H	3.386586	4.943507	4.280275	0.000000	
10 H	2.137790	4.284429	4.937049	2.477069	0.000000
11 O	1.363840	2.728885	4.571179	4.472895	2.524656
12 C	2.392432	2.542383	4.871957	5.746535	3.941254
13 H	3.262736	3.621948	5.955719	6.482698	4.404164
14 H	2.720415	2.341371	4.671938	6.022461	4.441127
15 H	2.720414	2.341371	4.671938	6.022460	4.441127
16 H	3.874329	4.280124	2.475705	2.482741	4.296390

	11	12	13	14	15	16
11 O	0.000000					
12 C	1.418333	0.000000				
13 H	2.010248	1.086586	0.000000			
14 H	2.083332	1.093058	1.777654	0.000000		
15 H	2.083332	1.093058	1.777654	1.783099	0.000000	
16 H	5.235147	6.104263	7.087535	6.119162	6.119162	0.000000

Internal coordinates for the vibrationally average structure at 0K (Sz)

		1	2	3	4	5
1	C	0.000000				
2	C	1.398248	0.000000			
3	C	2.427196	1.391229	0.000000		
4	C	2.792604	2.406445	1.398963	0.000000	
5	C	2.424130	2.784267	2.421410	1.388776	0.000000
6	C	1.398919	2.415415	2.801124	2.416546	1.402003
7	H	1.082496	2.148846	3.400700	3.874983	3.412621
8	H	2.146935	1.086311	2.151279	3.394489	3.870555
9	H	3.878537	3.393031	2.158125	1.085952	2.141779
10	H	3.397732	3.868918	3.412544	2.162400	1.084827
11	O	2.450044	3.700384	4.167061	3.627937	2.344528
12	C	2.859185	4.255795	5.072391	4.821871	3.659949
13	H	3.917729	5.307189	6.036758	5.630248	4.355616
14	H	2.857366	4.196929	5.141510	5.067180	4.040589
15	H	2.857368	4.196930	5.141510	5.067180	4.040589
16	H	3.409809	2.153709	1.084468	2.160833	3.404039

		6	7	8	9	10
6	C	0.000000				
7	H	2.166077	0.000000			
8	H	3.395248	2.458446	0.000000		
9	H	3.397508	4.960933	4.295934	0.000000	
10	H	2.144609	4.299055	4.955150	2.486826	0.000000
11	O	1.368902	2.741197	4.588653	4.485607	2.528447
12	C	2.407704	2.573309	4.908744	5.769404	3.948189
13	H	3.274476	3.652535	5.990426	6.497326	4.402998
14	H	2.740379	2.376989	4.717837	6.055262	4.455128
15	H	2.740380	2.376992	4.717839	6.055262	4.455128
16	H	3.885592	4.293810	2.483535	2.491614	4.311588

		11	12	13	14	15	16
11	O	0.000000					
12	C	1.420733	0.000000				
13	H	2.012740	1.085302	0.000000			
14	H	2.086828	1.090674	1.772651	0.000000		
15	H	2.086828	1.090674	1.772651	1.776042	0.000000	
16	H	5.251243	6.136649	7.114286	6.162302	6.162302	0.000000

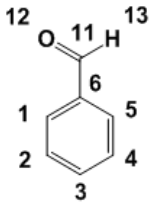
Internal coordinates for the vibr. average structure at 298.15K (Sa)

		1	2	3	4	5
1	C	0.000000				
2	C	1.396488	0.000000			
3	C	2.423276	1.389559	0.000000		
4	C	2.789205	2.405012	1.398165	0.000000	
5	C	2.422385	2.783428	2.419777	1.387555	0.000000
6	C	1.398871	2.414814	2.798514	2.414013	1.400636
7	H	1.080872	2.145351	3.395227	3.869961	3.409249
8	H	2.145376	1.085667	2.149529	3.392531	3.869073
9	H	3.873360	3.390010	2.156440	1.084175	2.138604
10	H	3.395493	3.867321	3.410441	2.161020	1.084069
11	O	2.450000	3.699230	4.164129	3.625358	2.343223
12	C	2.869331	4.263768	5.072691	4.815698	3.650748
13	H	3.914305	5.300926	6.021669	5.608544	4.332160
14	H	2.865764	4.207498	5.144113	5.060739	4.027685
15	H	2.865767	4.207500	5.144115	5.060740	4.027686
16	H	3.403710	2.149613	1.082414	2.158700	3.400624

		6	7	8	9	10
6	C	0.000000				
7	H	2.164426	0.000000			
8	H	3.394277	2.455534	0.000000		
9	H	3.393031	4.954134	4.292564	0.000000	
10	H	2.142650	4.295326	4.952910	2.483948	0.000000
11	O	1.368528	2.740316	4.587174	4.481123	2.526691
12	C	2.404862	2.591408	4.920698	5.758894	3.932437
13	H	3.258922	3.658898	5.989096	6.470753	4.373371
14	H	2.730770	2.394306	4.734897	6.044875	4.434387
15	H	2.730772	2.394311	4.734900	6.044876	4.434387
16	H	3.880928	4.286150	2.479576	2.490113	4.307989

		11	12	13	14	15	16
11	O	0.000000					
12	C	1.406224	0.000000				
13	H	1.991475	1.072788	0.000000			
14	H	2.059722	1.069364	1.746181	0.000000		
15	H	2.059722	1.069364	1.746181	1.735293	0.000000	
16	H	5.246268	6.135707	7.097678	6.165255	6.165257	0.000000

Benzaldehyde, b3lyp/aug-cc-pvtz



Electric dipole

Property at reference geometry, Unit: Debye	
X= -3.2913 Y= -1.1911 Z= -0.0000	**Total: 3.5002**
Temperature: 0K, Unit: Debye	
X= -3.2289 Y= -1.1434 Z= -0.0000	**Total: 3.425**
Temperature: 298K, Unit: Debye	
X= -3.1978 Y= -1.1314 Z= -0.0012	**Total: 3.390**

Internal coordinates for the Equilibrium structure (Se)

		1	2	3	4	5
1	C	0.000000				
2	C	1.384793	0.000000			
3	C	2.407823	1.394761	0.000000		
4	C	2.790414	2.415972	1.390309	0.000000	
5	C	2.416819	2.781758	2.402594	1.388891	0.000000
6	C	1.398135	2.408701	2.779954	2.414396	1.395244
7	H	1.081191	2.155007	3.396948	3.871400	3.388495
8	H	2.141982	1.081525	2.148951	3.393636	3.863266
9	H	3.871741	3.395948	2.147585	1.081333	2.146991
10	H	3.395587	3.864963	3.387422	2.149252	1.083242
11	C	2.501152	3.767595	4.257511	3.760141	2.480313
12	O	2.896845	4.277901	5.058386	4.794457	3.609191
13	H	3.453076	4.592232	4.814982	4.016301	2.629208
14	H	3.385936	2.148527	1.081809	2.144884	3.383051

		6	7	8	9	10
6	C	0.000000				
7	H	2.139885	0.000000			
8	H	3.390648	2.489021	0.000000		
9	H	3.395188	4.952730	4.286117	0.000000	
10	H	2.146327	4.276198	4.946482	2.479015	0.000000
11	C	1.477661	2.695065	4.640705	4.626074	2.674802
12	O	2.387450	2.606337	4.957976	5.731565	3.883783
13	H	2.184067	3.782997	5.550913	4.687794	2.351533
14	H	3.861761	4.291224	2.471447	2.471775	4.282031

		11	12	13	14
11	C	0.000000			
12	O	1.209342	0.000000		
13	H	1.108751	2.012693	0.000000	
14	H	5.339316	6.123655	5.876451	0.000000

Internal coordinates for the vibrationally average structure at 0K (Sz)

		1	2	3	4	5
1	C	0.000000				
2	C	1.389240	0.000000			
3	C	2.415308	1.399197	0.000000		
4	C	2.799652	2.424371	1.395268	0.000000	
5	C	2.425465	2.791624	2.410620	1.393123	0.000000
6	C	1.403061	2.416659	2.788445	2.421676	1.399837
7	H	1.085444	2.162458	3.408325	3.884889	3.401002
8	H	2.149514	1.085885	2.156812	3.406136	3.877491
9	H	3.885026	3.408115	2.155723	1.085379	2.153766
10	H	3.408457	3.879350	3.399619	2.156814	1.087762
11	C	2.509528	3.780538	4.272457	3.774186	2.490956
12	O	2.904847	4.290252	5.072222	4.806980	3.618108
13	H	3.463904	4.607515	4.831703	4.031227	2.640006
14	H	3.396797	2.155447	1.085609	2.152477	3.394441

		6	7	8	9	10
6	C	0.000000				
7	H	2.148052	0.000000			
8	H	3.402612	2.497549	0.000000		
9	H	3.406044	4.970265	4.302114	0.000000	
10	H	2.154509	4.292590	4.965228	2.486959	0.000000
11	C	1.484089	2.703413	4.656707	4.643458	2.687264
12	O	2.392819	2.614760	4.973575	5.747290	3.894143
13	H	2.191476	3.794297	5.569618	4.705604	2.363010
14	H	3.874052	4.305590	2.480028	2.481140	4.297212

		11	12	13	14
11	C	0.000000			
12	O	1.207216	0.000000		
13	H	1.111722	2.012632	0.000000	
14	H	5.358064	6.141304	5.897057	0.000000

Internal coordinates for the vibr. average structure at 298.15K (Sa)

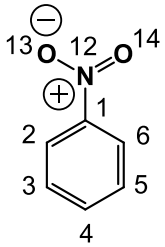
		1	2	3	4	5
1	C	0.000000				
2	C	1.387781	0.000000			
3	C	2.411738	1.397322	0.000000		
4	C	2.796687	2.422892	1.394707	0.000000	
5	C	2.424522	2.790782	2.408739	1.391144	0.000000
6	C	1.402925	2.415866	2.785814	2.419184	1.399405
7	H	1.084304	2.159235	3.403286	3.880798	3.399420
8	H	2.147578	1.085159	2.155143	3.404322	3.875924
9	H	3.880494	3.405324	2.154571	1.083812	2.149761

10	H	3.407387	3.877821	3.397014	2.154257	1.087070
11	C	2.509085	3.779139	4.269612	3.771915	2.490985
12	O	2.903961	4.287642	5.065181	4.797757	3.609715
13	H	3.454889	4.599588	4.825712	4.028797	2.639889
14	H	3.390915	2.151174	1.083316	2.150210	3.390325

		6	7	8	9	10
6	C	0.000000				
7	H	2.147468	0.000000			
8	H	3.401081	2.493616	0.000000		
9	H	3.401767	4.964606	4.299292	0.000000	
10	H	2.154110	4.291357	4.962973	2.482103	0.000000
11	C	1.483863	2.703271	4.654406	4.639465	2.688331
12	O	2.386547	2.619120	4.972130	5.735433	3.884852
13	H	2.184553	3.783569	5.559863	4.703761	2.369232
14	H	3.869128	4.298106	2.476541	2.479863	4.292439

		11	12	13	14
11	C	0.000000			
12	O	1.196770	0.000000		
13	H	1.100492	1.989304	0.000000	
14	H	5.352927	6.132269	5.889322	0.000000

Nitrobenzene, b3lyp/aug-cc-pvtz



Electric dipole

Property at reference geometry, Unit: Debye

X= 0.0000 Y= -0.0000 Z= -4.7066

Temperature: 0K, Unit: Debye

X= -0.0000 Y= 0.0000 Z= -4.6664

Temperature: 298K, Unit: Debye

X= 0.0003 Y= -0.0000 Z= -4.6435

Internal coordinates for the Equilibrium structure (Se)

		1	2	3	4	5
1	C	0.000000				
2	C	1.387820	0.000000			
3	C	2.386192	1.387820	0.000000		
4	C	2.750974	2.409169	1.391537	0.000000	
5	C	2.386192	2.791419	2.413929	1.391537	0.000000
6	C	1.387820	2.430054	2.791419	2.409169	1.387820
7	H	2.137572	1.078512	2.160327	3.397857	3.869605
8	H	3.368361	2.139699	1.080908	2.148699	3.393497
9	H	3.832398	3.387185	2.145626	1.081423	2.145626
10	H	3.368361	3.872324	3.393497	2.148699	1.080908
11	H	2.137572	3.396891	3.869605	3.397857	2.160327
12	N	1.476821	2.467360	3.735610	4.227795	3.735610
13	O	2.313451	2.718497	4.104947	4.916231	4.698534
14	O	2.313451	3.556791	4.698534	4.916231	4.104947

		6	7	8	9	10
6	C	0.000000				
7	H	3.396891	0.000000			
8	H	3.872324	2.490980	0.000000		
9	H	3.387185	4.293282	2.473088	0.000000	
10	H	2.139699	4.950501	4.286564	2.473088	0.000000
11	H	1.078512	4.269732	4.950501	4.293282	2.490980
12	N	2.467360	2.658539	4.604551	5.309219	4.604551
13	O	3.556791	2.395721	4.762780	5.975863	5.653632
14	O	2.718497	3.870726	5.653632	5.975863	4.762780

		11	12	13	14
11	H	0.000000			
12	N	2.658539	0.000000		
13	O	3.870726	1.222281	0.000000	
14	O	2.395721	1.222281	2.164783	0.000000

Internal coordinates for the vibrationally average structure at 0K (Sz)

		1	2	3	4	5
1	C	0.000000				
2	C	1.391879	0.000000			
3	C	2.392916	1.392302	0.000000		
4	C	2.758536	2.416763	1.395768	0.000000	
5	C	2.392916	2.800388	2.421428	1.395768	0.000000
6	C	1.391879	2.438094	2.800388	2.416763	1.392302
7	H	2.144486	1.082261	2.167874	3.409079	3.882312
8	H	3.378588	2.146755	1.084626	2.155594	3.404335
9	H	3.843723	3.398157	2.152472	1.085186	2.152472
10	H	3.378588	3.885011	3.404335	2.155594	1.084626
11	H	2.144486	3.408130	3.882312	3.409079	2.167874
12	N	1.485308	2.477698	3.750150	4.243844	3.750150
13	O	2.321907	2.729165	4.120024	4.932836	4.713610
14	O	2.321907	3.567626	4.713610	4.932836	4.120024

		6	7	8	9	10
6	C	0.000000				
7	H	3.408130	0.000000			
8	H	3.885011	2.499758	0.000000		
9	H	3.398157	4.307641	2.480959	0.000000	
10	H	2.146755	4.966927	4.300388	2.480959	0.000000
11	H	1.082261	4.283699	4.966927	4.307641	2.499758
12	N	2.477698	2.668477	4.621967	5.329030	4.621967
13	O	3.567626	2.405970	4.780757	5.996292	5.671683
14	O	2.729165	3.881354	5.671683	5.996292	4.780757

		11	12	13	14
11	H	0.000000			
12	N	2.668477	0.000000		
13	O	3.881354	1.223001	0.000000	
14	O	2.405970	1.223001	2.165469	0.000000

Internal coordinates for the vibr. average structure at 298.15K (Sa)

		1	2	3	4	5
1	C	0.000000				
2	C	1.388331	0.000000			
3	C	2.389454	1.391225	0.000000		
4	C	2.756479	2.412966	1.390983	0.000000	
5	C	2.389454	2.792034	2.411488	1.390983	0.000000
6	C	1.388331	2.430011	2.792034	2.412966	1.391225
7	H	2.138204	1.079659	2.165207	3.402561	3.871381
8	H	3.371086	2.142676	1.080346	2.146196	3.389996
9	H	3.839658	3.392931	2.147228	1.083178	2.147228

10	H	3.371086	3.872376	3.389996	2.146196	1.080346
11	H	2.138204	3.397681	3.871381	3.402561	2.165207
12	N	1.484821	2.475271	3.747044	4.241300	3.747044
13	O	2.310008	2.727439	4.116848	4.923785	4.697921
14	O	2.310008	3.549688	4.697921	4.923785	4.116848

		6	7	8	9	10
6	C	0.000000				
7	H	3.397681	0.000000			
8	H	3.872376	2.496592	0.000000		
9	H	3.392931	4.299921	2.471752	0.000000	
10	H	2.142676	4.951716	4.281557	2.471752	0.000000
11	H	1.079659	4.270999	4.951716	4.299921	2.496592
12	N	2.475271	2.663805	4.615423	5.324478	4.615423
13	O	3.549688	2.411080	4.778854	5.986028	5.650797
14	O	2.727439	3.858101	5.650797	5.986028	4.778854

		11	12	13	14
11	H	0.000000			
12	N	2.663805	0.000000		
13	O	3.858101	1.203693	0.000000	
14	O	2.411080	1.203693	2.124008	0.000000

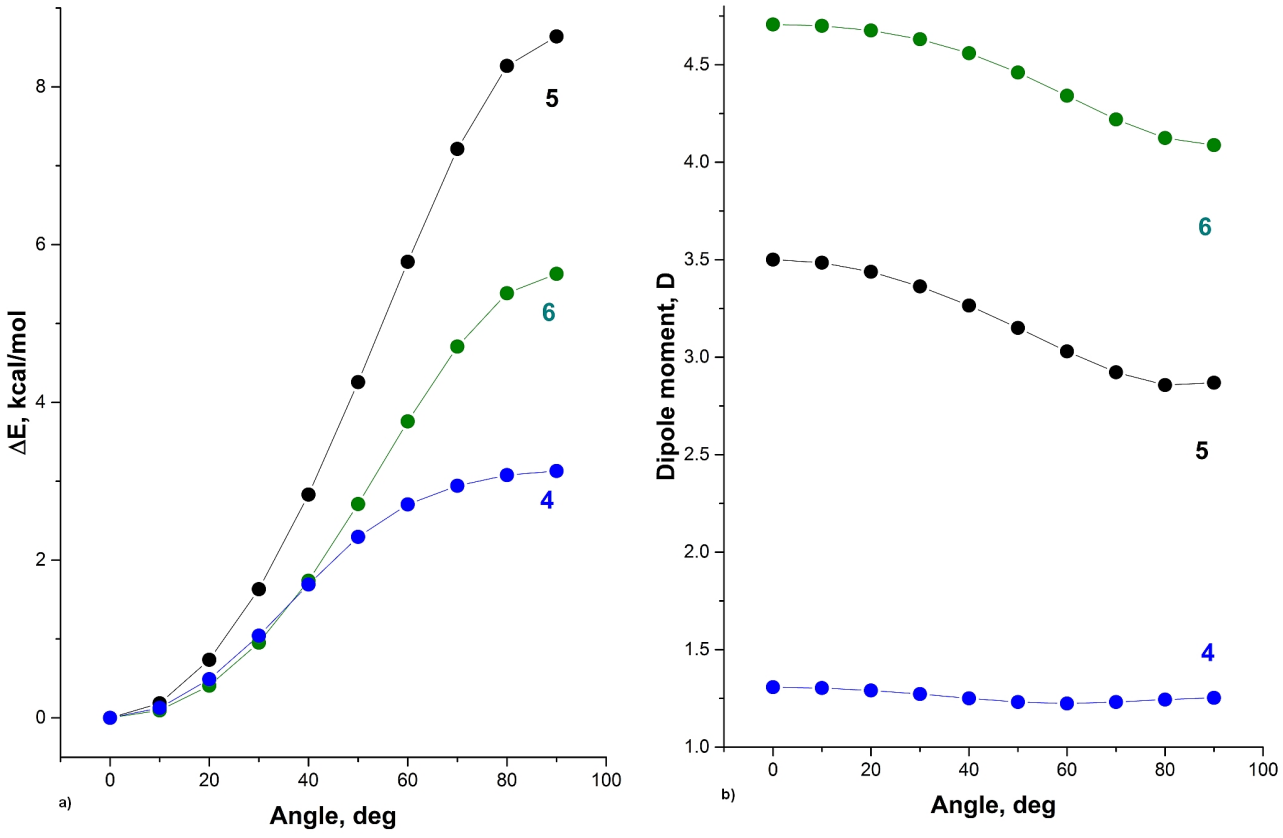


Fig. 1S. Anisole (**4**, blue), benzaldehyde (**5**, black) and nitrobenzene (**6**, green). a) PES in the gas phase; b) Dipole moments of the rotamers corresponding to PES.

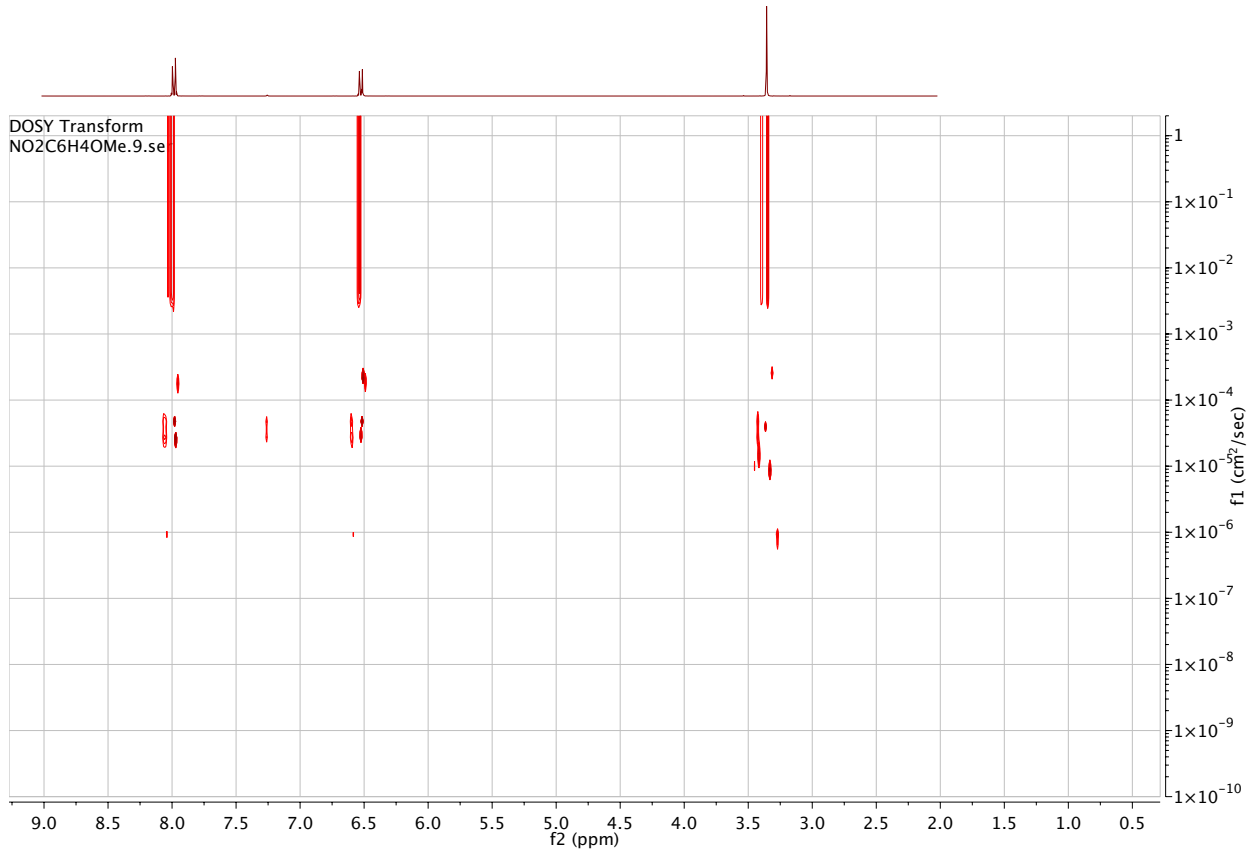


Fig. 2S. DOSY H-NMR spectrum of *p*-nitroanisole (**10**) in benzene.

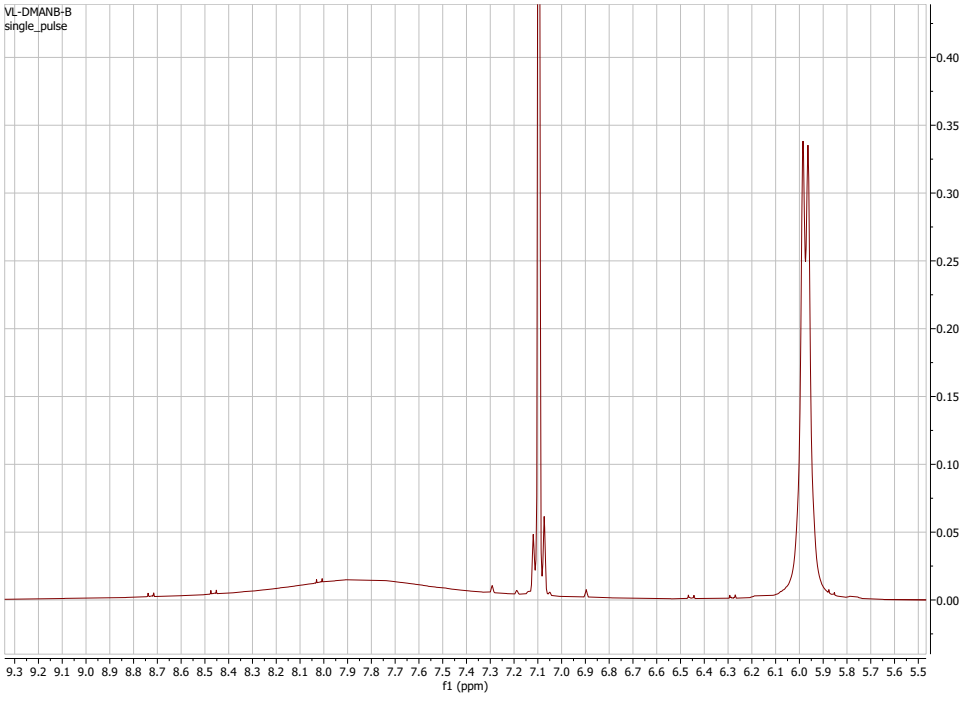


Fig. 3S. 1H-NMR spectrum of p-nitroso-N,N-dimethylaminobenzene (**14**) in benzene-d_6 at 295°C.

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