Electronic Supplementary Material (ESI) for Faraday Discussions.

On the development of a chemical shift-based scale for weak halogen bonding interactions; a ^{15}N-NMR and DFT study

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Supporting Information

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1. Observed chemical shifts

Table S1: Chemical shifts of the nitrogen and 2H in pyridine when mixed with various halogen bond donors following 5:1 stoichiometric experiments in toluene-d_8. In addition, the Hammett para-constant σ_{para} and the changes in chemical shift $\Delta\delta$ between pyridine mixed with halogen bond donors and pyridine mixed with the same equivalents of benzene are displayed. The substituents under "R" and halogens under "X" correspond to the structure displayed in Figure 1.

R	X	σ	$^{1H}\delta$ (ppm)	$^{15N}\delta$ (ppm)	$^{1H}\Delta\delta$ (ppm)	$^{15N}\Delta\delta$ (ppm)
(benzene reference)		-	*8.1997*	*-58.0056*	*0*	*0*
OCH_3	I	-0.27	7.9363	-59.2809	-0.2634	-1.2753
	Br		8.0569	-58.5915	-0.1428	-0.5859
	Cl		8.1008	-59.0427	-0.0989	-1.0371
CH_3	I	-0.17	7.9869	-58.7460	-0.2128	-0.7404
	Br		7.9647	-58.5445	-0.2350	-0.5389
	Cl		8.1434	-58.2335	-0.0563	-0.2279
H	I	0	7.9894	-58.9422	-0.2103	-0.9366
	Br		8.0756	-58.5297	-0.1241	-0.5241
	Cl		8.1442	-58.2789	-0.0555	-0.2733
F	I	0.06	7.9898	-59.0868	-0.2099	-1.0812
	Br		8.0848	-58.3691	-0.1149	-0.3635
	Cl		8.1531	-58.2873	-0.0466	-0.2817
OCF_3	I	0.35	8.0140	-60.1671	-0.1857	-2.1615
	Br		8.0989	-58.7858	-0.1008	-0.7802
	Cl		8.1600	-58.4837	-0.0397	-0.4781
CF_3	I	0.54	8.0115	-59.3602	-0.1882	-1.3546
	Br		8.0977	-58.4912	-0.1020	-0.4856
	Cl		8.1504	-58.2889	-0.0493	-0.2833
(C_6F_5)	I	-	7.7945	-67.0214	-0.4052	-9.0158
	Br		7.9728	-59.1034	-0.2269	-1.0978
	Cl		8.0309	-58.2871	-0.1688	-0.2815

Table S2: Chemical shifts of the nitrogen and 2H in pyridine when mixed with various halogen bond donors following 5:1 stoichiometric experiments in acetonitrile-d_3. In addition, the Hammett para-constant σ_{para} and the changes in chemical shift $\Delta\delta$ between pyridine mixed with halogen bond donors and pyridine mixed with the same equivalents of benzene are displayed. The substituents under "R" and halogens under "X" correspond to the structure displayed in FIgure 1.

R	X	σ	$^{1H}\delta$ (ppm)	$^{15N}\delta$ (ppm)	$^{1H}\Delta\delta$ (ppm)	$^{15N}\Delta\delta$ (ppm)
(benzene reference)		-	9.0142	-60.7775	*0*	*0*
OCH_3	I	-0.27	8.4538	-61.1981	0.5605	0.4206
	Br		8.6299	-60.5959	0.3844	-0.1816
	Cl		8.5376	-60.4980	0.4766	-0.2795
CH_3	I	-0.17	8.4794	-60.6136	0.5348	-0.1639
	Br		8.4786	-60.1747	0.5357	-0.6028
	Cl		8.6642	-60.4805	0.3500	-0.2970
H	I	0	8.5464	-60.4733	0.4679	-0.3042
	Br		8.6284	-60.4523	0.3858	-0.3252
	Cl		8.5665	-60.5222	0.4477	-0.2553
F	I	0.06	8.5251	-60.9733	0.4892	0.1959
	Br		8.6160	-60.7238	0.3982	-0.0537
	Cl		8.6798	-60.6732	0.3344	-0.1043
OCF_3	I	0.35	8.6628	-61.3577	0.3514	0.5803
	Br		8.5883	-60.5150	0.4260	-0.2625
	Cl		8.6433	-60.3475	0.3710	-0.4300
CF_3	I	0.54	8.4714	-61.3331	0.5428	0.5557
	Br		8.5530	-61.2109	0.4612	0.4334
	Cl		8.6428	-60.4614	0.3714	-0.3161
(C_6F_5)	I	-	8.3456	-66.5245	0.6686	5.7471
	Br		8.4560	-61.5097	0.5583	0.7322
	Cl		8.5090	-60.8302	0.5053	0.0527

Table S3: Chemical shifts of the nitrogen and 2H in pyridine when mixed with various halogen bond donors following 5:1 stoichiometric experiments in DMSO-d_3. In addition, the Hammett para-constant σ_{para} and the changes in chemical shift Δδ between pyridine mixed with halogen bond donors and pyridine mixed with the same equivalents of benzene are displayed. The substituents under "R" and halogens under "X" correspond to the structure displayed in Figure 1.

R	X	σ	^{1H}δ (ppm)	^{15N}δ (ppm)	^{1H}Δδ (ppm)	^{15N}Δδ (ppm)
(benzene reference)		-	8.7467	-60.6011	*0*	*0*
OCH_3	I	-0.27	8.2698	-60.9608	-0.4770	-0.3597
	Br		8.3851	-60.7012	-0.3616	-0.1001
	Cl		8.4675	-60.6346	-0.2792	-0.0336
CH_3	I	-0.17	8.3422	-60.1871	-0.4046	0.4140
	Br		8.4405	-59.9424	-0.3063	0.6587
	Cl		8.5454	-60.1418	-0.2014	0.4593
H	I	0	8.3361	-60.7310	-0.4106	-0.1299
	Br		8.4301	-60.5691	-0.3167	0.0320
	Cl		8.5233	-60.4072	-0.2235	0.1939
F	I	0.06	8.3196	-60.4930	-0.4271	0.1081
	Br		8.4160	-60.6623	-0.3307	-0.0612
	Cl		8.4810	-60.5853	-0.2658	0.0158
OCF_3	I	0.35	8.3089	-60.2588	-0.4378	0.3423
	Br		8.3960	-60.0950	-0.3508	0.5061
	Cl		8.4615	-58.0799	-0.2853	0.5212
CF_3	I	0.54	8.2951	-60.6759	-0.4517	-0.0749
	Br		8.3688	-60.2988	-0.3779	0.3023
	Cl		8.4324	-60.0330	-0.3144	0.5681
(C_6F_5)	I	-	8.1254	-63.4702	-0.6213	-2.8692
	Br		8.2554	-60.6733	-0.4914	-0.0723
	Cl		8.3334	-60.3015	-0.4133	0.2996

Table S4: Chemical shifts of the nitrogen and 2H in pyridine when mixed with various iodobenzenes following 3:1 stoichiometric experiments in toluene-d_8. In addition, the Hammett para-constant σ_{para} and the changes in chemical shift $\Delta\delta$ between pyridine mixed with halogen bond donors and pyridine mixed with the same equivalents of benzene are displayed. The substituents under "R" and halogens under "X" correspond to the structure displayed in Figure 1.

R	σ	$^{1H}\delta$ (ppm)	$^{15N}\delta$ (ppm)	$^{1H}\Delta\delta$ (ppm)	$^{15N}\Delta\delta$ (ppm)
(benzene reference)	-	8.1920	-58.1670	0	0.0280
		8.1920	-58.1975	0	-0.0025
		8.1930	-58.2215	0.0010	-0.0265
OCH_3	-0.27	8.0130	-58.9105	-0.1790	-0.7155
		8.0145	-58.9320	-0.1775	-0.7370
		8.0145	-58.9245	-0.1775	-0.7295
CH_3	-0.17	8.0345	-58.5035	-0.1575	-0.3085
		8.0350	-58.5780	-0.1570	-0.3830
		8.0335	-58.5600	-0.1585	-0.3650
H	0	8.0325	-58.7680	-0.1595	-0.5730
		8.0315	-58.7795	-0.1605	-0.5845
		8.0335	-58.7845	-0.1585	-0.5895
F	0.06	8.0495	-58.8340	-0.1425	-0.6390
		8.0465	-58.8560	-0.1455	-0.6610
		8.0495	-58.8720	-0.1425	-0.6770
Cl	0.23	8.0155	-58.9225	-0.1765	-0.7035
		8.0145	-58.9905	-0.1775	-0.7715
		8.0080	-58.9855	-0.1840	-0.7665
OCF_3	0.35	8.0540	-59.0215	-0.1380	-0.8265
		8.0550	-59.0095	-0.1370	-0.8145
		8.0565	-59.0075	-0.1355	-0.8125
CF_3	0.54	8.0535	-59.0510	-0.1385	-0.8560
		8.0535	-59.0220	-0.1385	-0.8270
		8.0515	-59.0175	-0.1405	-0.8225

R	σ	^{1H}δ (ppm)	^{15N}δ (ppm)	^{1H}Δδ (ppm)	^{15N}Δδ (ppm)
OCH_2CH_3	-0.24	8.0295	-58.9870	-0.1625	-0.7680
		8.0250	-58.9905	-0.1670	-0.7715
		8.0270	-59.0170	-0.1650	-0.7980

Table S5: Chemical shifts of the nitrogen and 2H in pyridine when mixed with various para-substituted phenols following 3:1 stoichiometric experiments in toluene-d_8. In addition, the Hammett para-constant σ_{para} and the changes in chemical shift $\Delta\delta$ between pyridine mixed with halogen bond donors and pyridine mixed with the same equivalents of benzene are displayed. The substituents under "R" and halogens under "X" correspond to the structure displayed in Figure 1.

R	σ	$^{1H}\delta$ (ppm)	$^{15N}\delta$ (ppm)	$^{1H}\Delta\delta$ (ppm)	$^{15N}\Delta\delta$ (ppm)
(benzene reference)	-	8.1920	-58.1670	0	0.0280
		8.1920	-58.1975	0	-0.0025
		8.1930	-58.2215	0.0010	-0.0265
OCH_3	-0.27	7.8045	-82.4545	-0.3875	-24.2595
		7.8090	-82.4065	-0.3830	-24.2115
		7.8045	-82.5245	-0.3875	-24.3295
CH_3	-0.17	7.7790	-83.2410	-0.4130	-25.0460
		7.7840	-82.8600	-0.4080	-24.6650
		7.7810	-83.0940	-0.4110	-24.8990
H	0	7.7140	-84.2600	-0.4780	-26.0650
		7.7170	-84.2125	-0.4750	-26.0175
		7.7150	-84.2760	-0.4770	-26.0810
F	0.06	7.7260	-85.5895	-0.4660	-27.3945
		7.7240	-85.6455	-0.4680	-27.4505
		7.7260	-85.5625	-0.4660	-27.3675
Cl	0.23	7.6485	-86.6055	-0.5435	-28.4105
		7.6510	-86.4915	-0.5410	-28.2965
		7.6515	-86.4055	-0.5405	-28.2105
OCF_3	0.35	7.6945	-86.8615	-0.4975	-28.6665
		7.6945	-86.9165	-0.4975	-28.7215
		7.6990	-86.7195	-0.4930	-28.5245

R	σ	^{1H}δ (ppm)	^{15N}δ (ppm)	^{1H}Δδ (ppm)	^{15N}Δδ (ppm)
CF_3	0.54	7.7060	-88.5670	-0.4860	-30.3720
		7.7160	-87.5290	-0.4760	-29.3340
		7.7090	-88.2060	-0.4830	-30.0110
OCH_2CH_3	-0.24	7.8175	-82.1410	-0.3745	-23.9460
		7.8140	-82.2675	-0.3780	-24.0725
		7.8150	-82.0470	-0.3770	-23.8520
(C_6F_5)	-	7.7140	-124.790	-0.4780	-66.5950

2. Computed electronic energies, Gibbs free energies, BSSE, NAP, chemical shifts and complexations shifts

Table S6: Calculated absolute electronic energies E_e, Gibbs free energies $G(298)$, and basis set superposition errors BSSE for the compounds investigated in this study. The substituents under "R" and halogens under "X" correspond to the structure displayed in Figure 1. All values are given in Hartree units.

		E_e	$G(298)$			
Pyridine		-248.27556669	-248.214115			
		Halobenzene		Halobenzene-pyridine complex		
X	R	E_e	$G(298)$	E_e	$G(298)$	BSSE
I	H	-7150.87892577	-7150.820668	-7399.15920688	-7399.026576	0.000679
	OCH_3	-7265.40209411	-7265.315926	-7513.68201593	-7513.520539	0.000662
	OCH_2CH_3	-7304.71769091	-7304.605868	-7552.99755110	-7552.810152	0.000660
	CH_3	-7190.19304383	-7190.109950	-7438.47308046	-7438.315201	0.000655
	$CH(CH_3)_2$	-7268.81371240	-7268.678721	-7517.09363449	-7516.884324	0.000576
	F	-7250.12236332	-7250.073702	-7498.40323600	-7498.279570	0.000706
	Cl	-7610.44454720	-7610.398106	-7858.72558324	-7858.604047	0.000706
	OCF_3	-7563.16097268	-7563.102881	-7811.44200808	-7811.307596	0.000672
	$COOCH_3$	-7378.76322051	-7378.669884	-7627.04416581	-7626.875390	0.000681
	$COCH_3$	-7303.52753299	-7303.438180	-7551.80861151	-7551.644139	0.000670
	CF_3	-7487.94206436	-7487.884464	-7736.22341853	-7736.090498	0.000705
	CN	-7243.12232060	-7243.068202	-7491.40422390	-7491.274551	0.000698
	NO_2	-7355.39158801	-7355.335520	-7603.67386110	-7603.542469	0.000716
Br	H	-2805.60842779	-2805.548950	-3053.88644195	-3053.751489	0.000458
	OCH_3	-2920.13113367	-2920.043692	-3168.40894100	-3168.248143	0.000454
	OCH_2CH_3	-2959.44673102	-2959.333564	-3207.72448027	-3207.537645	0.000443
	CH_3	-2844.92239987	-2844.839932	-3093.20023672	-3093.041703	0.000419
	$CH(CH_3)_2$	-2923.54302209	-2923.406888	-3171.82081334	-3171.607753	0.000411

	F	-2904.85164392	-2904.801751	-3153.13011375	-3153.007568	0.000499
	Cl	-3265.17389558	-3265.126233	-3513.45247580	-3513.331944	0.000477
	OCF_3	-3217.89105812	-3217.831740	-3466.16987472	-3466.036571	0.000454
	$COOCH_3$	-3033.49273543	-3033.398101	-3281.77130994	-3281.603225	0.000439
	$COCH_3$	-2958.25706885	-2958.166790	-3206.53574851	-3206.371637	0.000432
	CF_3	-3142.67154520	-3142.612745	-3390.95045364	-3390.817558	0.000447
	CN	-2897.85188795	-2897.796529	-3146.13114342	-3146.002321	0.000456
	NO_2	-3010.12114760	-3010.063804	-3258.40070619	-3258.269789	0.000486
Cl	H	-691.80292038	-691.741711	-940.07960339	-939.944792	0.000643
	OCH_3	-806.32538231	-806.236138	-1054.60194562	-1054.440848	0.001060
	OCH_2CH_3	-845.64099789	-845.525847	-1093.91750095	-1093.730744	0.000650
	CH_3	-731.11682767	-731.032574	-979.39336250	-979.236786	0.000618
	$CH(CH_3)_2$	-809.73744491	-809.599625	-1058.01400536	-1057.805301	0.000644
	F	-791.04604457	-790.994402	-1039.32304625	-1039.197216	0.000690
	Cl	-1151.36836738	-1151.318266	-1399.64544579	-1399.522156	0.000674
	OCF_3	-1104.08557295	-1104.024480	-1352.36289519	-1352.225634	0.000736
	$COOCH_3$	-919.68734883	-919.591177	-1167.96448198	-1167.797118	0.000661
	$COCH_3$	-844.45170183	-844.359858	-1092.72889164	-1092.565212	0.000661
	CF_3	-1028.86611429	-1028.805566	-1277.14351629	-1277.011746	0.000702
	CN	-784.04652810	-783.989401	-1032.32414890	-1032.192173	0.000699
	NO_2	-896.31581271	-896.256697	-1144.59363475	-1144.459770	0.000703

Table S7: The calculated change of the natural atomic population (NAP) of the pyridine N atom, Δn(N), the π part Δn_π(N) of Δn(N), and the changes of the NAP at the halogen atoms Δ(nX) (X = I, Br, Cl) in the molecules investigated in this study. Δn(N) and Δn_π(N) are given relative to free pyridine, Δn(X) relative to the corresponding compound with R = H. For the Δn(X), the notations C and H refer to the halobenzene-pyridine complex and the free halobenzene, respectively. All values scaled by a factor of 100. The substituents under "R" and halogens under "X" correspond to the structure displayed in Figure 1.

	X = I				X = Br				X = Cl			
	$100 \cdot \Delta n$(N)	$100 \cdot \Delta n_\pi$(N)	$100 \cdot \Delta n$(I)		$100 \cdot \Delta n$(N)	$100 \cdot \Delta n_\pi$(N)	$100 \cdot \Delta n$(Br)		$100 \cdot \Delta n$(N)	$100 \cdot \Delta n_\pi$(N)	$100 \cdot \Delta n$(Cl)	
R			C	H			C	H			C	H
H	0.80	2.03	0.00	0.00	0.11	0.76	0.00	0.00	-0.31	0.04	0.00	0.00
OCH_3	0.71	1.90	-0.13	0.59	0.02	0.68	0.65	0.62	-0.38	-0.02	0.67	0.62
OCH_2CH_3	0.69	1.87	-0.16	0.69	0.01	0.67	0.77	0.75	-0.39	-0.03	0.77	0.73
CH_3	0.72	1.91	-0.12	0.48	0.04	0.69	0.50	0.44	-0.37	-0.01	0.47	0.42
$CH(CH_3)_2$	0.71	1.90	-0.13	0.49	0.03	0.68	0.49	0.50	-0.37	-0.01	0.46	0.43
F	0.97	2.28	0.25	-0.95	0.26	0.92	-0.80	-0.86	-0.20	0.13	-0.71	-0.75
Cl	1.03	2.35	0.32	-1.47	0.32	0.98	-1.32	-1.31	-0.15	0.18	-1.23	-1.22
OCF_3	1.05	2.40	0.37	-1.53	0.41	1.09	-1.83	-1.41	-0.07	0.26	-1.68	-1.14
$COOCH_3$	1.05	2.36	0.33	-2.19	0.35	1.00	-2.01	-1.94	-0.12	0.21	-1.92	-1.75
$COCH_3$	1.09	2.41	0.38	-2.40	0.39	1.04	-2.22	-2.17	-0.09	0.23	-2.11	-1.91
CF_3	1.17	2.55	0.52	-2.62	0.47	1.15	-2.45	-2.47	-0.02	0.29	-2.34	-2.18
CN	1.31	2.75	0.72	-3.65	0.60	1.28	-3.47	-3.39	0.09	0.39	-3.20	-3.00
NO_2	1.43	2.91	0.88	-4.71	0.71	1.40	-4.36	-4.29	0.18	0.47	-4.04	-3.83

Table S8: The calculated chemical shielding σ and the change in chemical shift upon complexation Δδ at the N atom and the *ortho* H atom in the pyridine moiety for the halobenzene-pyridine complexes investigated in this study. Δδ given relative to the chemical shift in free pyridine. For free pyridine, the calculated shielding values are $\sigma(^{15}N)$ = –99.6517 and $\sigma(^{1}H)$ = 22.5326. All values are given in ppm. The substituents under "R" and halogens under "X" correspond to the structure displayed in Figure 1.

	X = I				X = Br				X = Cl			
R	$\sigma(^{15}N)$	$\sigma(^{1}H)$	$\Delta\delta(^{15}N)$	$\Delta\delta(^{1}H)$	$\sigma(^{15}N)$	$\sigma(^{1}H)$	$\Delta\delta(^{15}N)$	$\Delta\delta(^{1}H)$	$\sigma(^{15}N)$	$\sigma(^{1}H)$	$\Delta\delta(^{15}N)$	$\Delta\delta(^{1}H)$
H	-95.7897	22.5871	-3.8620	-0.0545	-99.5788	22.5018	-0.0729	0.0308	-101.8064	22.4686	2.1547	0.0640
OCH_3	-96.3123	22.5921	-3.3394	-0.0595	-99.9298	22.5118	0.2781	0.0208	-102.0816	22.4787	2.4299	0.0539
OCH_2CH_3	-96.3388	22.5918	-3.3129	-0.0592	-99.9801	22.5117	0.3284	0.0209	-102.1045	22.4792	2.4528	0.0534
CH_3	-96.1964	22.5932	-3.4553	-0.0606	-99.8518	22.5126	0.2001	0.0200	-102.012	22.4782	2.3603	0.0544
$CH(CH_3)_2$	-96.5561	22.6039	-3.0956	-0.0713	-99.7967	22.5093	0.1450	0.0233	-101.974	22.4747	2.3223	0.0579
F	-94.8637	22.6071	-4.7880	-0.0745	-98.8562	22.5229	-0.7955	0.0097	-101.3641	22.4866	1.7124	0.0460
Cl	-94.4717	22.6135	-5.1800	-0.0809	-98.5006	22.5309	-1.1511	0.0017	-101.1319	22.493	1.4802	0.0396
OCF_3	-94.3032	22.6083	-5.3485	-0.0757	-98.2464	22.5291	-1.4053	0.0035	-100.9009	22.4962	1.2492	0.0364
$COOCH_3$	-94.3236	22.5988	-5.3281	-0.0662	-98.3306	22.5157	-1.3211	0.0169	-100.9815	22.4772	1.3298	0.0554
$COCH_3$	-94.3101	22.5988	-5.3416	-0.0662	-98.1702	22.5165	-1.4815	0.0161	-100.9063	22.4775	1.2546	0.0551
CF_3	-93.6587	22.6050	-5.9930	-0.0724	-97.7201	22.5222	-1.9316	0.0104	-100.647	22.4819	0.9953	0.0507
CN	-92.8231	22.6192	-6.8286	-0.0866	-96.9877	22.5352	-2.6640	-0.0026	-100.1296	22.4933	0.4779	0.0393
NO_2	-92.1983	22.6154	-7.4534	-0.0828	-96.6463	22.5298	-3.0054	0.0028	-99.7796	22.4887	0.1279	0.0439

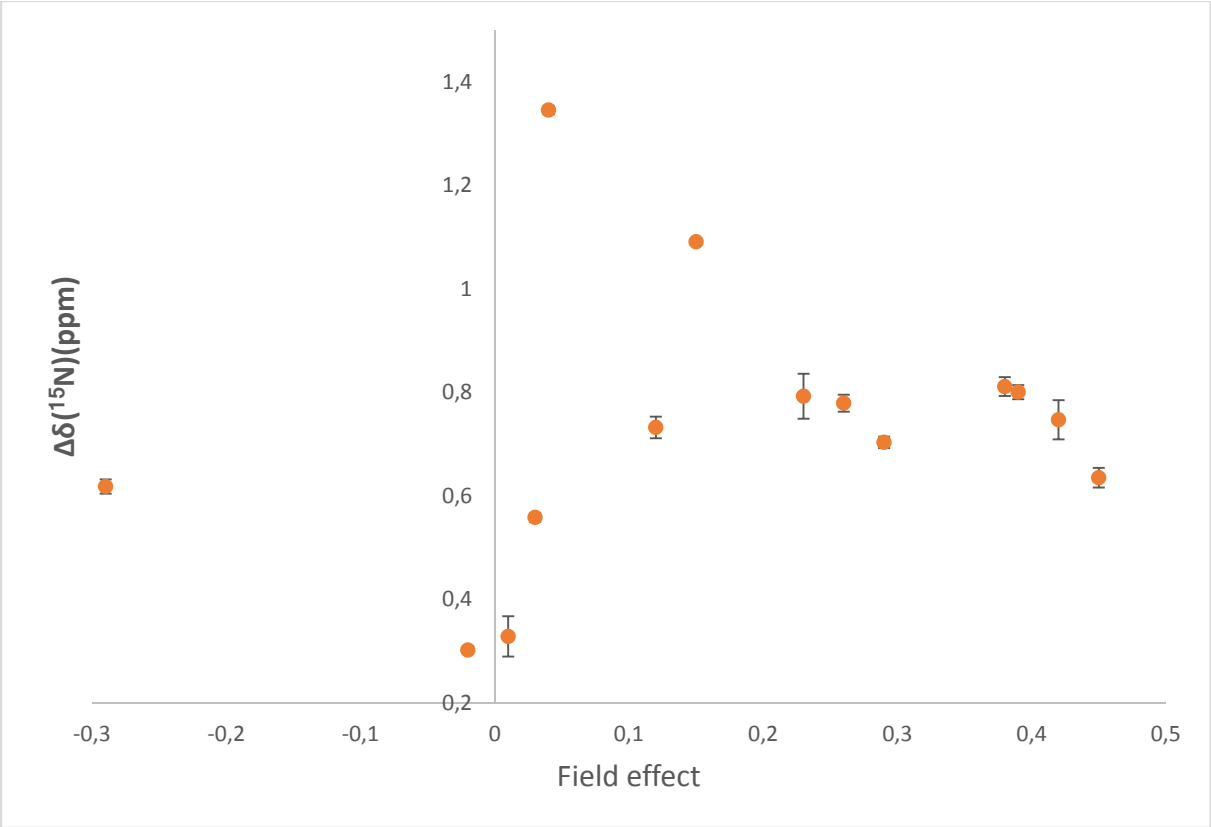

Figure S1. Plot of the change in ^{15}N chemical shift against Swain-Lupton field effect for the various para-substituted iodobenzenes.

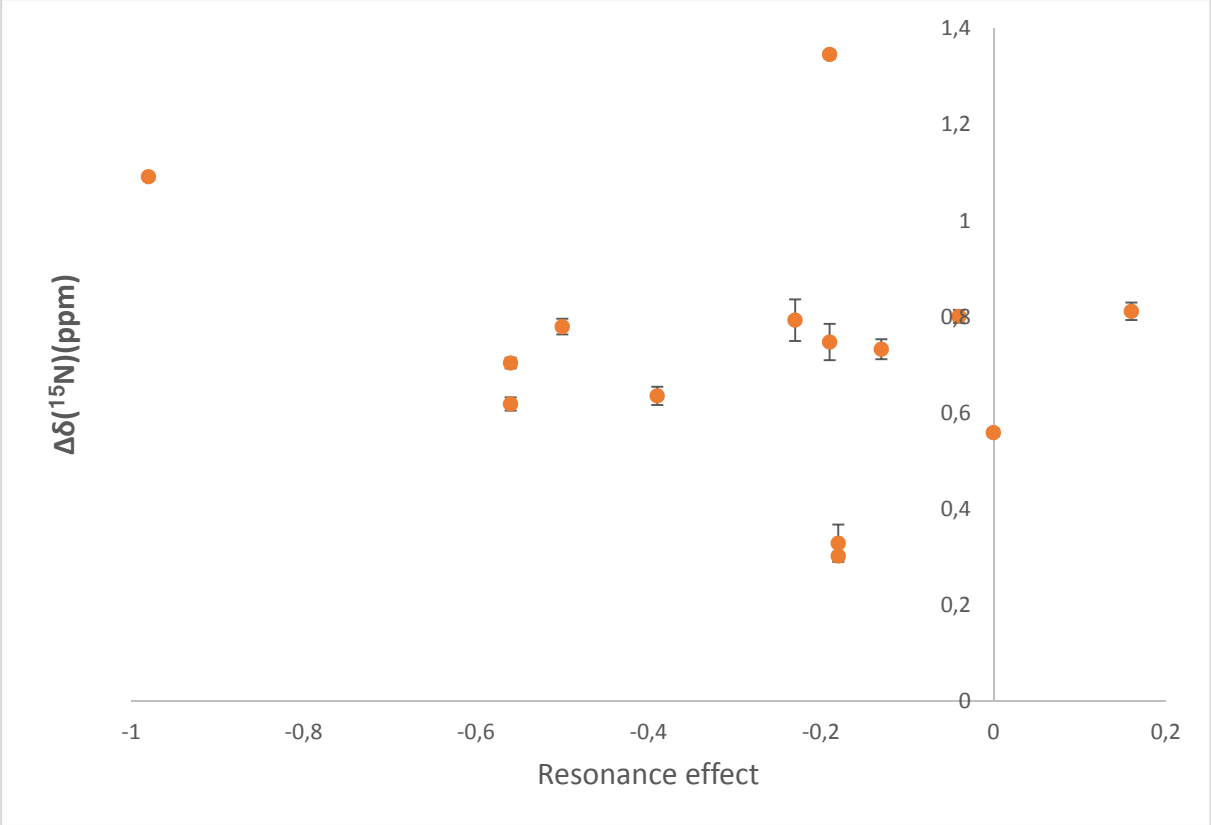

Figure S2. Plot of the change in ^{15}N chemical shift against Swain-Lupton resonance effect for the various para-substituted iodobenzenes.

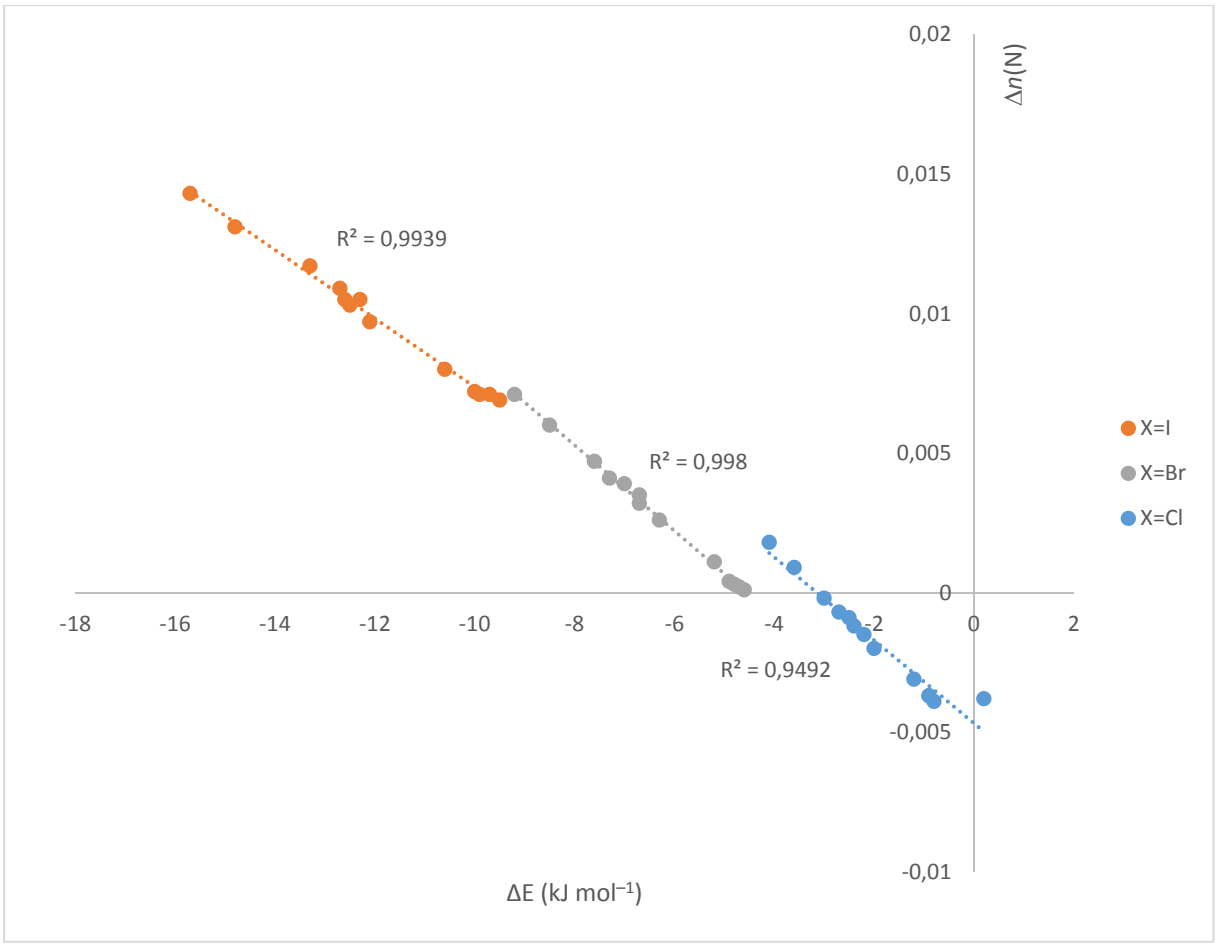

Figure S3. Plot of Δn(N) against ΔE for a series of iodo-, bromo- and chlorobenzenes (see table S7), and the R^2-values for their linear correlation.

3. NMR spectra (pyridine:halobenzene 1:5 mixtures)

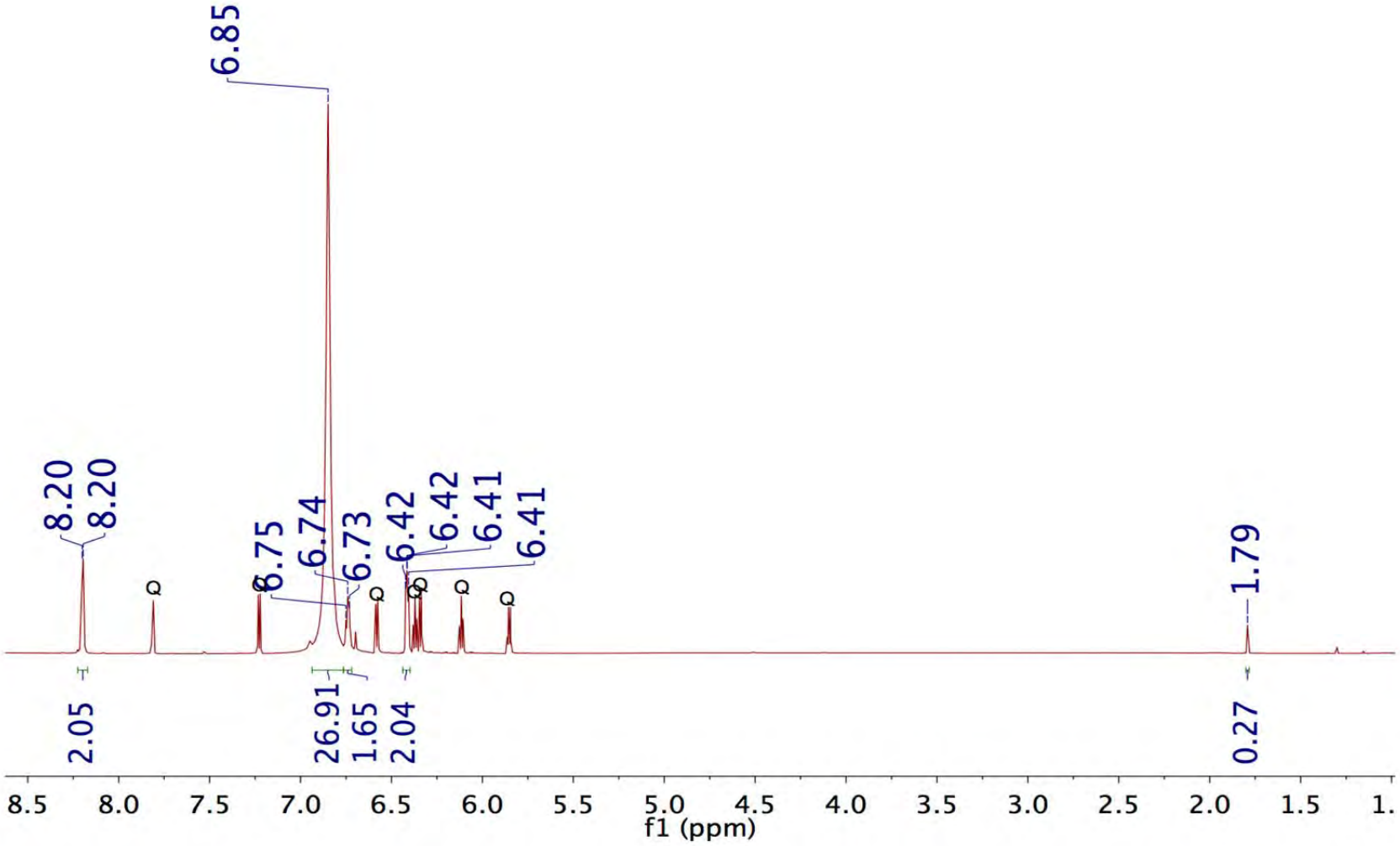

Figure S4: The ^{1}H NMR-spectrum of pyridine mixed with 5 equivalents of benzene in toluene-*d8*. Quinoline peaks are highlighted with "Q".

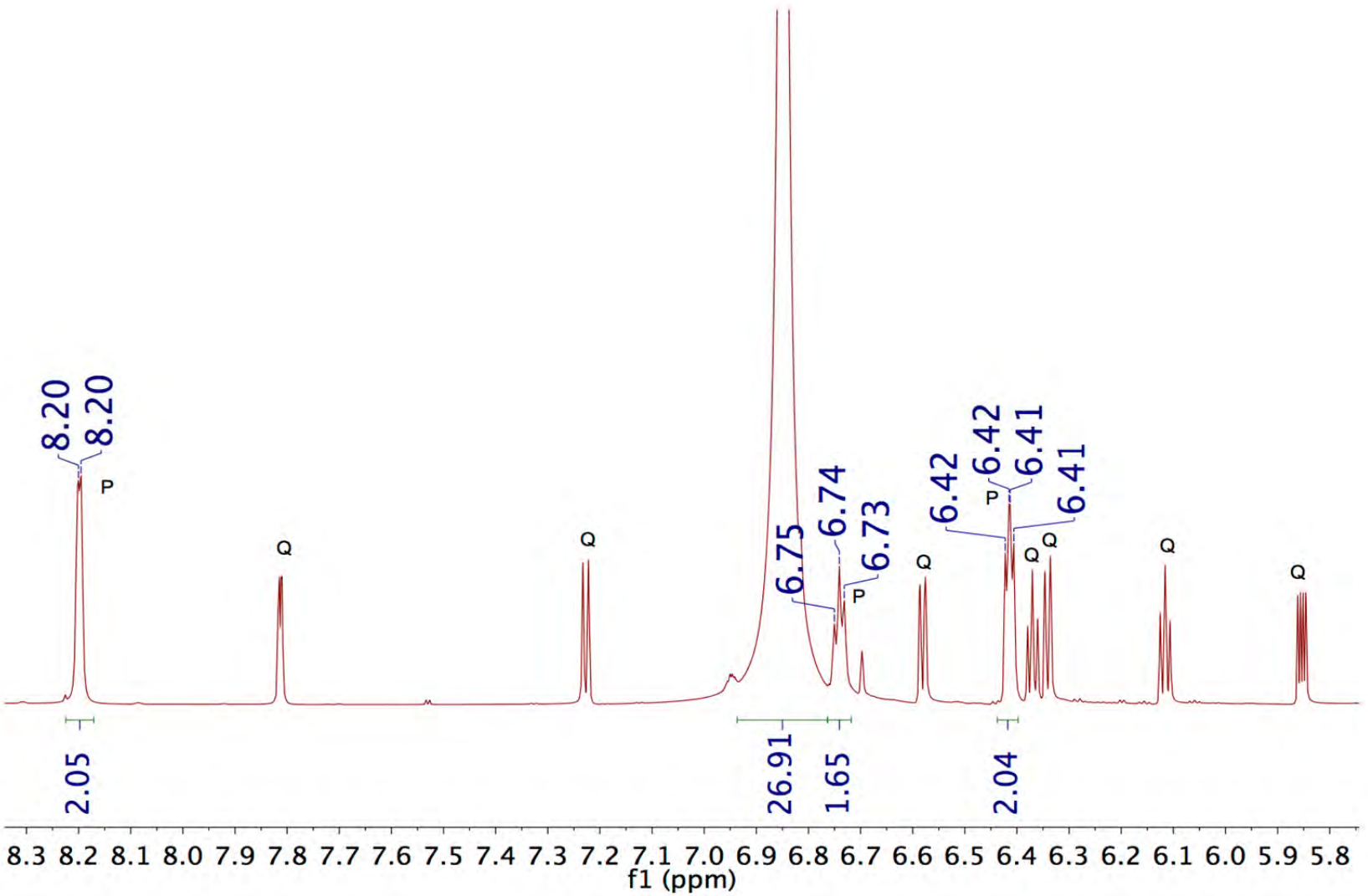

Figure S5: The aromatic region of the ^{1}H NMR-spectrum of pyridine mixed with 5 equivalents of benzene in toluene-*d8*. Quinoline and pyridine peaks are highlighted with "Q" and "P", respectively.

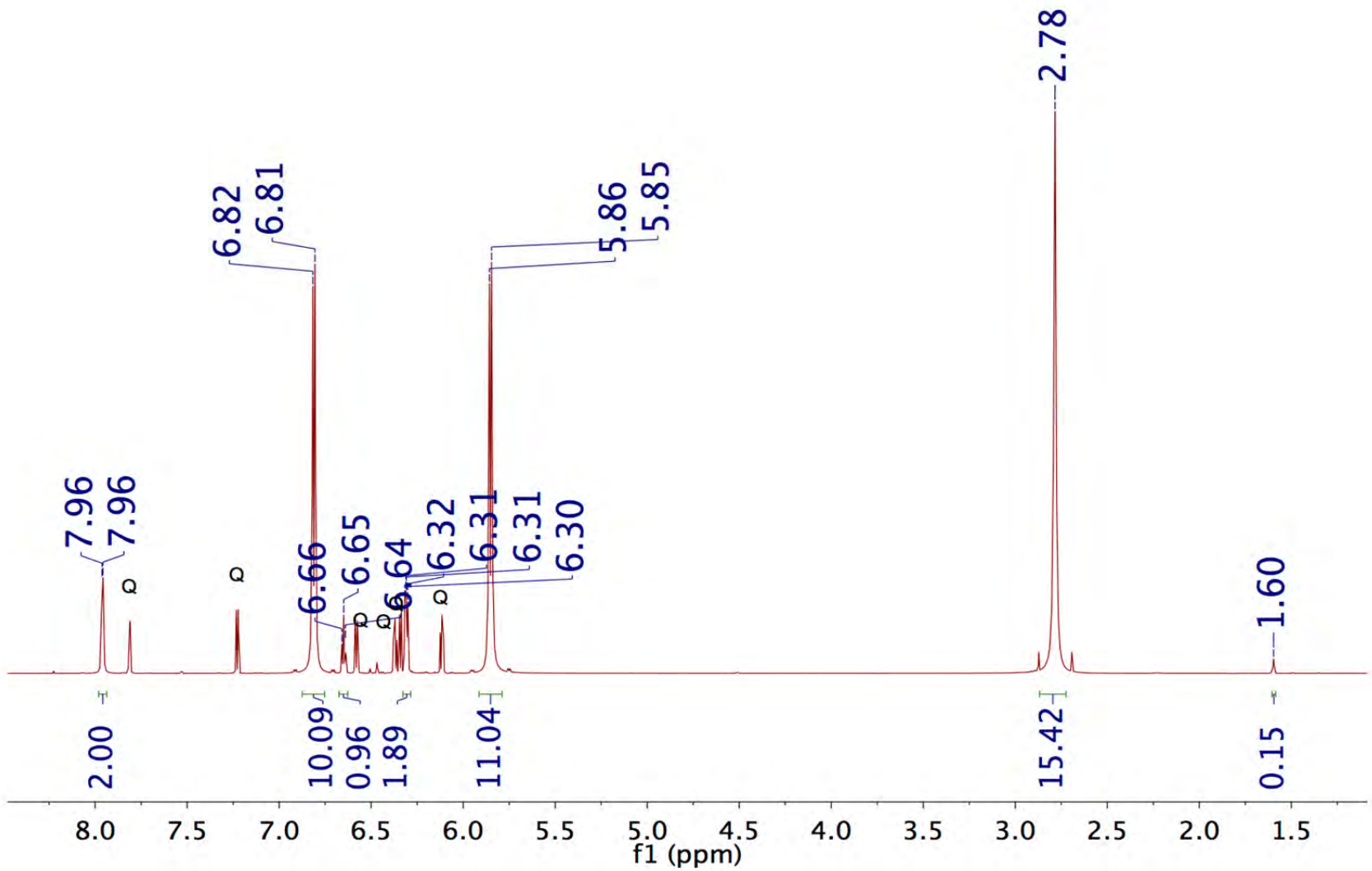

Figure S6: The 1H NMR-spectrum of pyridine mixed with 5 equivalents of 4-iodoanisole in toluene-*d8*. Quinoline peaks are highlighted with "Q".

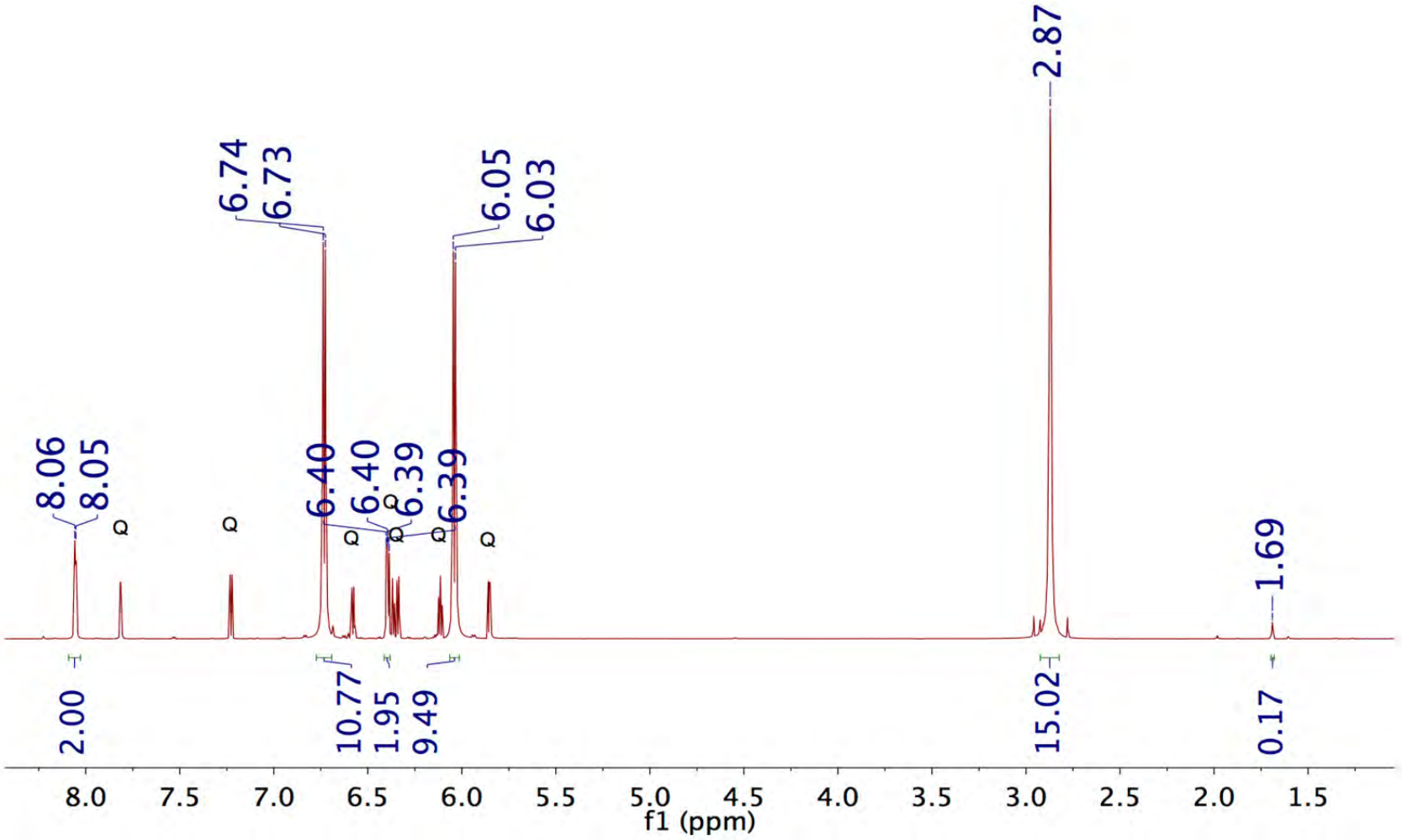

Figure S7: The 1H NMR-spectrum of pyridine mixed with 5 equivalents of 4-bromoanisole in toluene-*d8*. Quinoline peaks are highlighted with "Q".

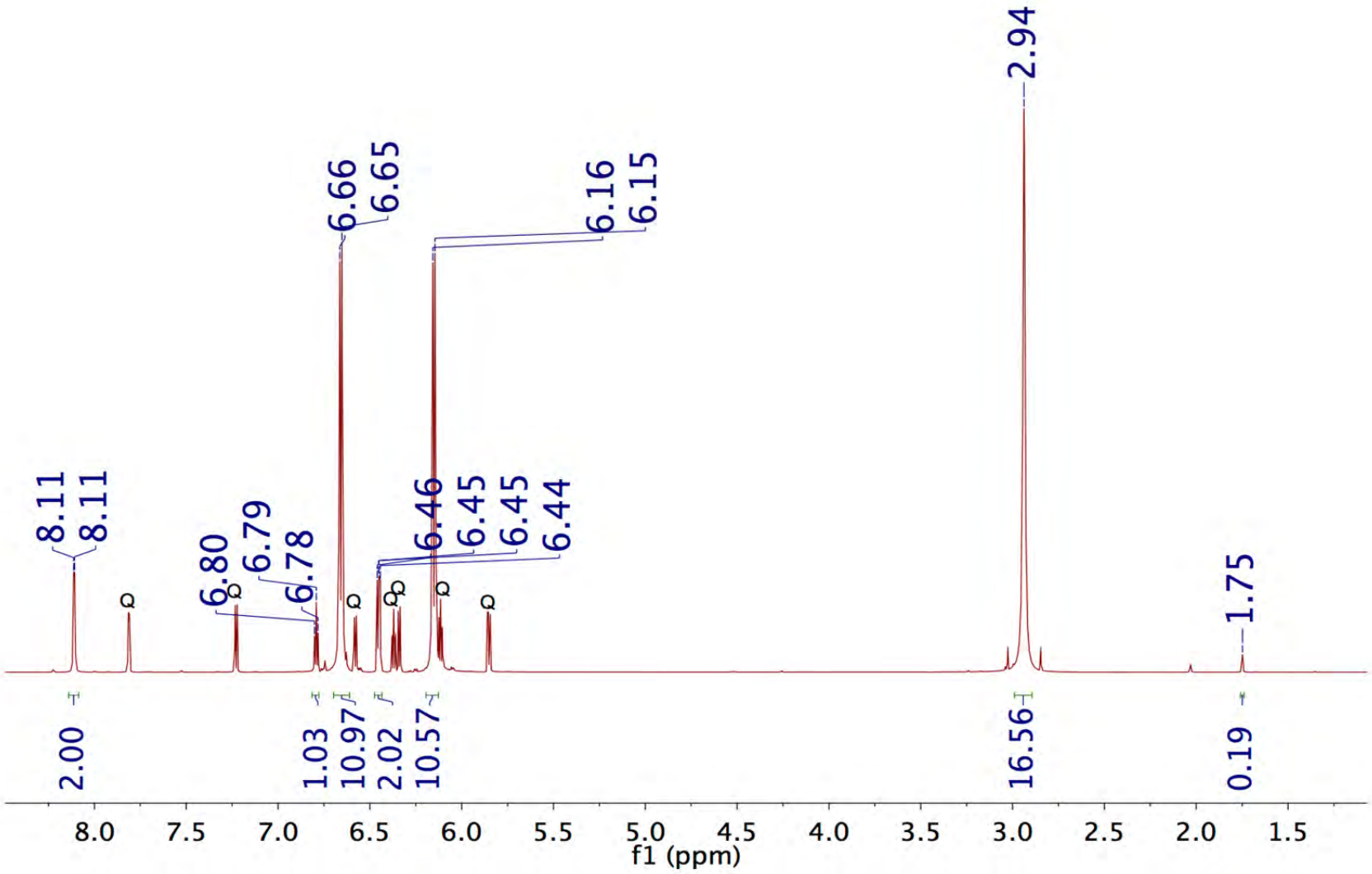

Figure S8: The 1H NMR-spectrum of pyridine mixed with 5 equivalents of 4-chloroanisole in toluene-*d8*. Quinoline peaks are highlighted with "Q".

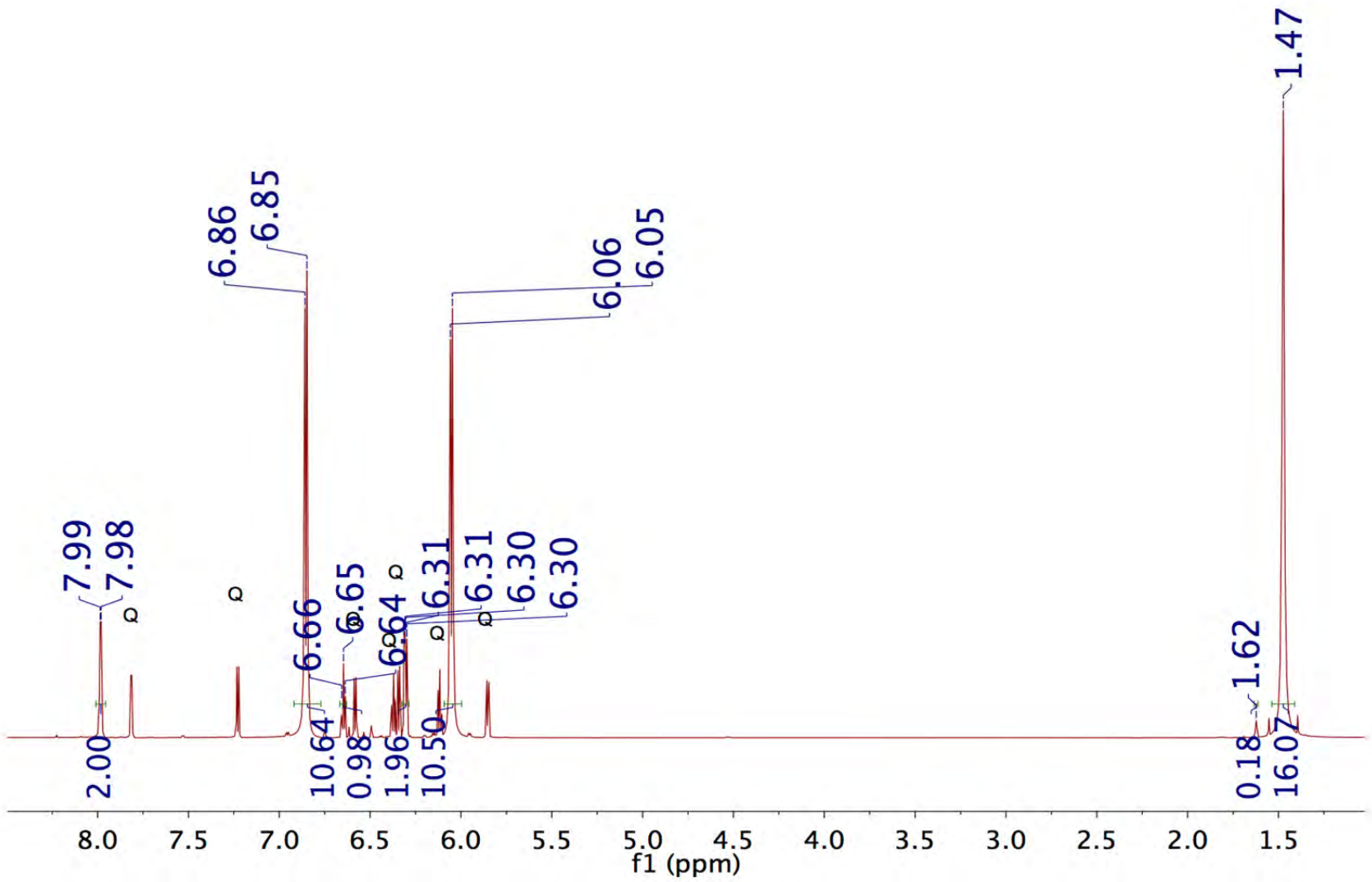

Figure S9: The 1H NMR-spectrum of pyridine mixed with 5 equivalents of 4-iodotoluene in toluene-*d8*. Quinoline peaks are highlighted with "Q".

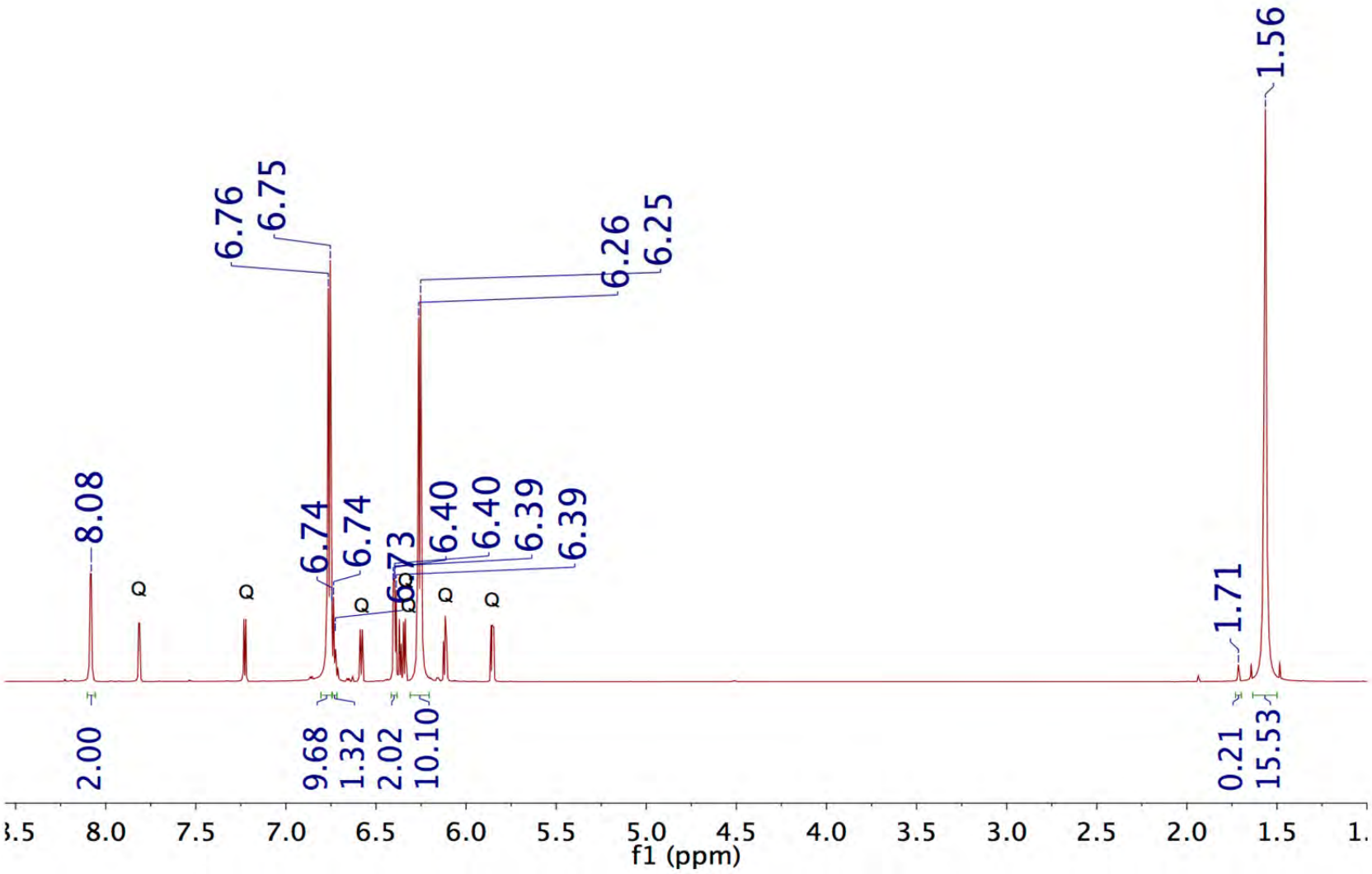

Figure S10: The 1H NMR-spectrum of pyridine mixed with 5 equivalents of 4-bromotoluene in toluene-*d8*. Quinoline peaks are highlighted with "Q".

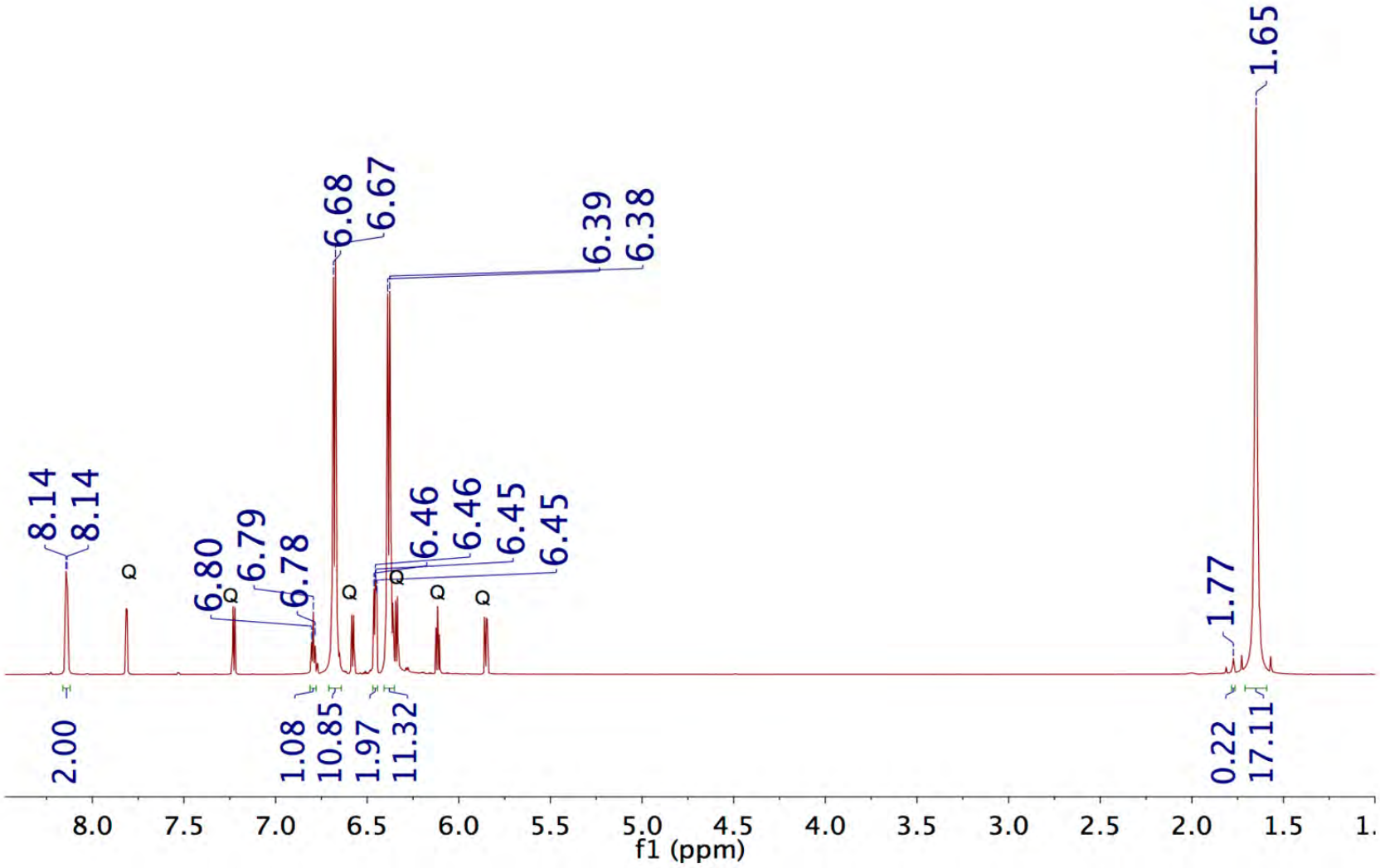

*Figure S7:*The 1H NMR-spectrum of pyridine mixed with 5 equivalents of 4-chlorotoluene in toluene-*d8*. Quinoline peaks are highlighted with "Q".

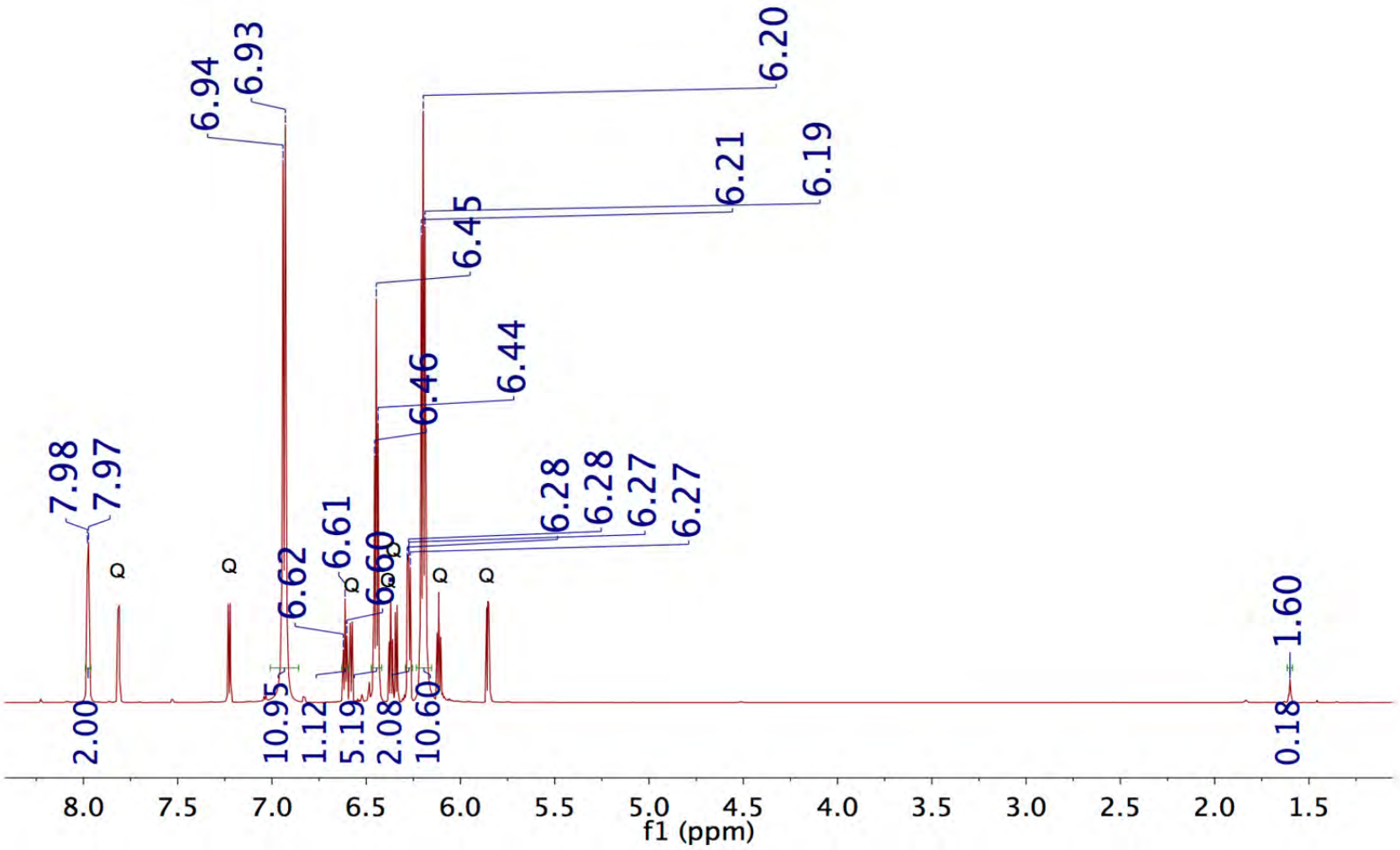

*Figure S8:*The 1H NMR-spectrum of pyridine mixed with 5 equivalents of 4-iodobenzene in toluene-*d8*. Quinoline peaks are highlighted with "Q".

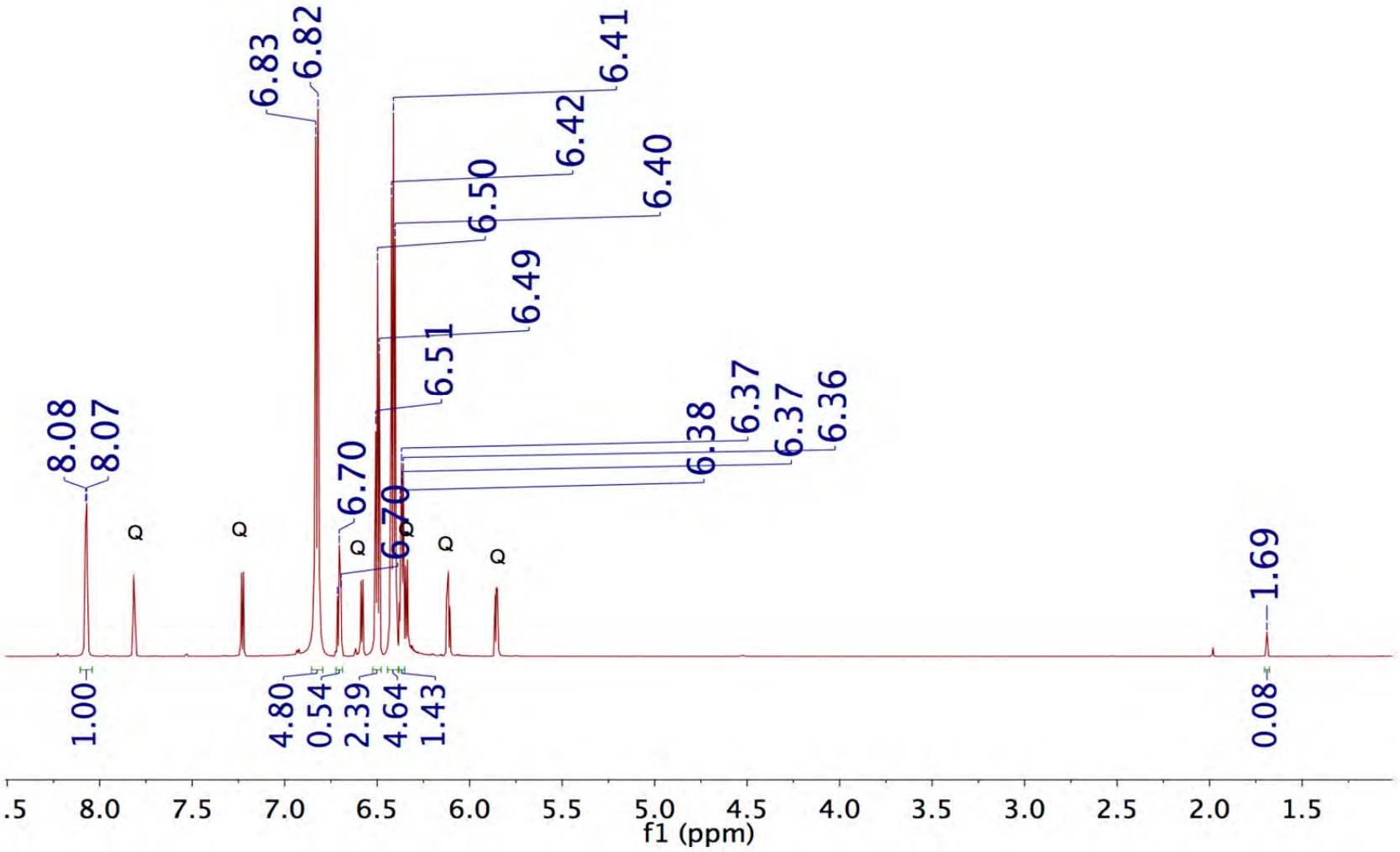

*Figure S9:*The 1H NMR-spectrum of pyridine mixed with 5 equivalents of 4-bromobenzene in toluene-*d8*. Quinoline peaks are highlighted with "Q".

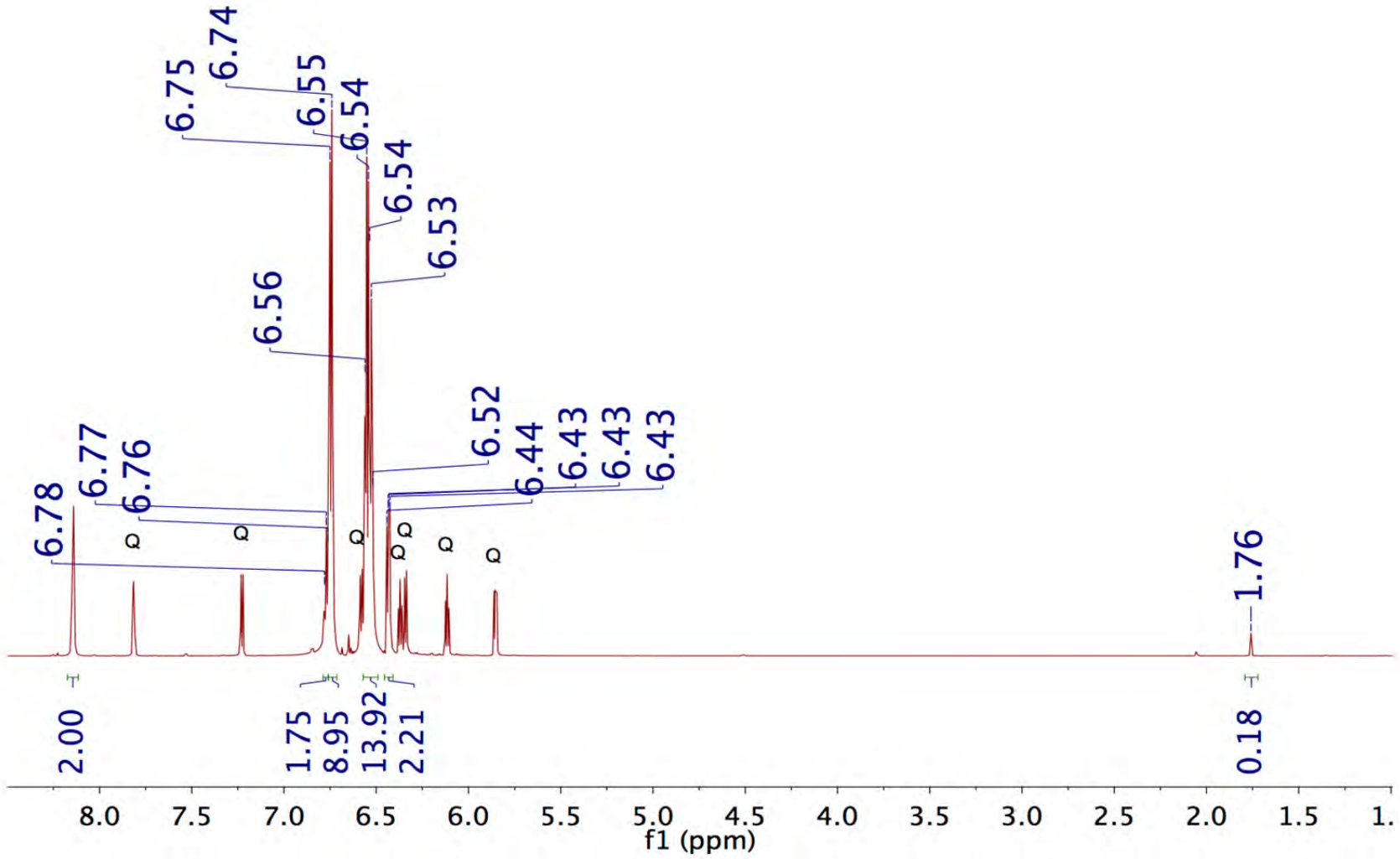

Figure S10: The 1H NMR-spectrum of pyridine mixed with 5 equivalents of 4-chlorobenzene in toluene-*d8*. Quinoline peaks are highlighted with "Q".

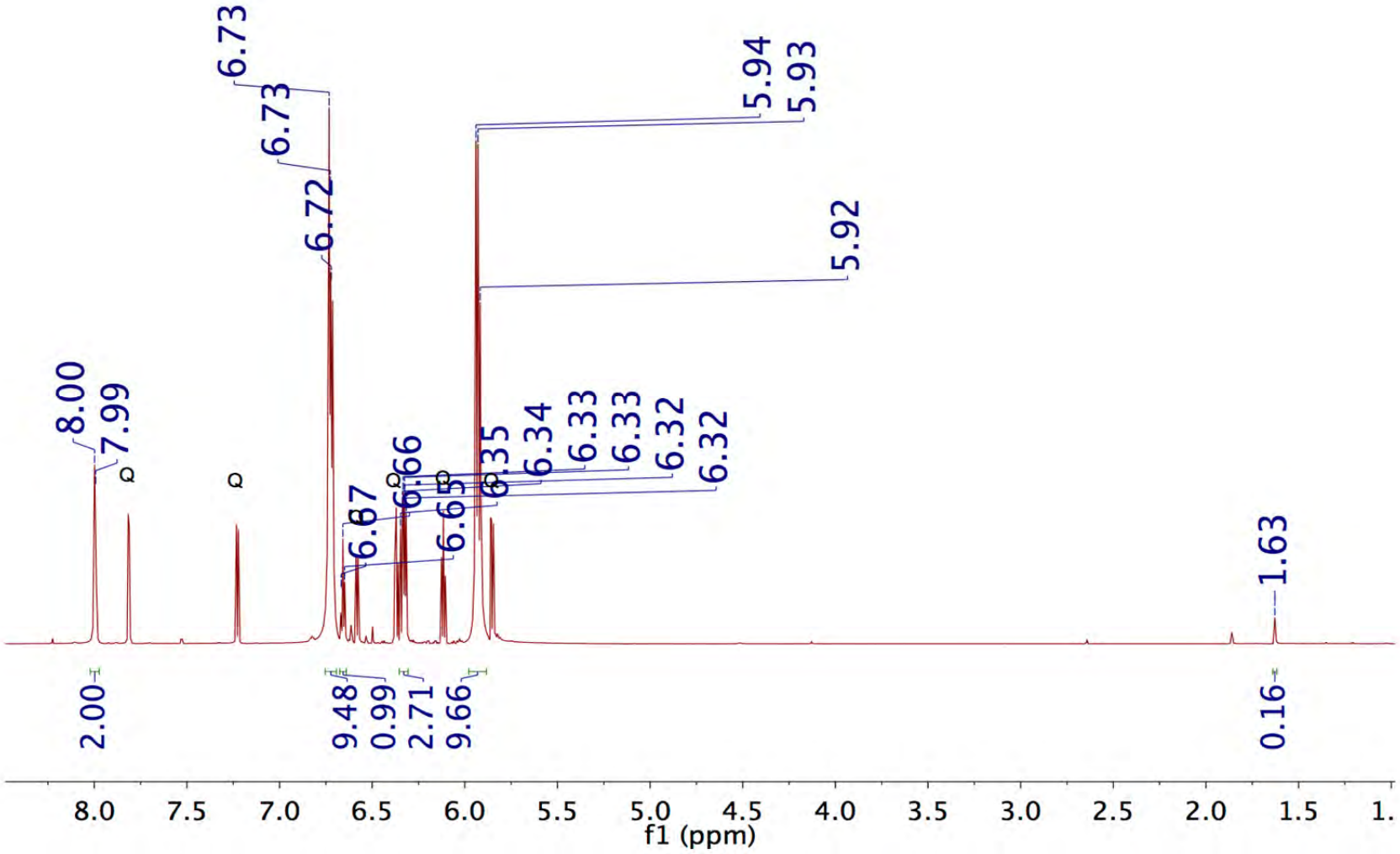

Figure S11: The 1H NMR-spectrum of pyridine mixed with 5 equivalents of 4-fluoroiodobenzene in toluene-*d8*. Quinoline peaks are highlighted with "Q".

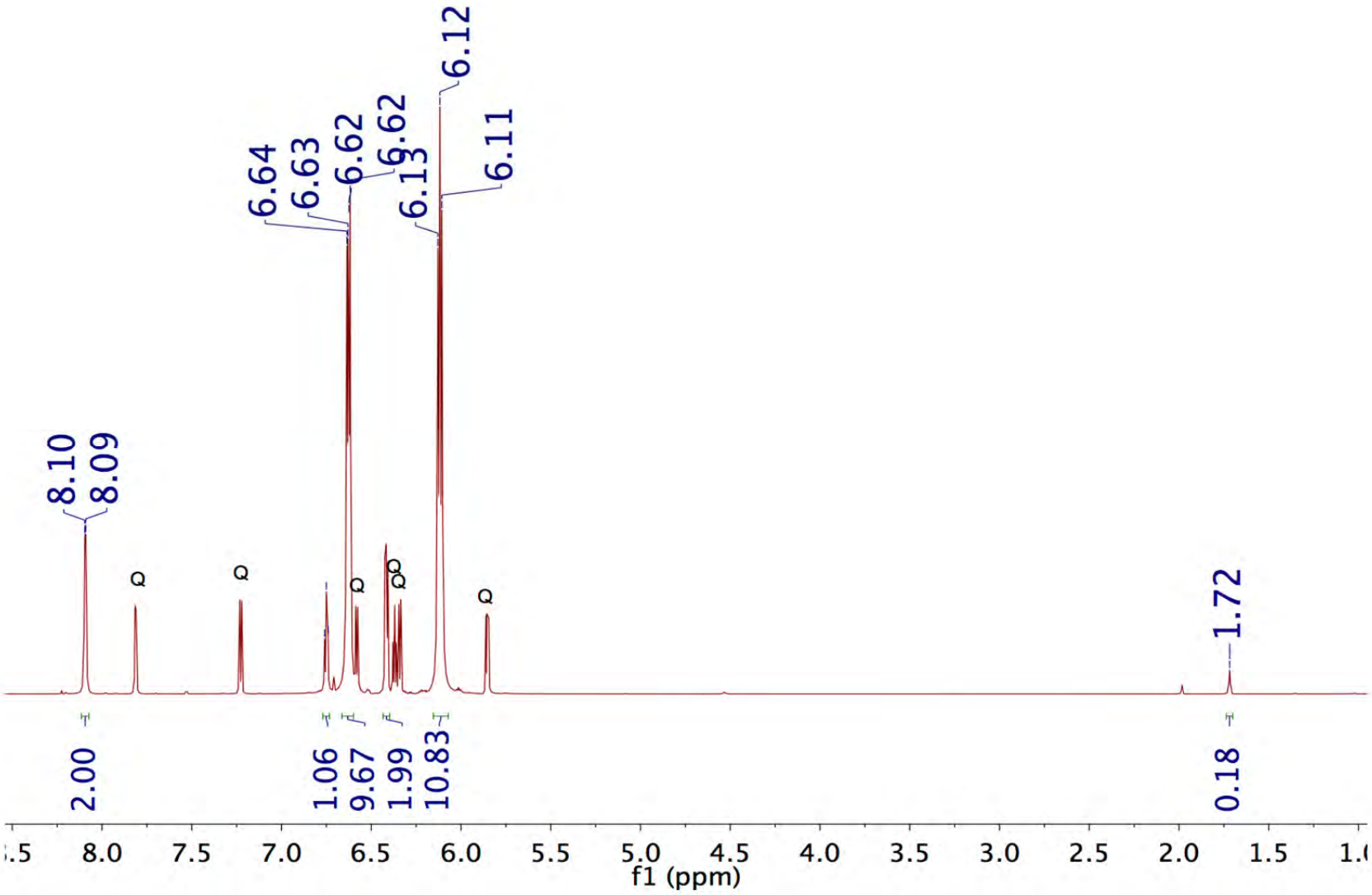

Figure S12: The 1H NMR-spectrum of pyridine mixed with 5 equivalents of 4-bromofluorobenzene in toluene-*d8*. Quinoline peaks are highlighted with "Q".

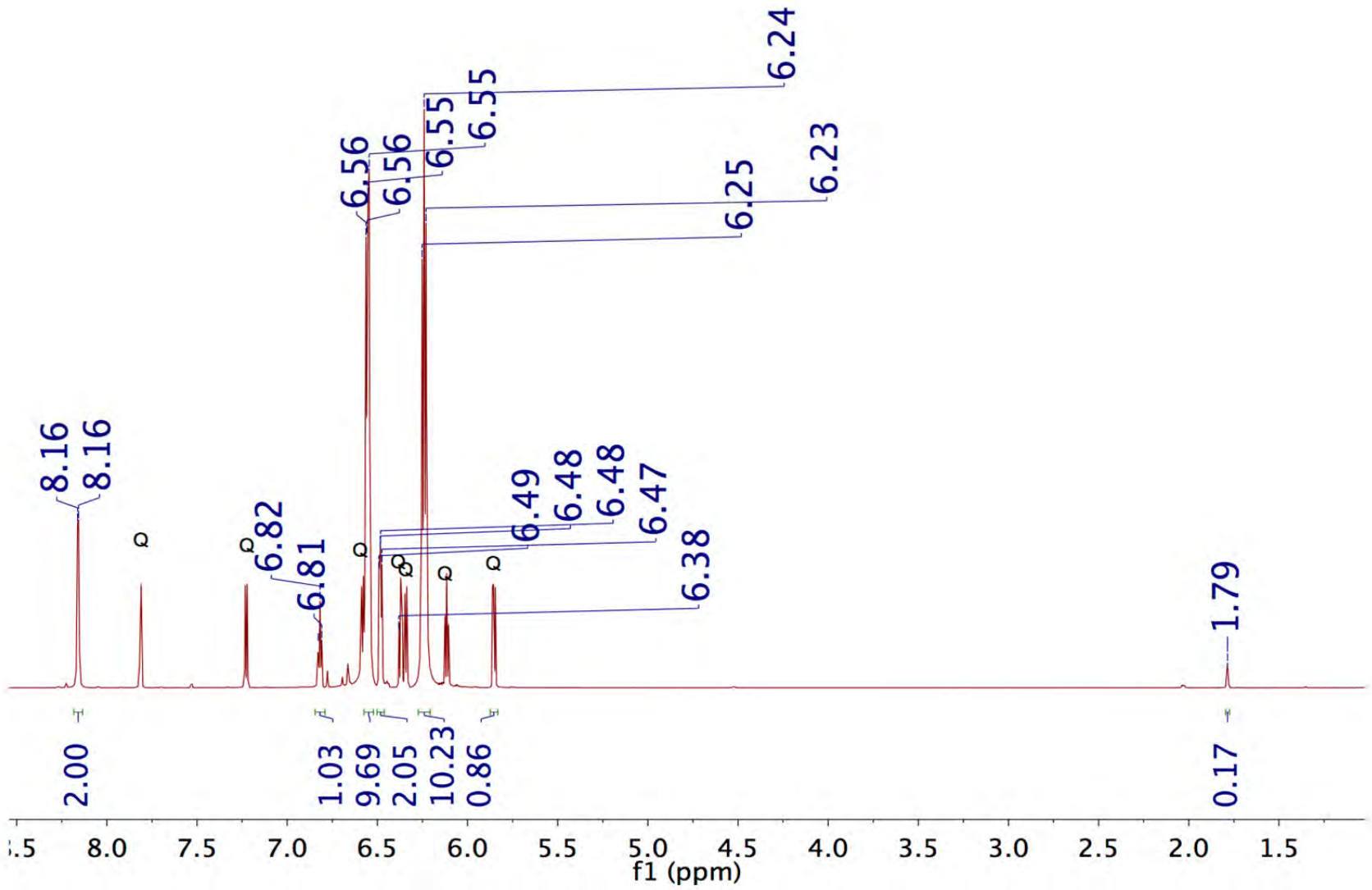

Figure S13: The 1H NMR-spectrum of pyridine mixed with 5 equivalents of 4-chlorofluorobenzene in toluene-*d8*. Quinoline peaks are highlighted with "Q".

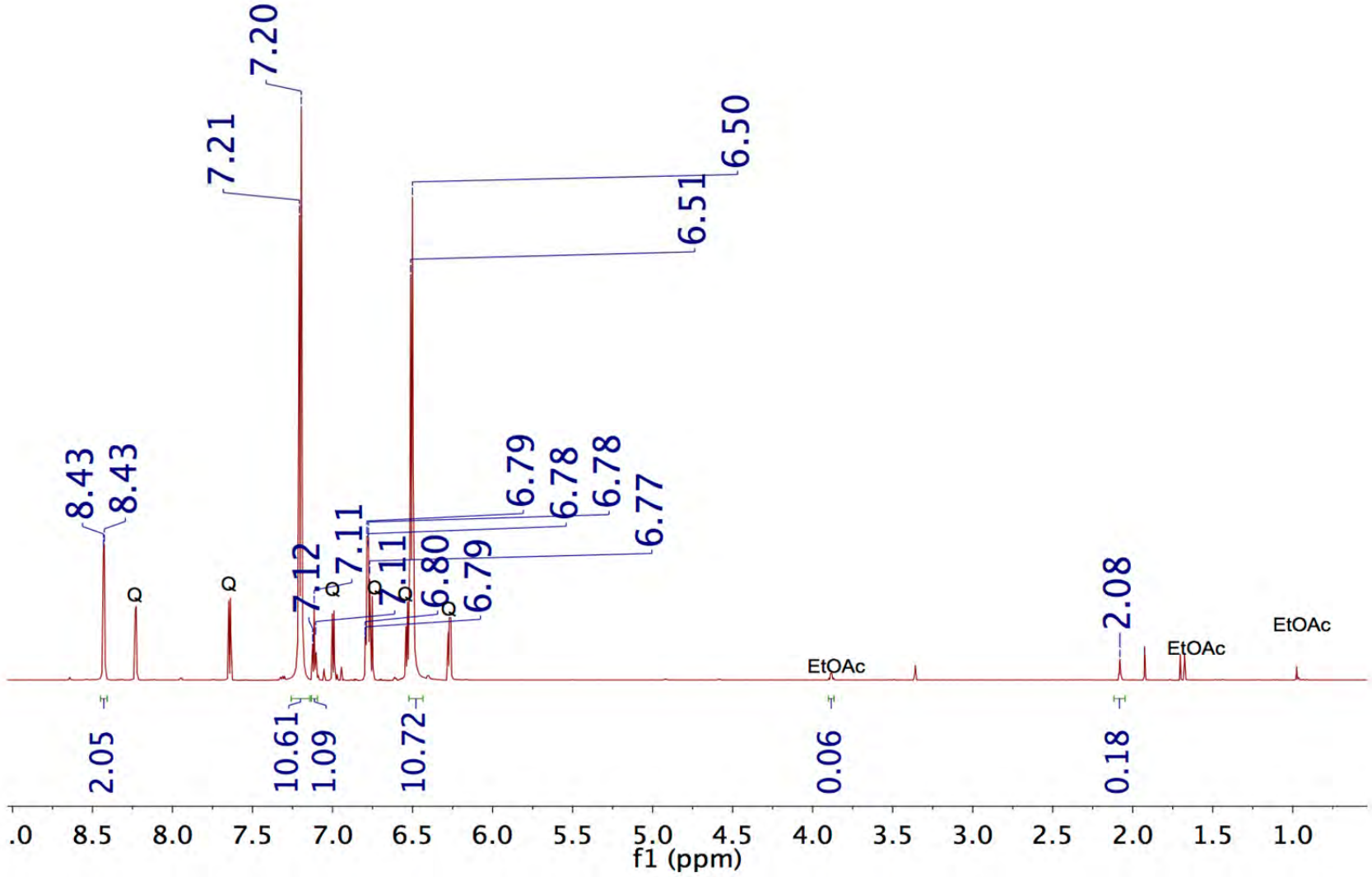

Figure S14: The 1H NMR-spectrum of pyridine mixed with 5 equivalents of 4-(trifluoromethoxy)iodobenzene in toluene-*d8*. Quinoline peaks are highlighted with "Q".

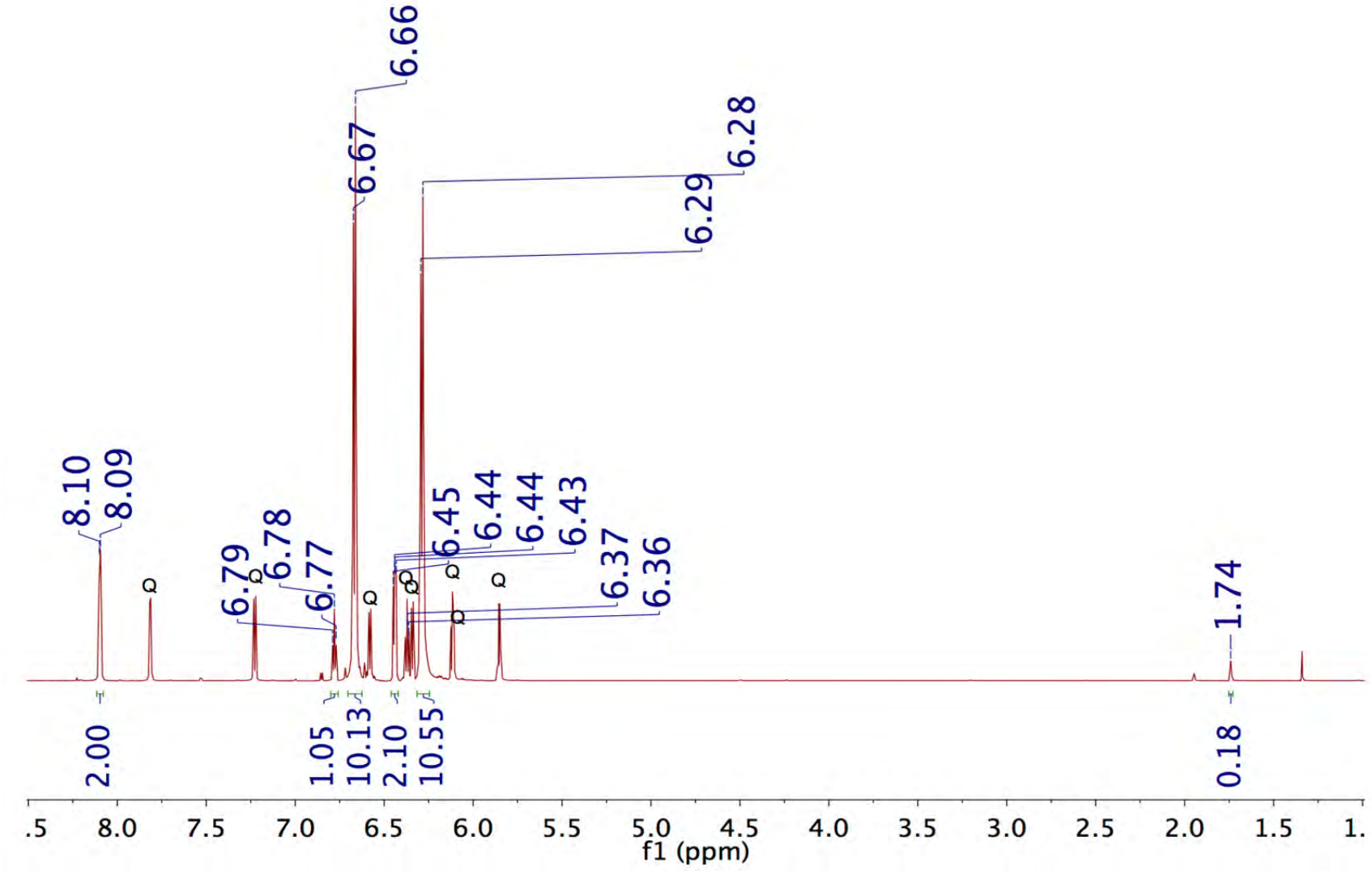

Figure S19: The 1H NMR-spectrum of pyridine mixed with 5 equivalents of 4-(trifluoromethoxy)bromobenzene in toluene-*d8*. Quinoline peaks are highlighted with "Q".

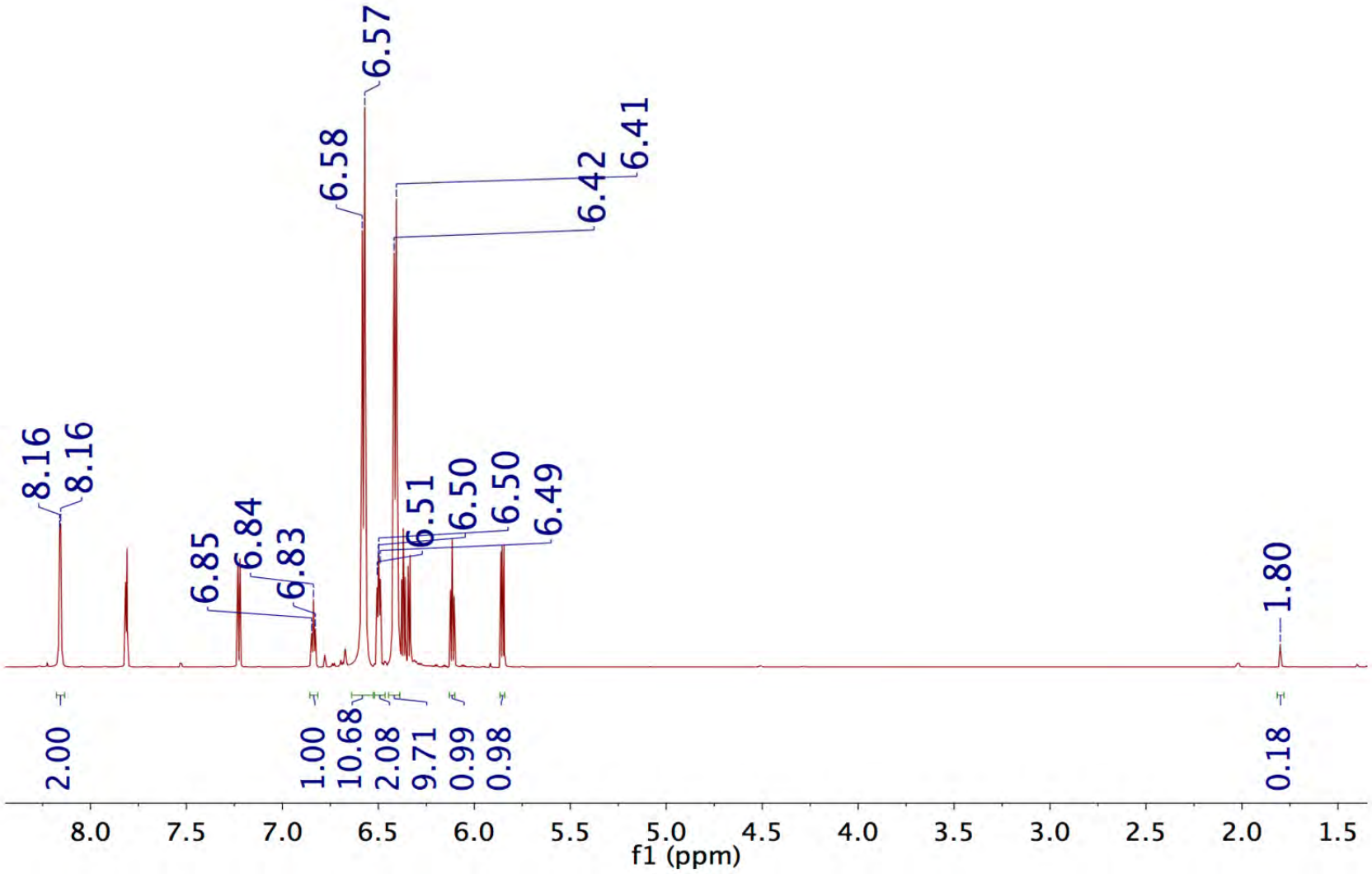

Figure S20: The 1H NMR-spectrum of pyridine mixed with 5 equivalents of 4-(trifluoromethoxy)chlorobenzene in toluene-*d8*. Quinoline peaks are highlighted with "Q".

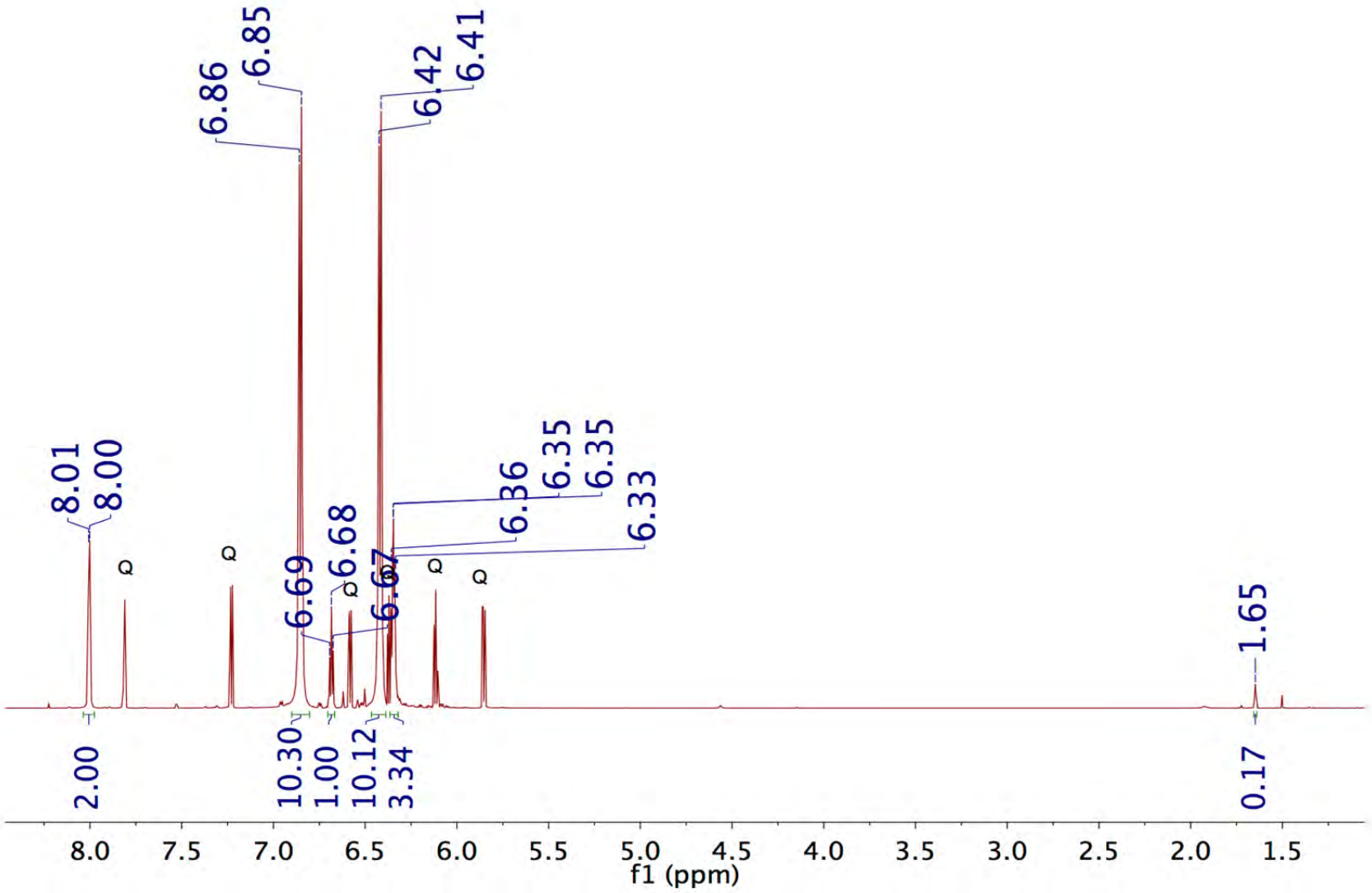

Figure S15: The 1H NMR-spectrum of pyridine mixed with 5 equivalents of 4-iodobenzotrifluoride in toluene-*d8*. Quinoline peaks are highlighted with "Q".

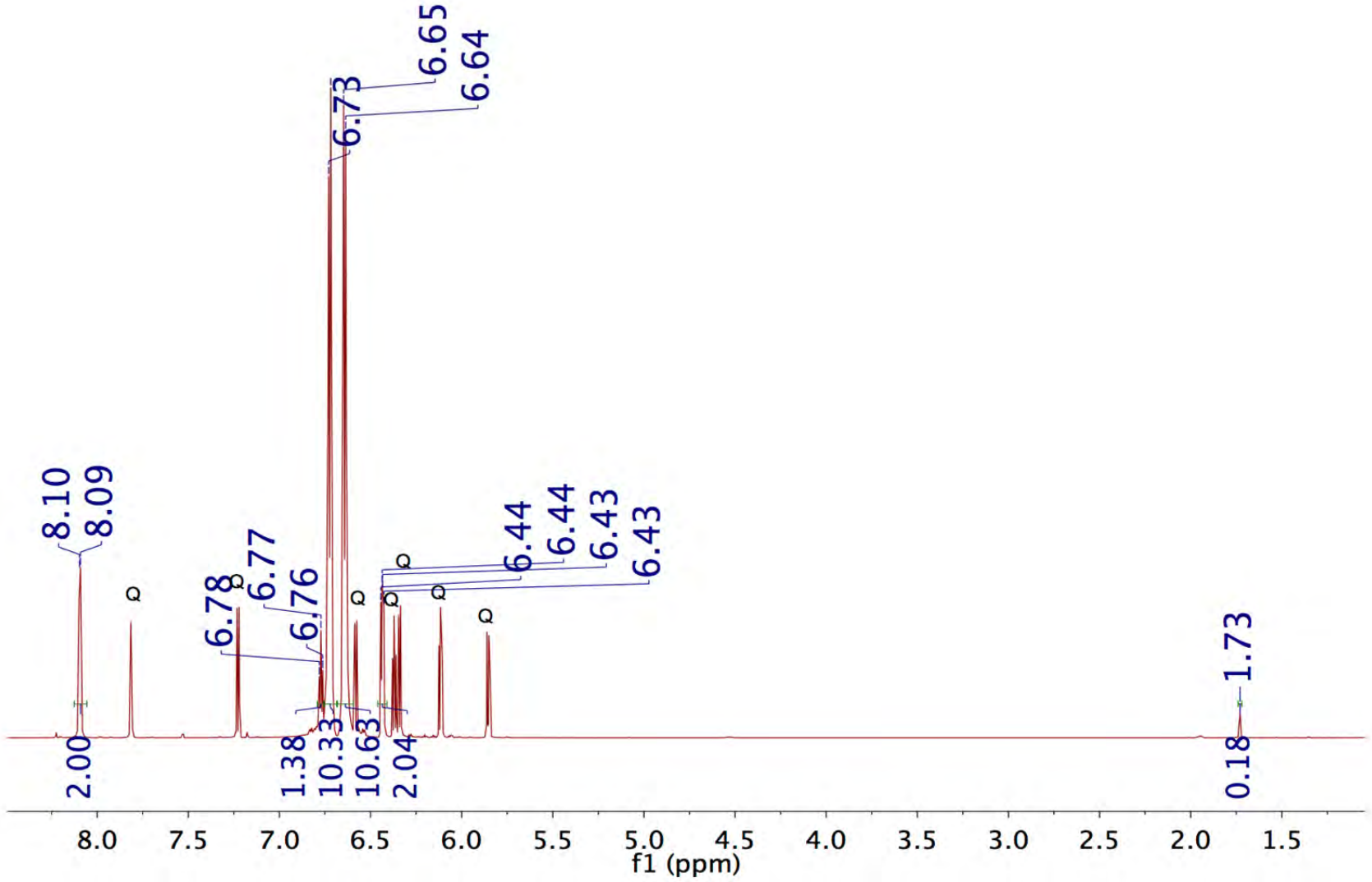

Figure S22: The 1H NMR-spectrum of pyridine mixed with 5 equivalents of 4-bromobenzotrifluoride in toluene-*d8*. Quinoline peaks are highlighted with "Q".

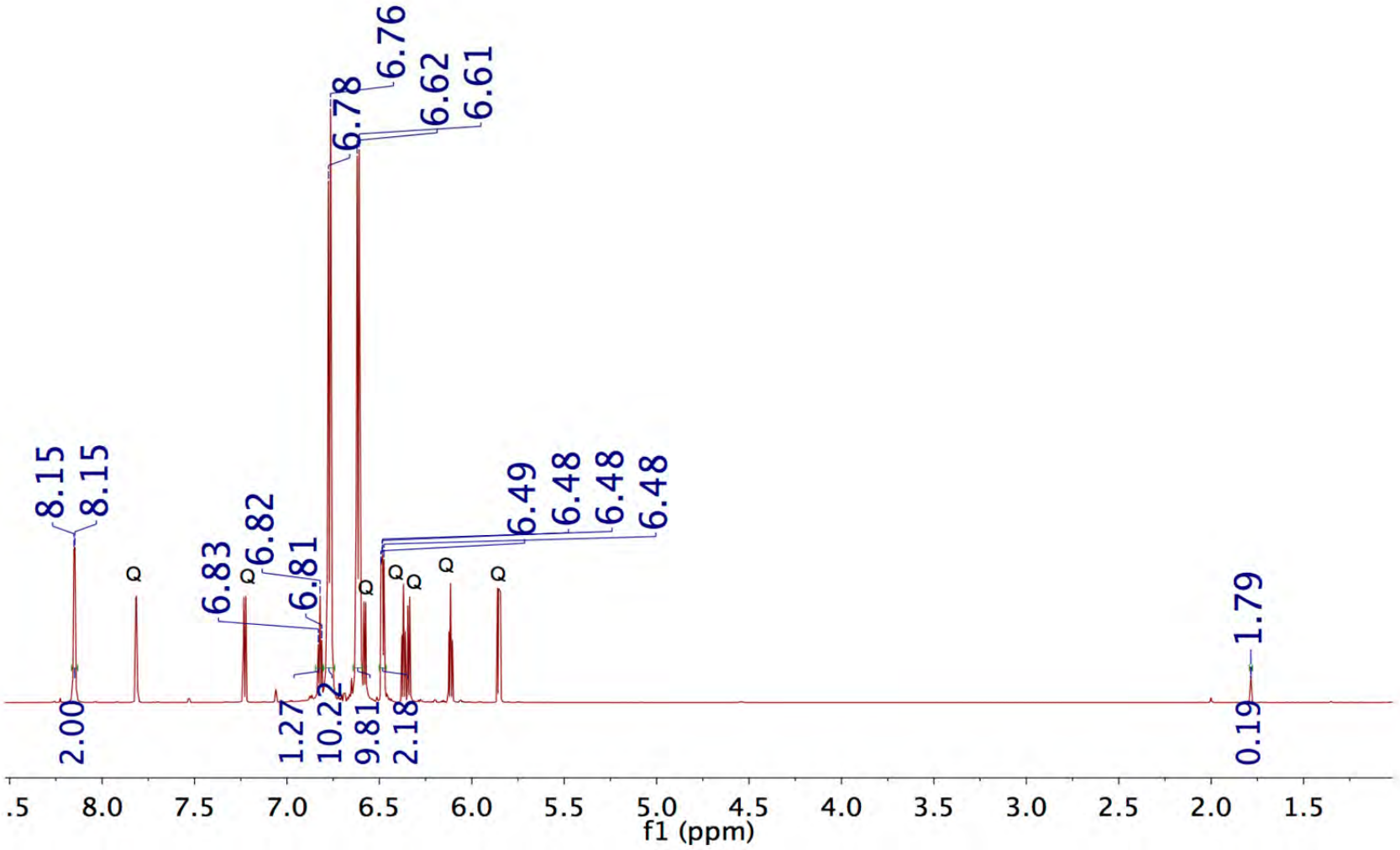

Figure S23: The 1H NMR-spectrum of pyridine mixed with 5 equivalents of 4-chlorobenzotrifluoride in toluene-*d8*. Quinoline peaks are highlighted with "Q".

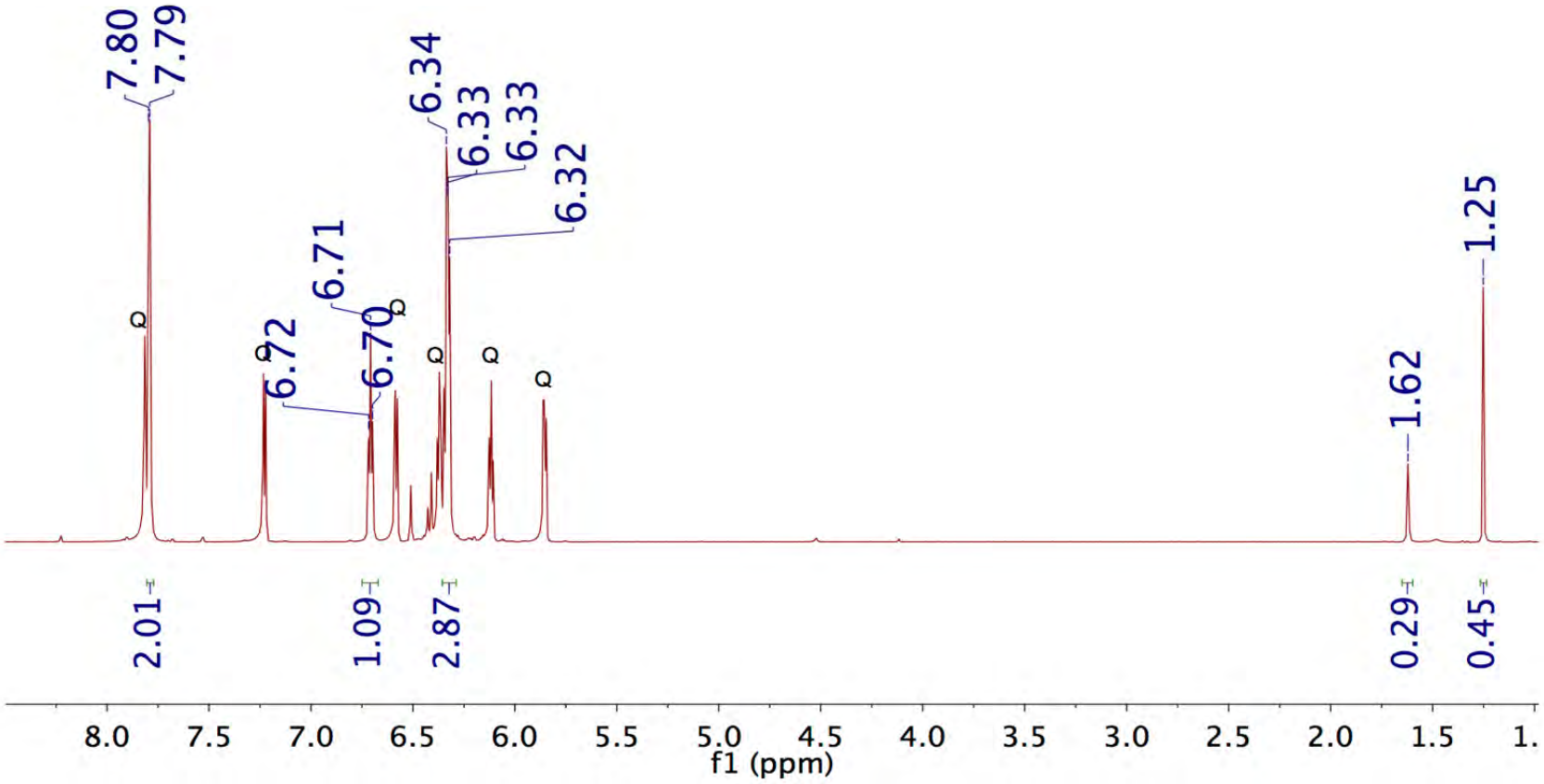

Figure S16: The 1H NMR-spectrum of pyridine mixed with 5 equivalents of iodopentafluorobenzene in toluene-*d8*. Quinoline peaks are highlighted with "Q".

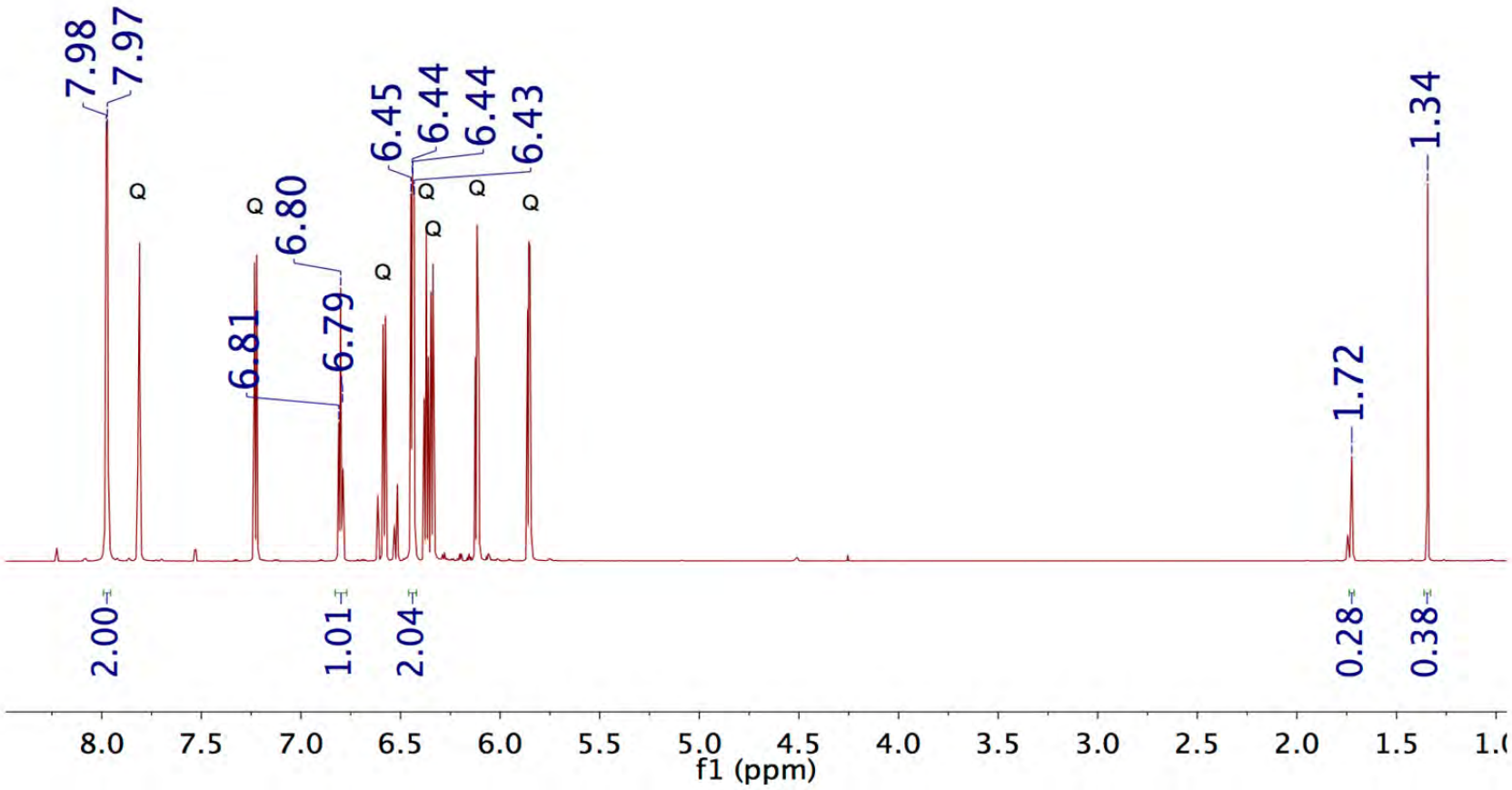

Figure S17: The 1H NMR-spectrum of pyridine mixed with 5 equivalents of bromopentafluorobenzene in toluene-*d8*. Quinoline peaks are highlighted with "Q".

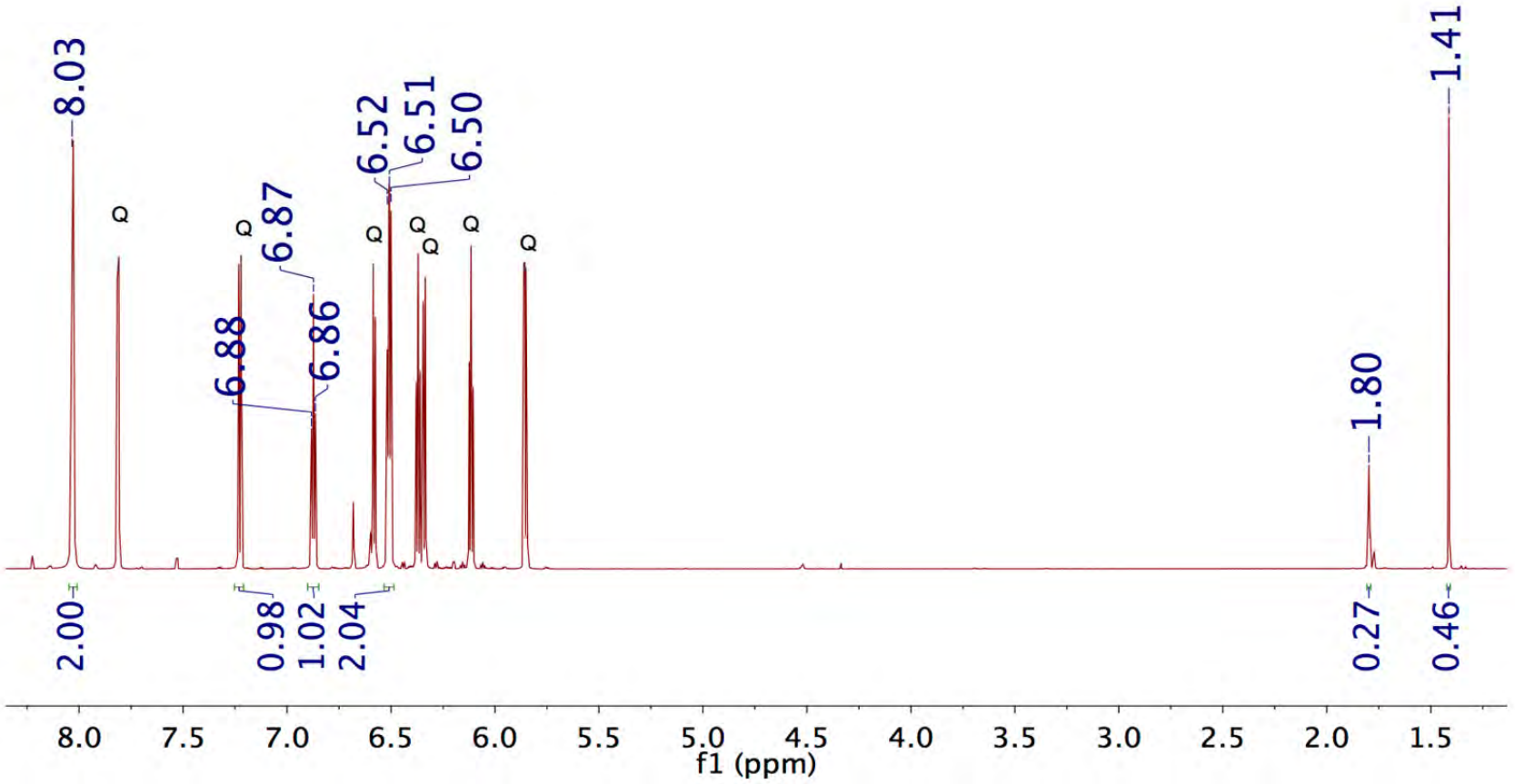

Figure S18: The 1H NMR-spectrum of pyridine mixed with 5 equivalents of chloroopentafluorobenzene in toluene-*d8*. Quinoline peaks are highlighted with "Q".

NMR data: **pyridine:iodobenzene (1:3) series**

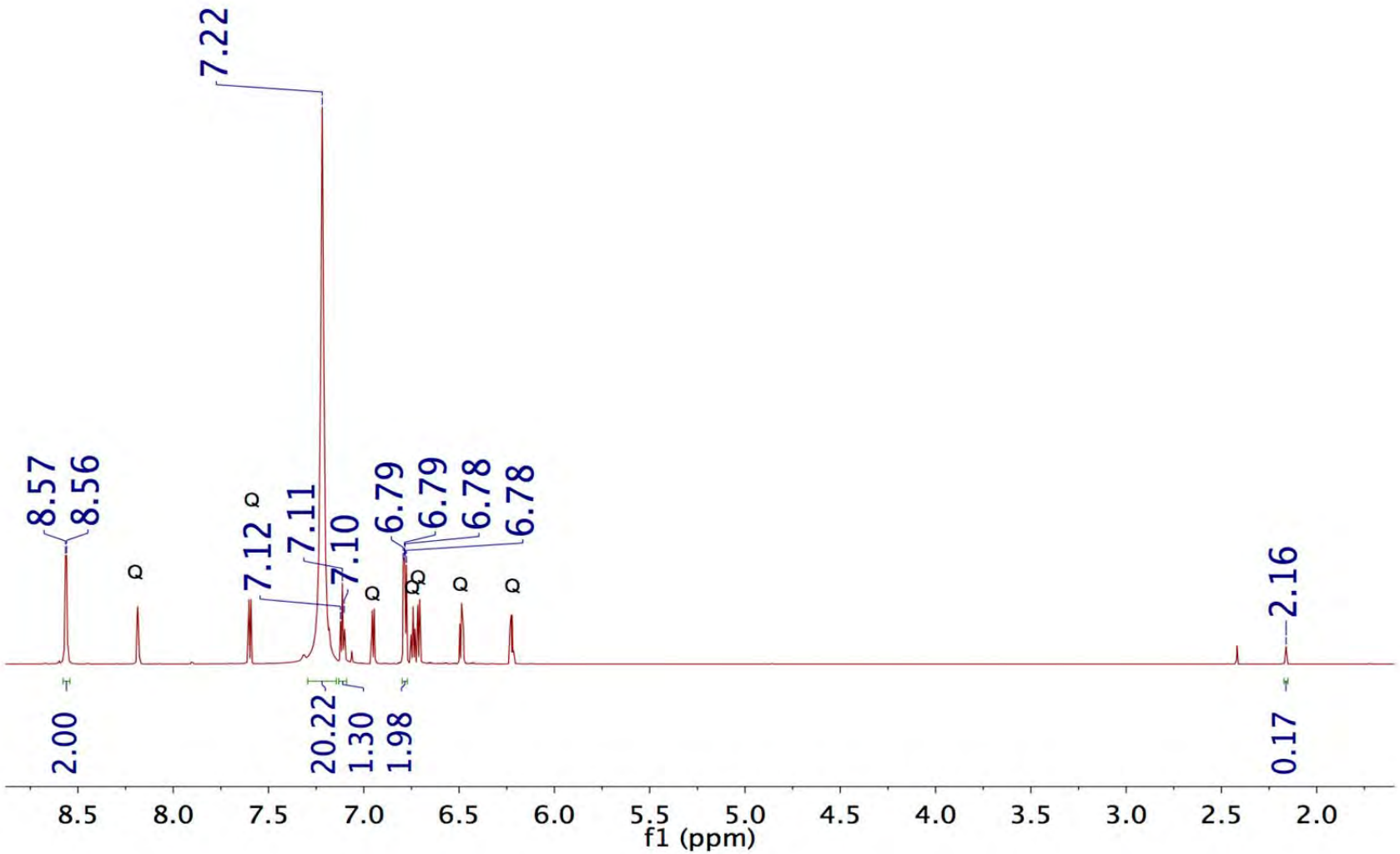

Figure S19: The 1H NMR-spectrum of pyridine mixed with 3 equivalents of benzene in toluene-*d8*. Quinoline peaks are highlighted with "Q".

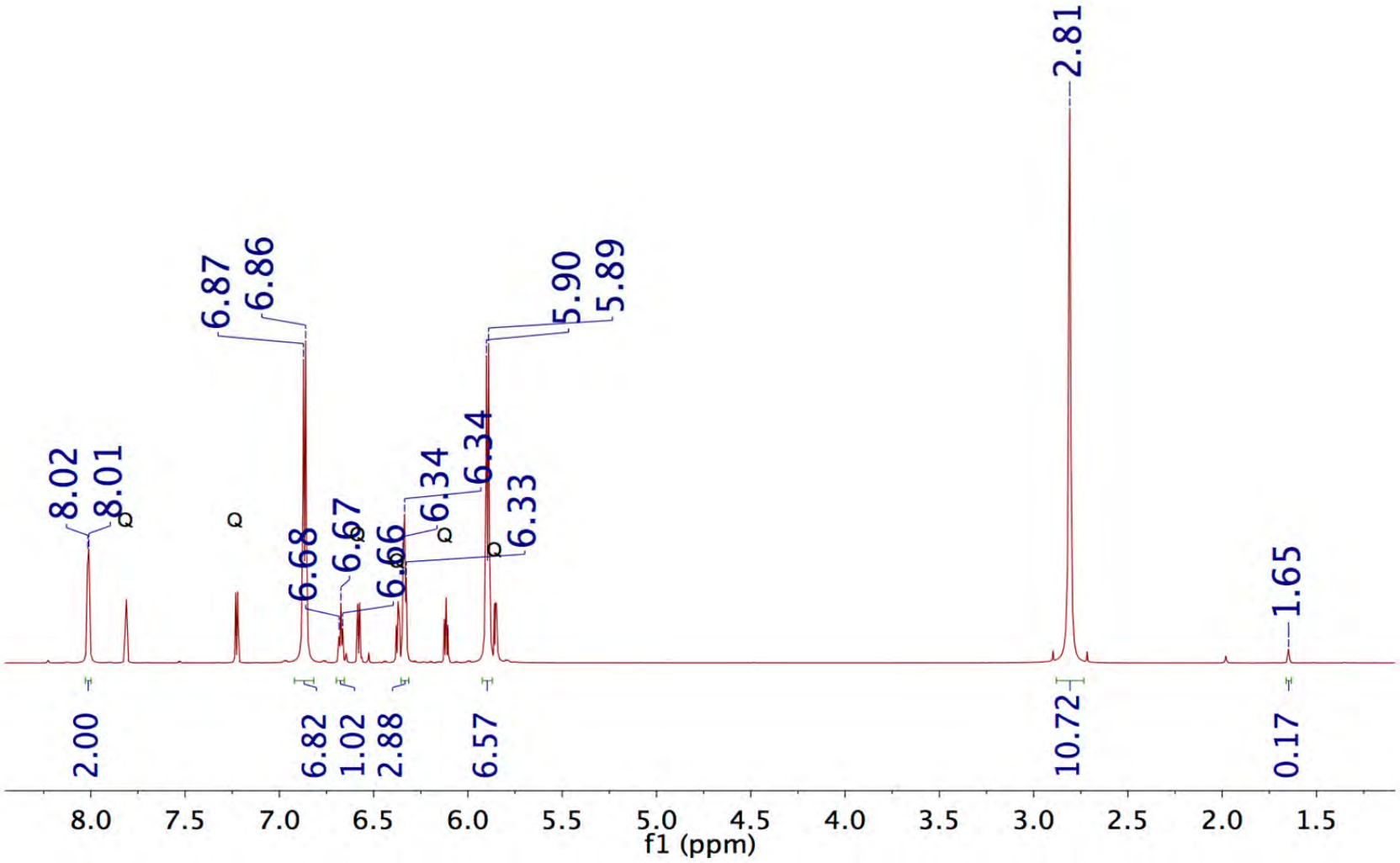

Figure S20: The 1H NMR-spectrum of pyridine mixed with 3 equivalents of 4-iodoanisole in toluene-*d8*. Quinoline peaks are highlighted with "Q".

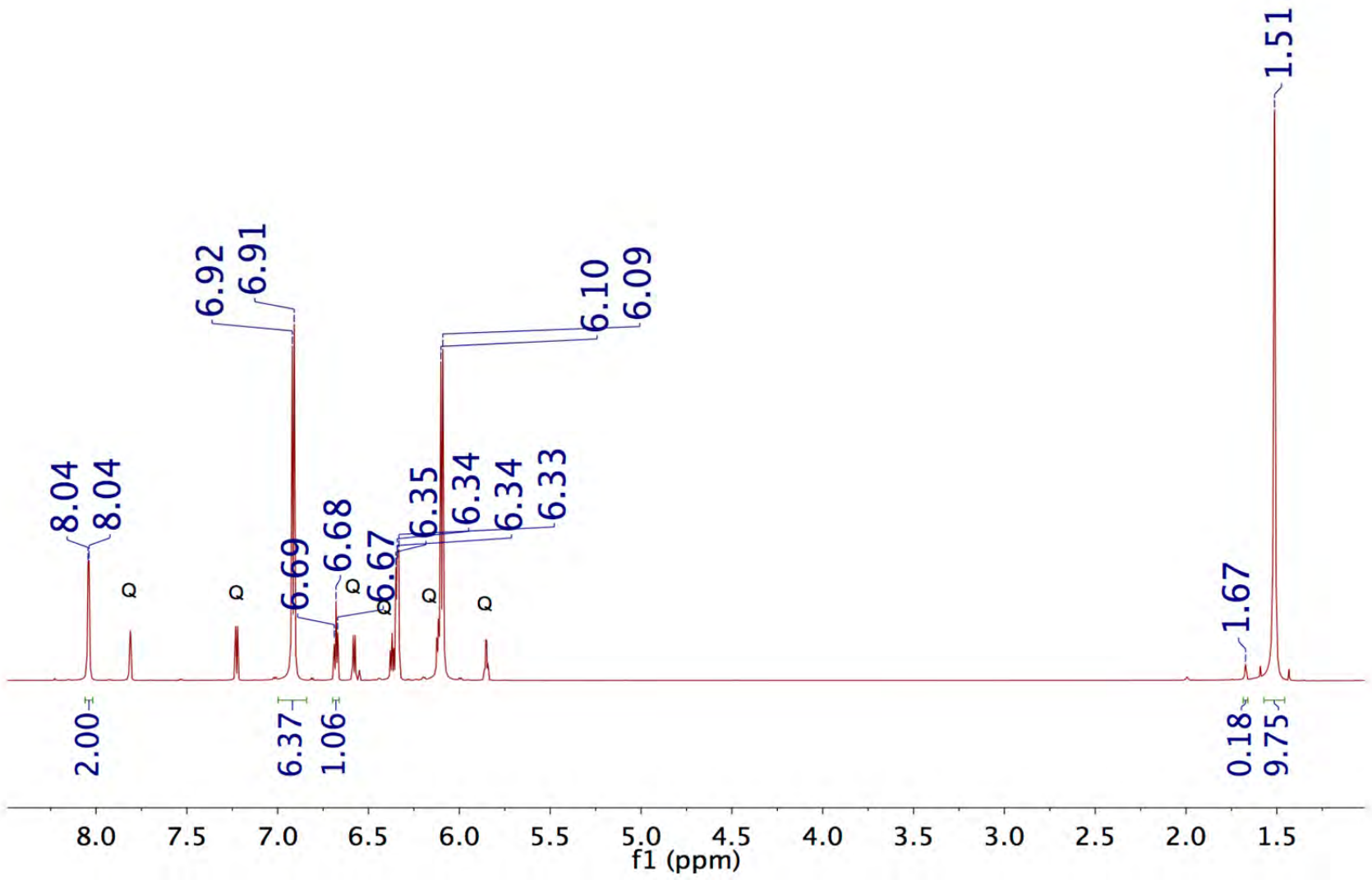

Figure S21: The 1H NMR-spectrum of pyridine mixed with 3 equivalents of 4-iodotoluene in toluene-*d8*. Quinoline peaks are highlighted with "Q".

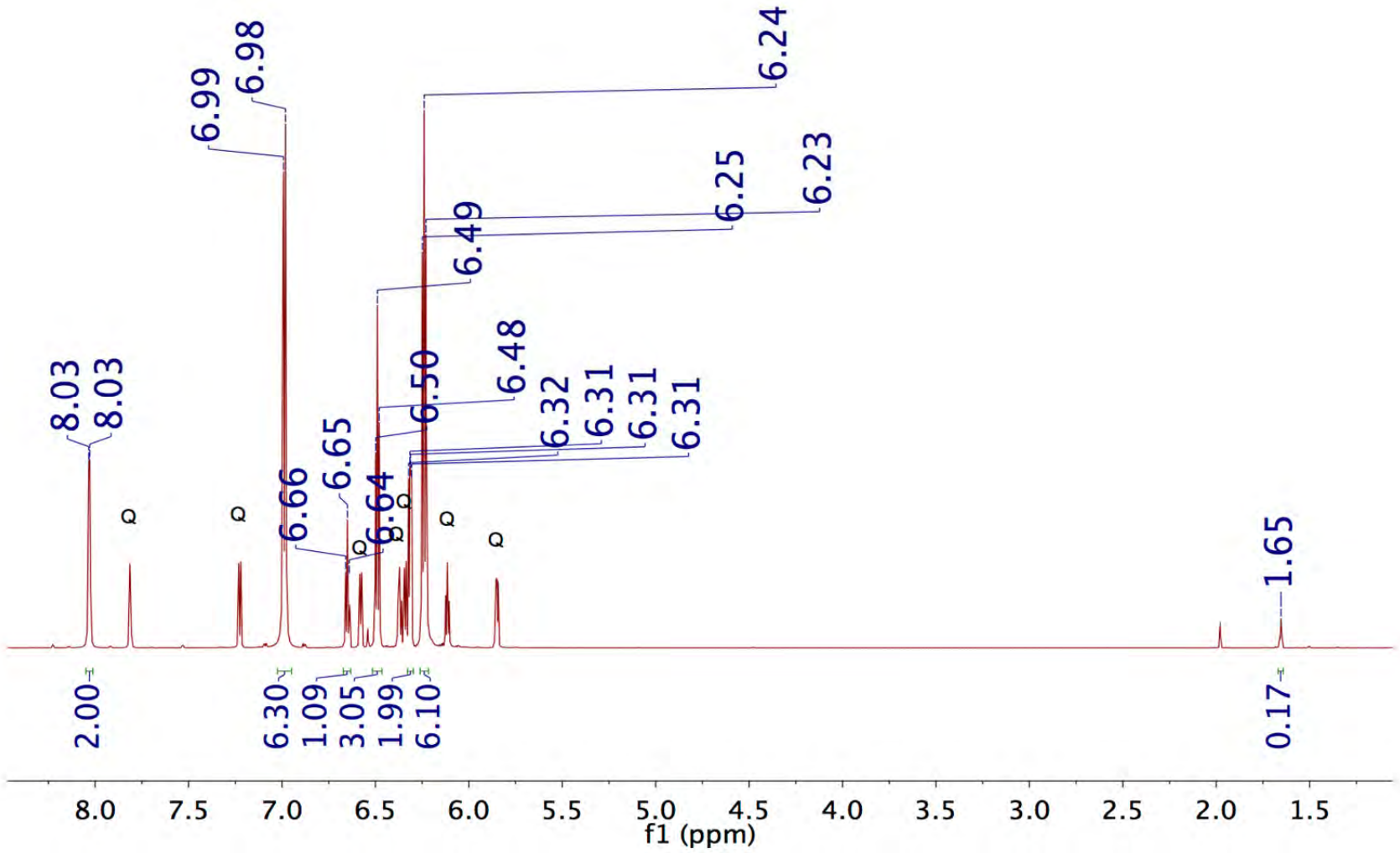

Figure S22: The 1H NMR-spectrum of pyridine mixed with 3 equivalents of iodobenzene in toluene-*d8*. Quinoline peaks are highlighted with "Q".

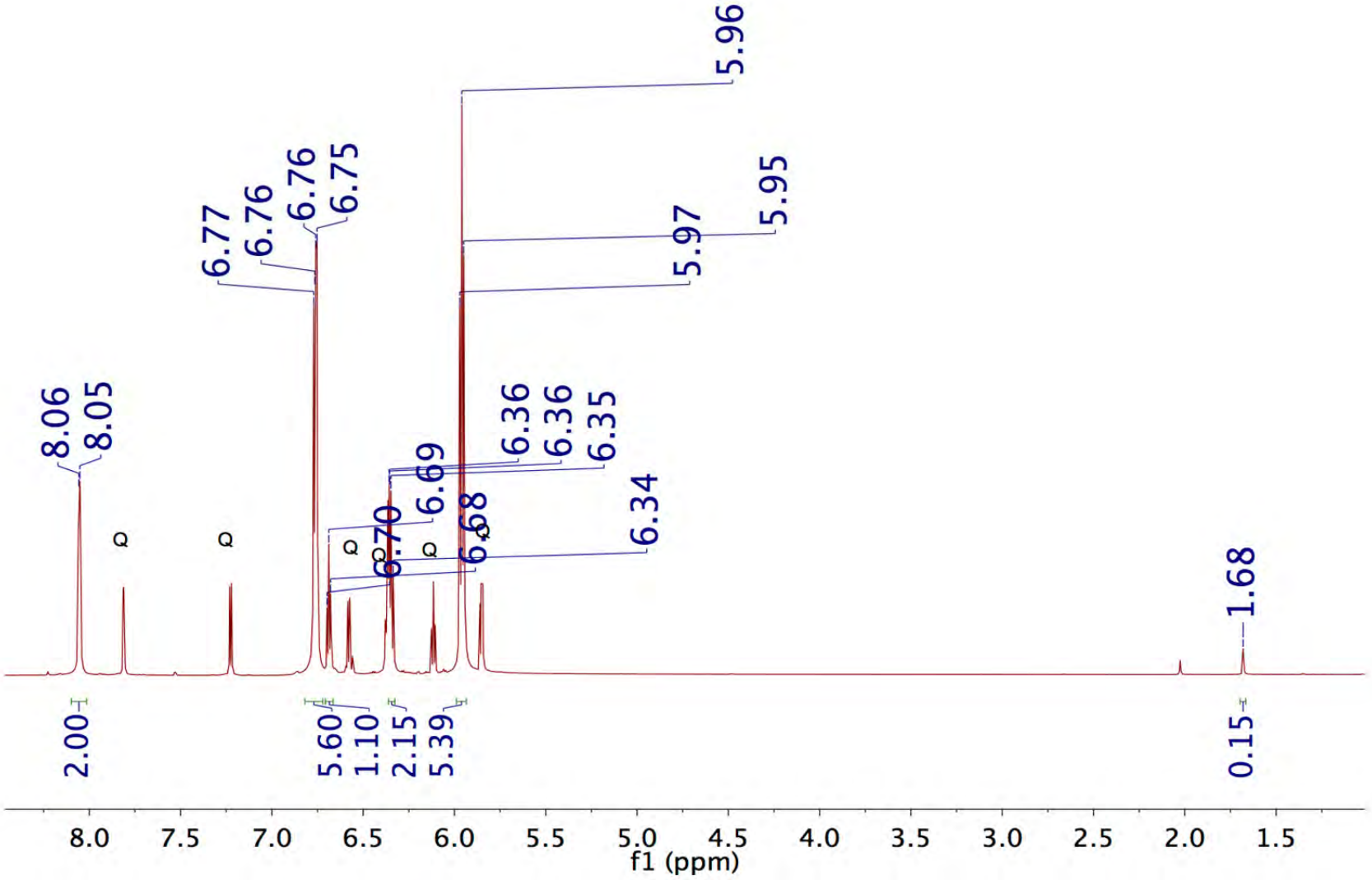

Figure S23: The 1H NMR-spectrum of pyridine mixed with 3 equivalents of 4-fluoroiodobenzene in toluene-*d8*. Quinoline peaks are highlighted with "Q".

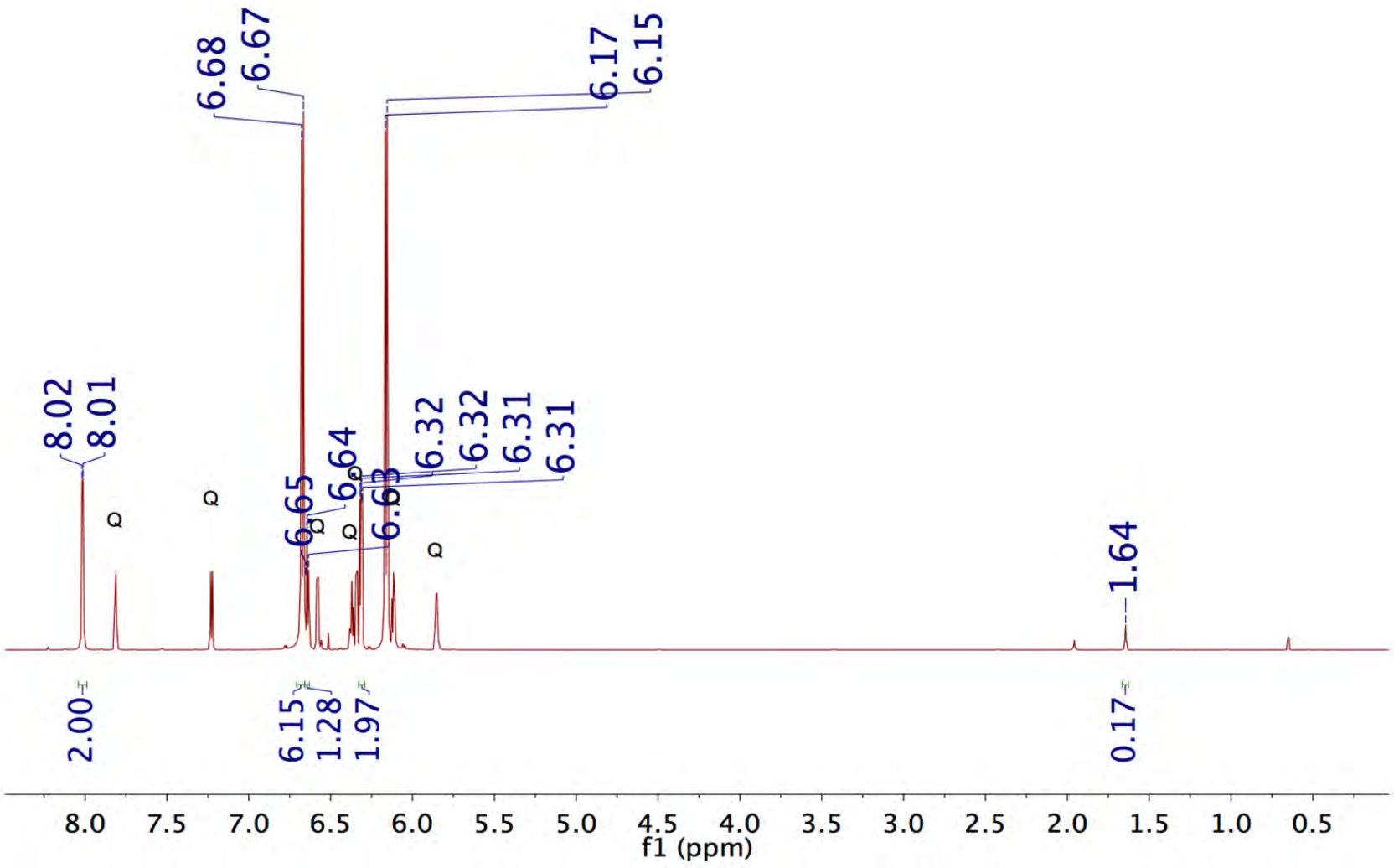

Figure S24: The 1H NMR-spectrum of pyridine mixed with 3 equivalents of 4-chloroiodobenzene in toluene-*d8*. Quinoline peaks are highlighted with "Q".

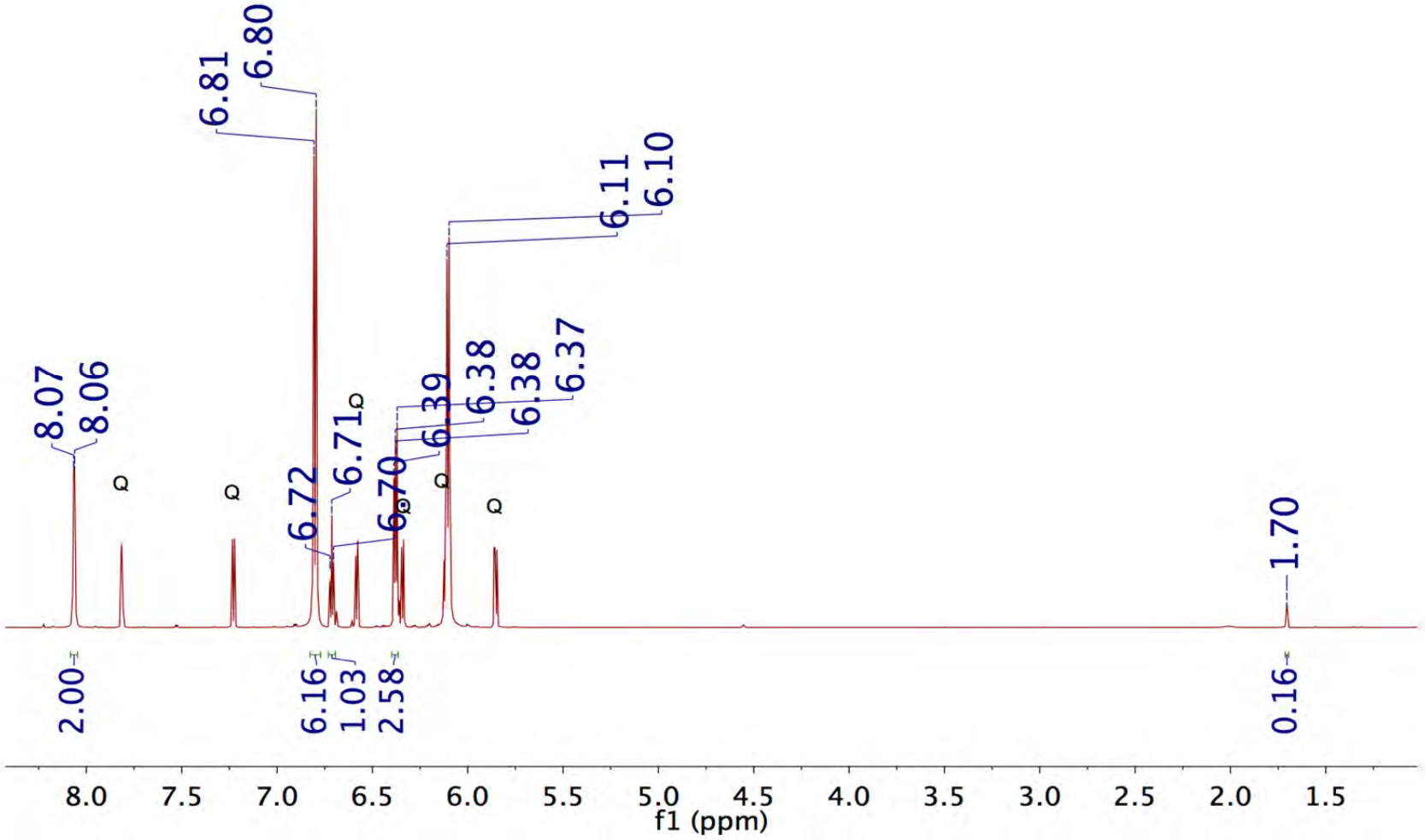

Figure S25: The 1H NMR-spectrum of pyridine mixed with 3 equivalents of 4-(trifluoromethoxy)iodobenzene in toluene-*d8*. Quinoline peaks are highlighted with "Q".

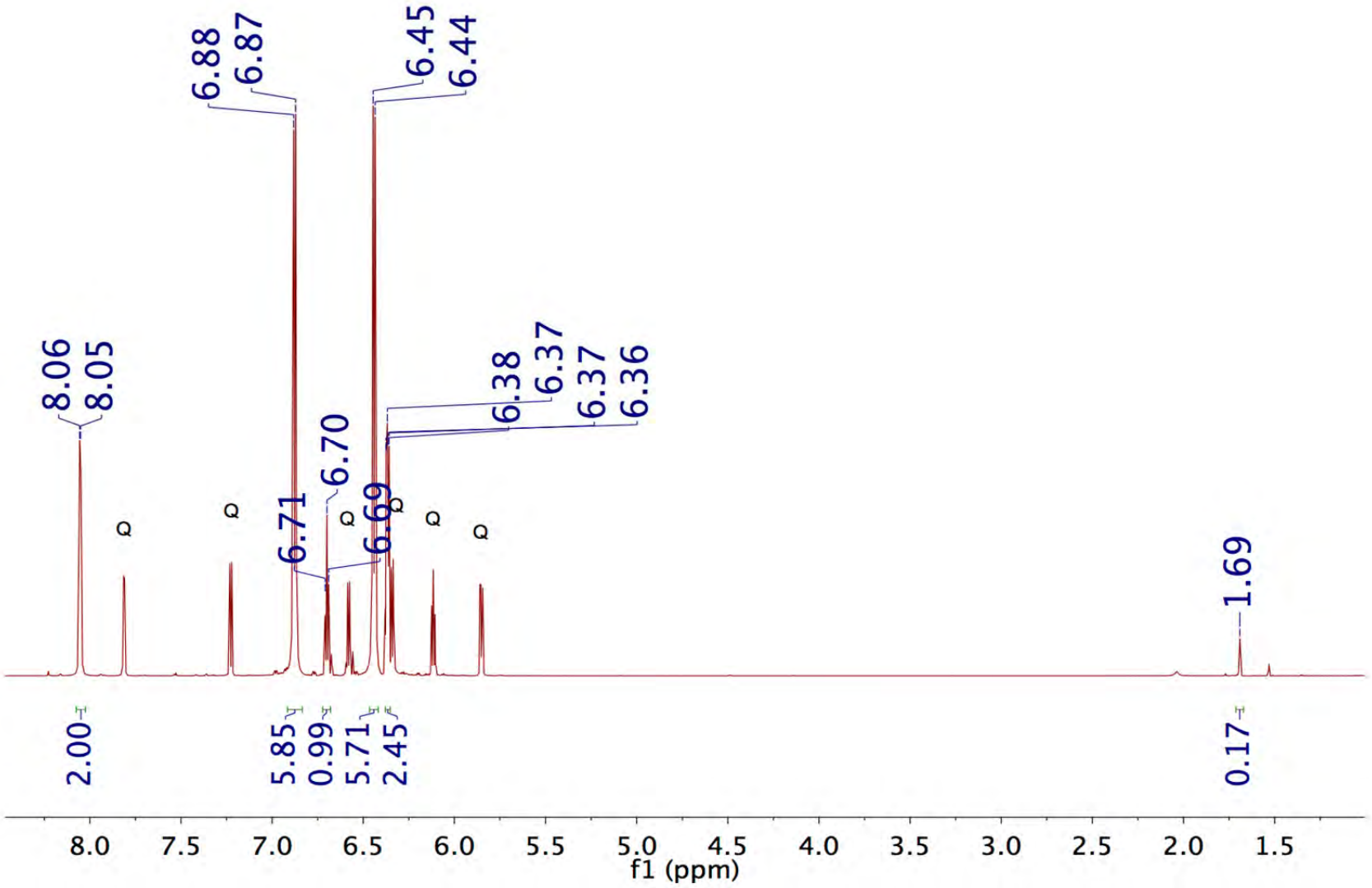

Figure S26: The 1H NMR-spectrum of pyridine mixed with 3 equivalents of 4-iodobenzetrifluoride in toluene-*d8*. Quinoline peaks are highlighted with "Q".

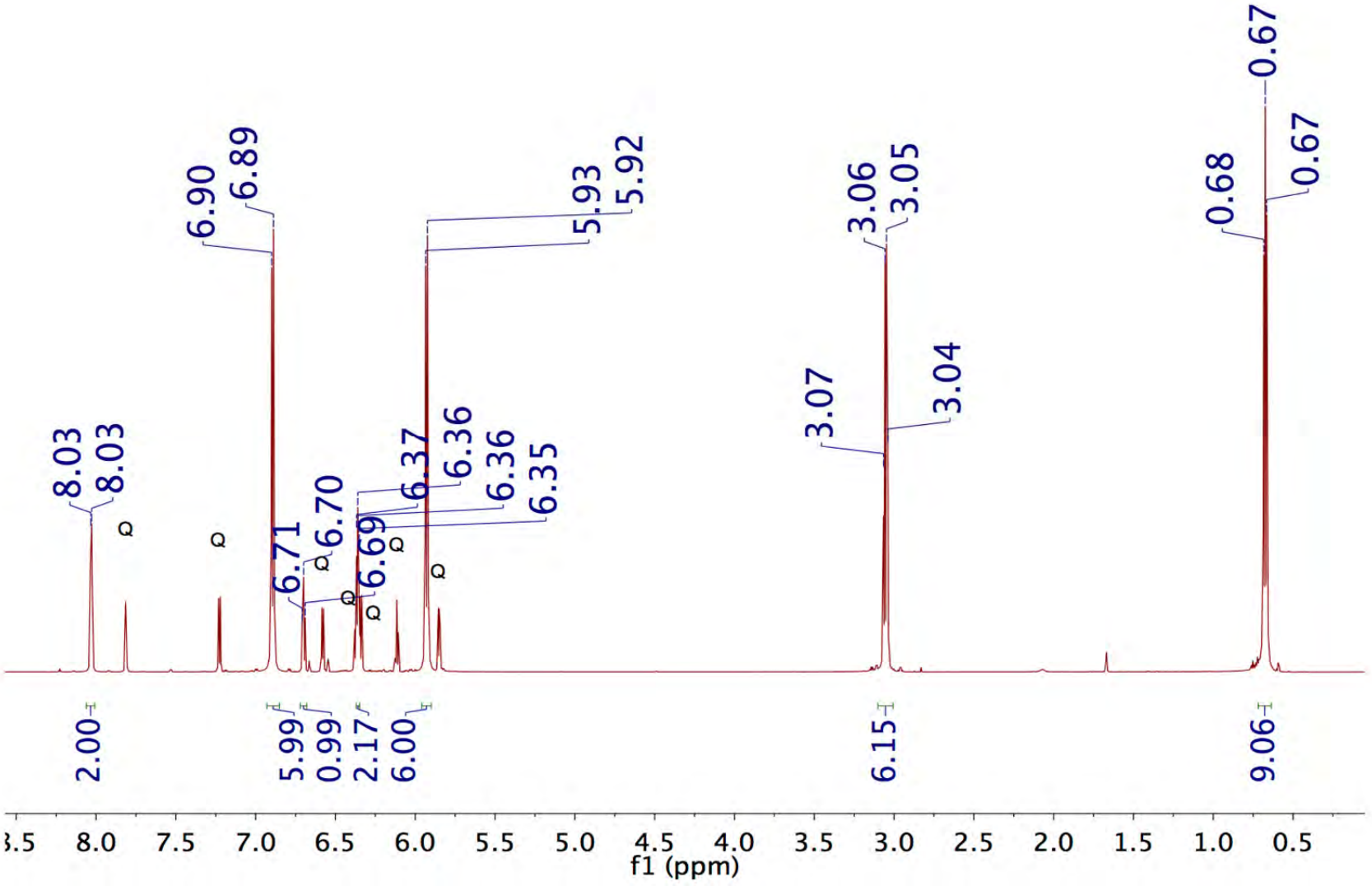

Figure S27: The 1H NMR-spectrum of pyridine mixed with 3 equivalents of 4-iodophenetole in toluene-*d8*. Quinoline peaks are highlighted with "Q".

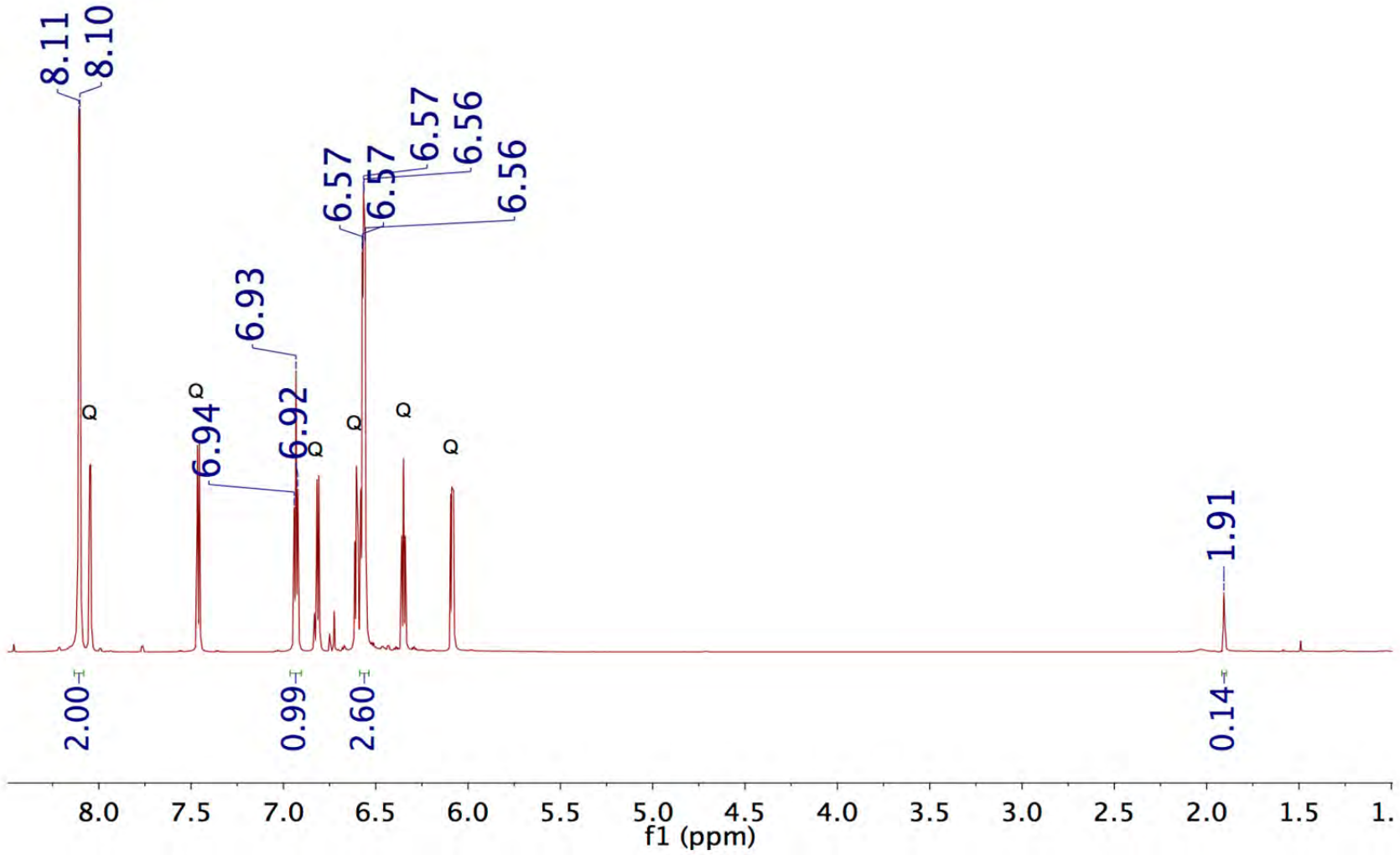

Figure S28: The 1H NMR-spectrum of pyridine mixed with 3 equivalents of iodopentafluorobenzene in toluene-*d8*. Quinoline peaks are highlighted with "Q".

NMR data: **pyridine:phenol (1:3) series**

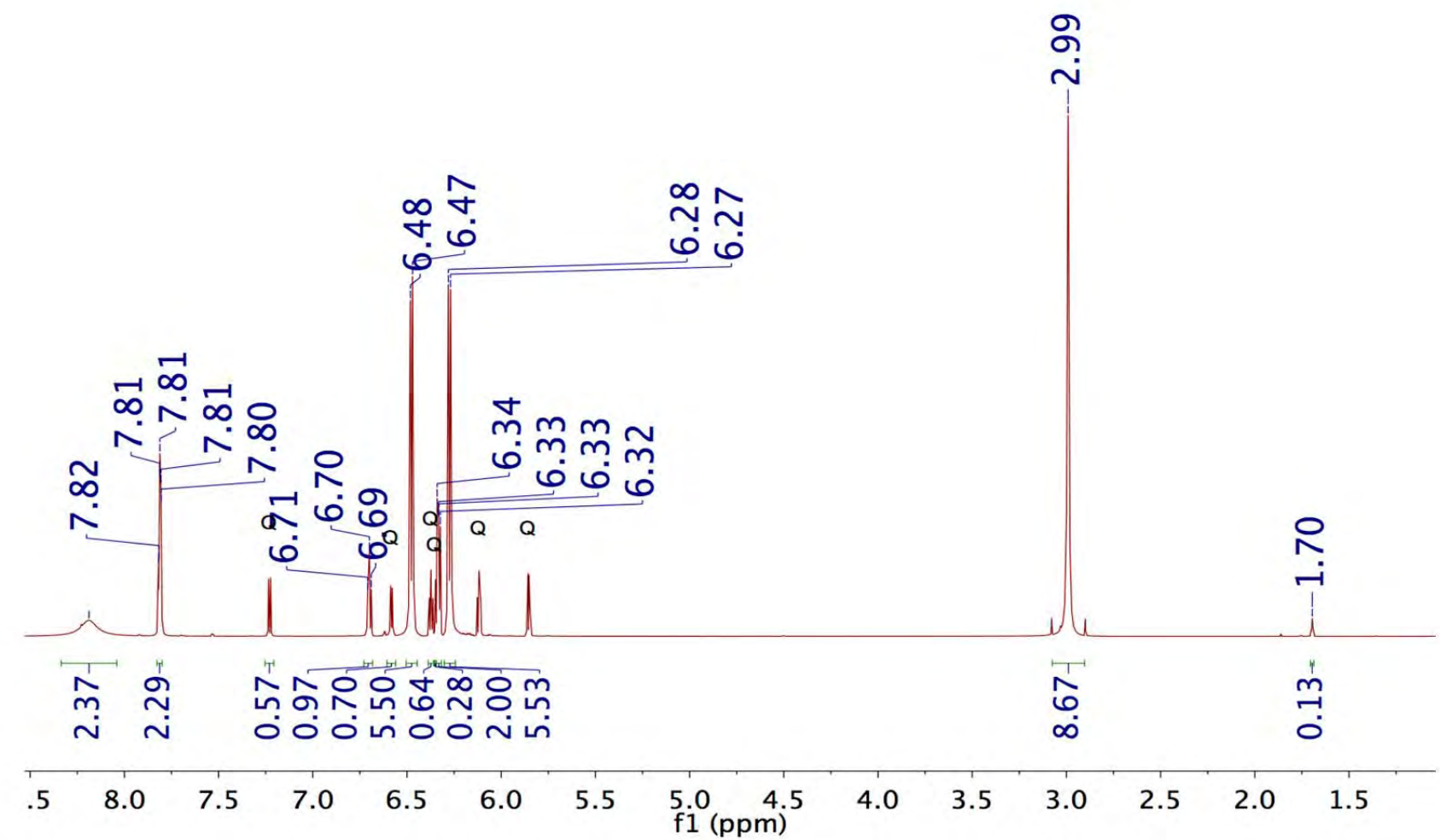

Figure S37: The 1H NMR-spectrum of pyridine mixed with 3 equivalents of 4-methoxyphenol in toluene-*d8*. Quinoline peaks are highlighted with "Q".

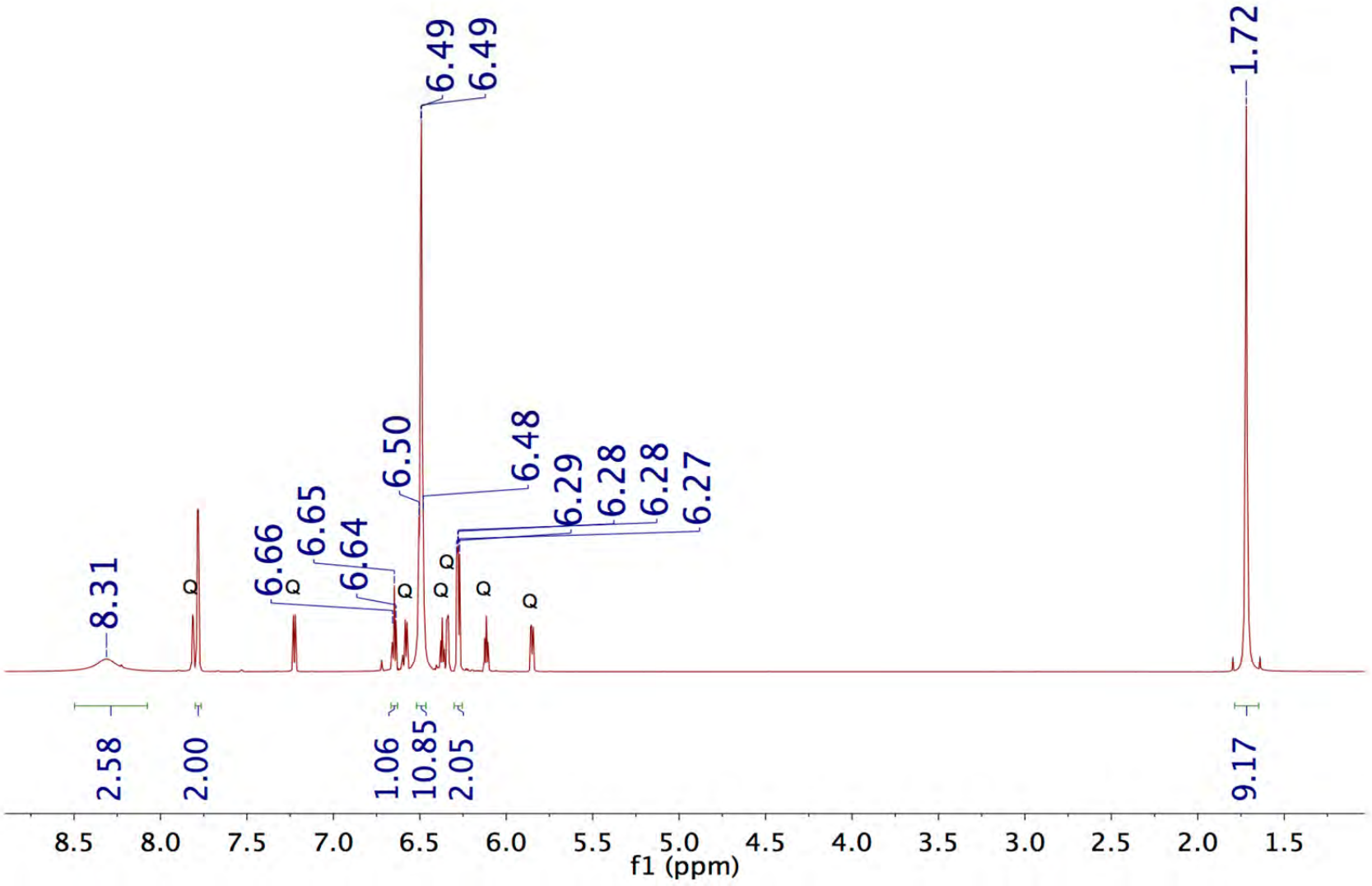

Figure S38: The 1H NMR-spectrum of pyridine mixed with 3 equivalents of *p*-cresol in toluene-*d8*. Quinoline peaks are highlighted with "Q".

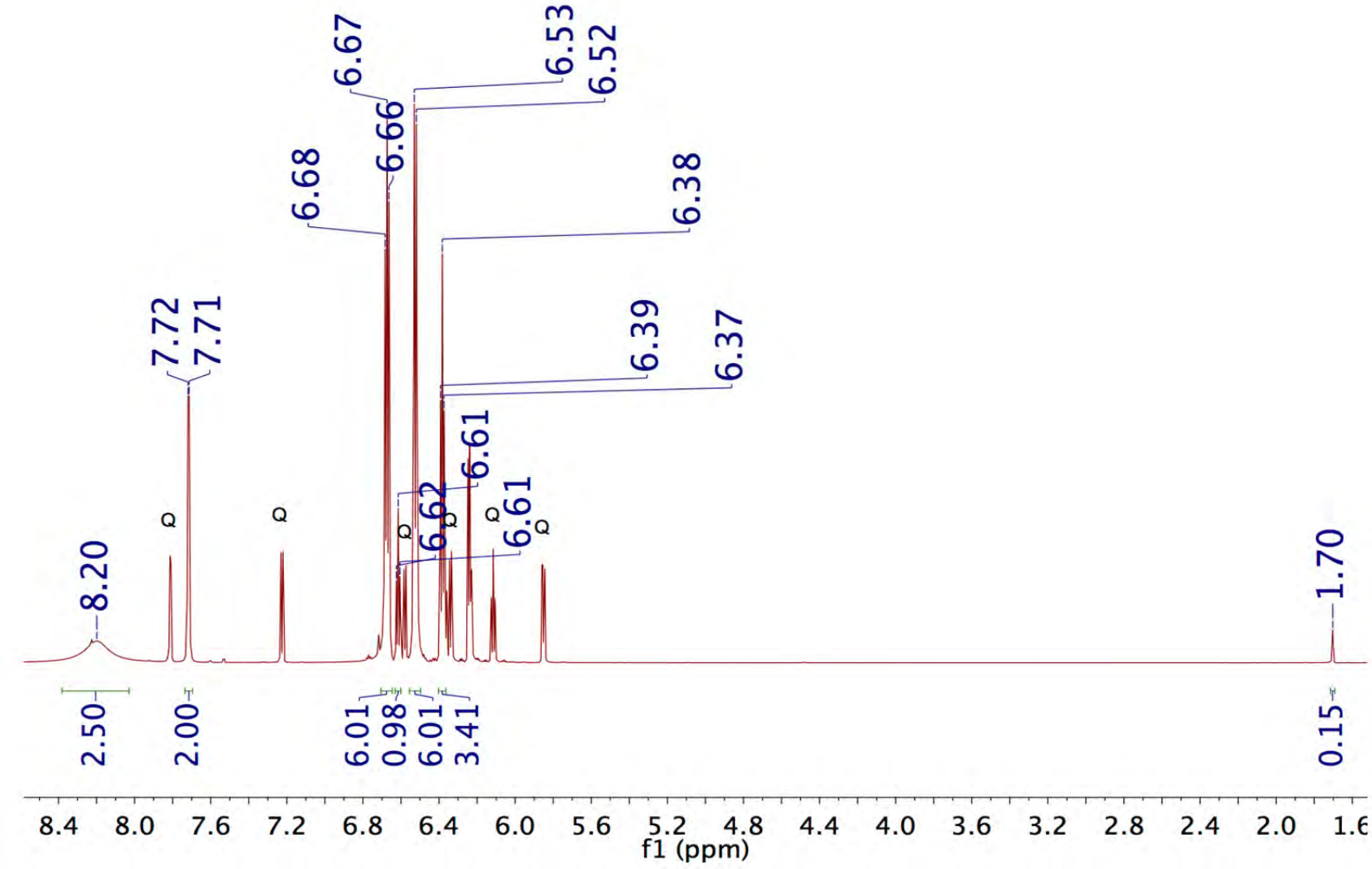

Figure S39: The 1H NMR-spectrum of pyridine mixed with 3 equivalents of phenol in toluene-*d8*. Quinoline peaks are highlighted with "Q".

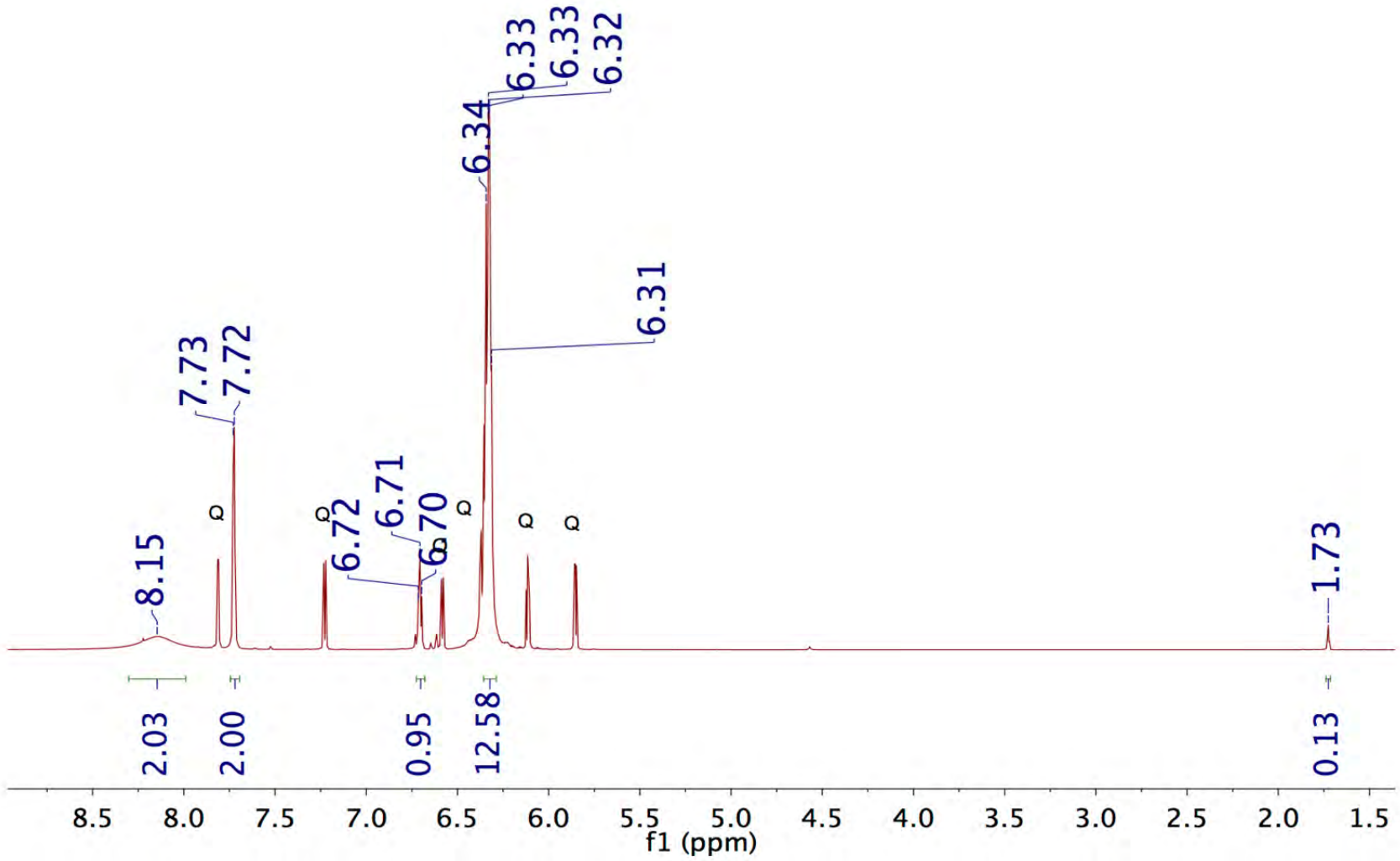

Figure S29: The 1H NMR-spectrum of pyridine mixed with 3 equivalents of 4-fluorophenol in toluene-*d8*. Quinoline peaks are highlighted with "Q".

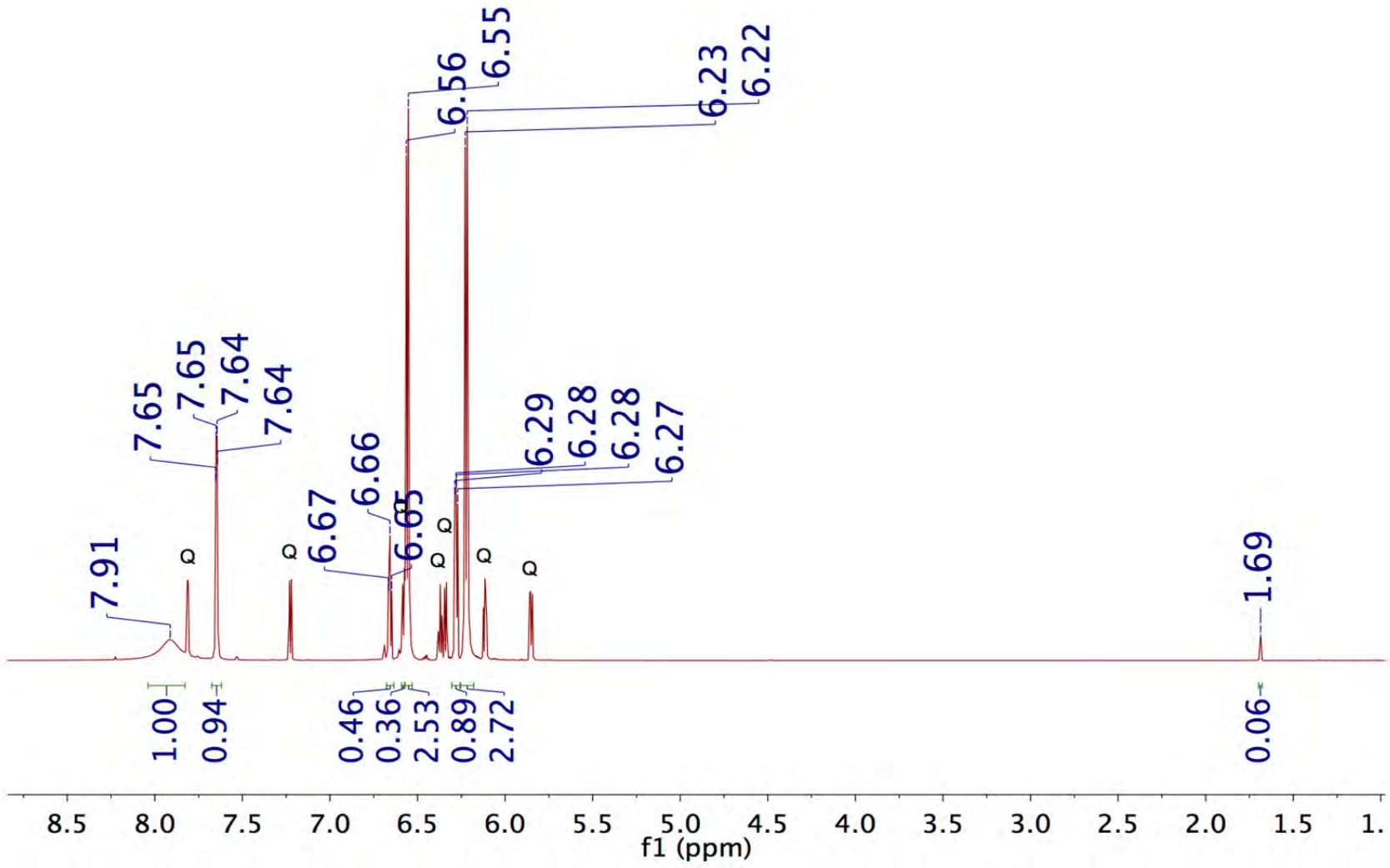

Figure S30: The 1H NMR-spectrum of pyridine mixed with 3 equivalents of 4-chlorophenol in toluene-*d8*. Quinoline peaks are highlighted with "Q".

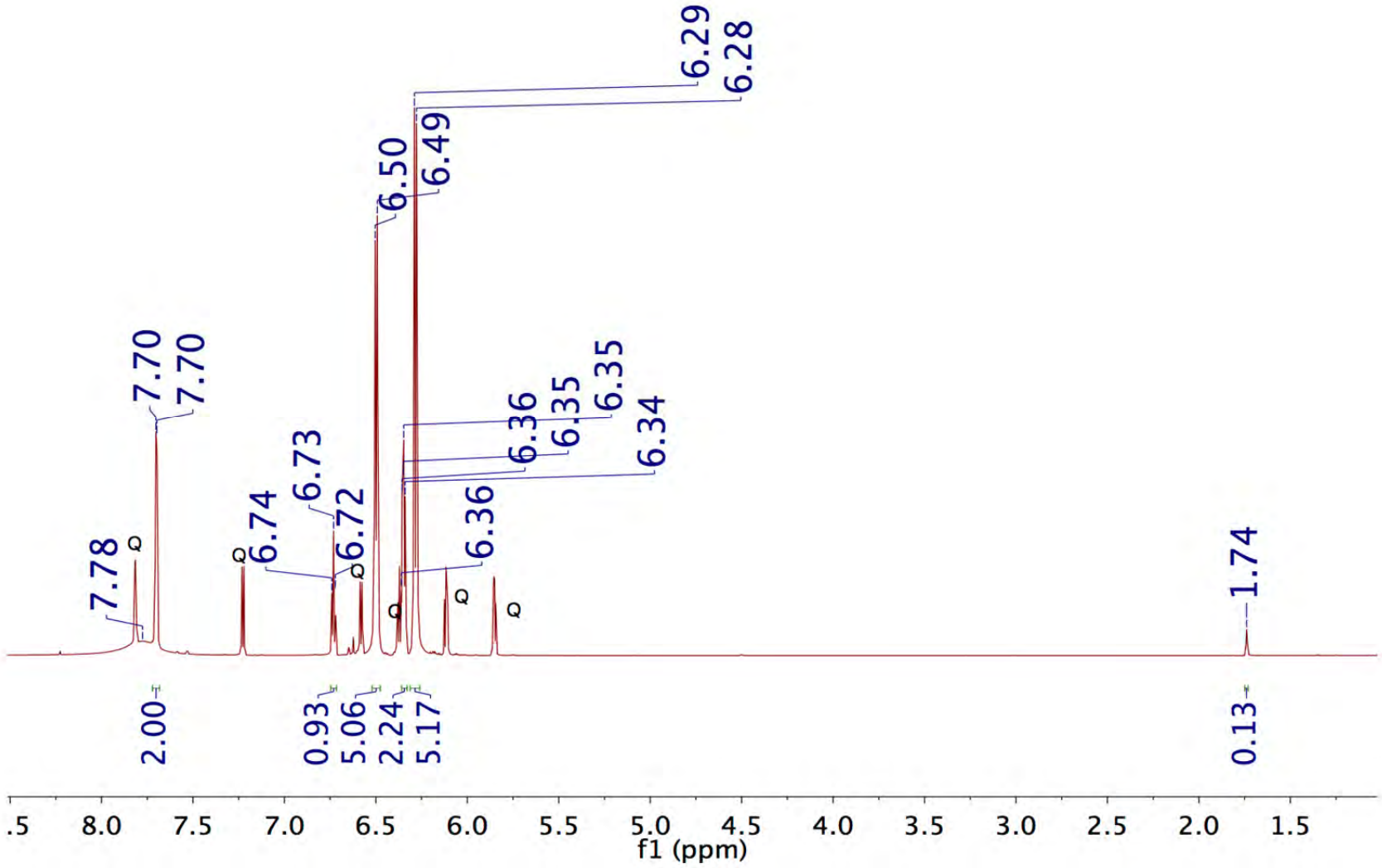

Figure S31: The 1H NMR-spectrum of pyridine mixed with 3 equivalents of 4-(trifluoromethoxy)phenol in toluene-*d8*. Quinoline peaks are highlighted with "Q".

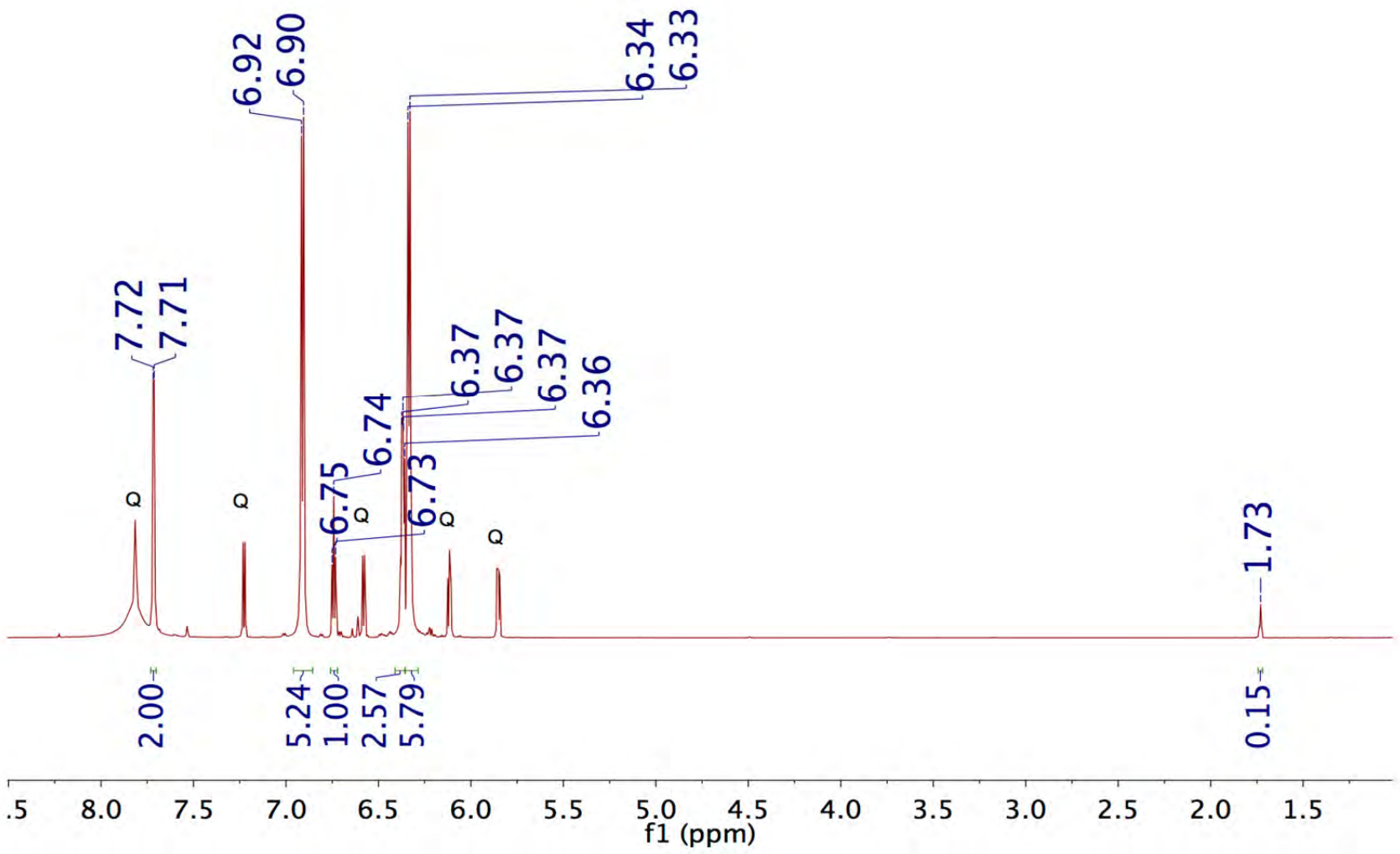

Figure S32: The 1H NMR-spectrum of pyridine mixed with 3 equivalents of 4-(trifluoromethyl)phenol in toluene-*d8*. Quinoline peaks are highlighted with "Q".

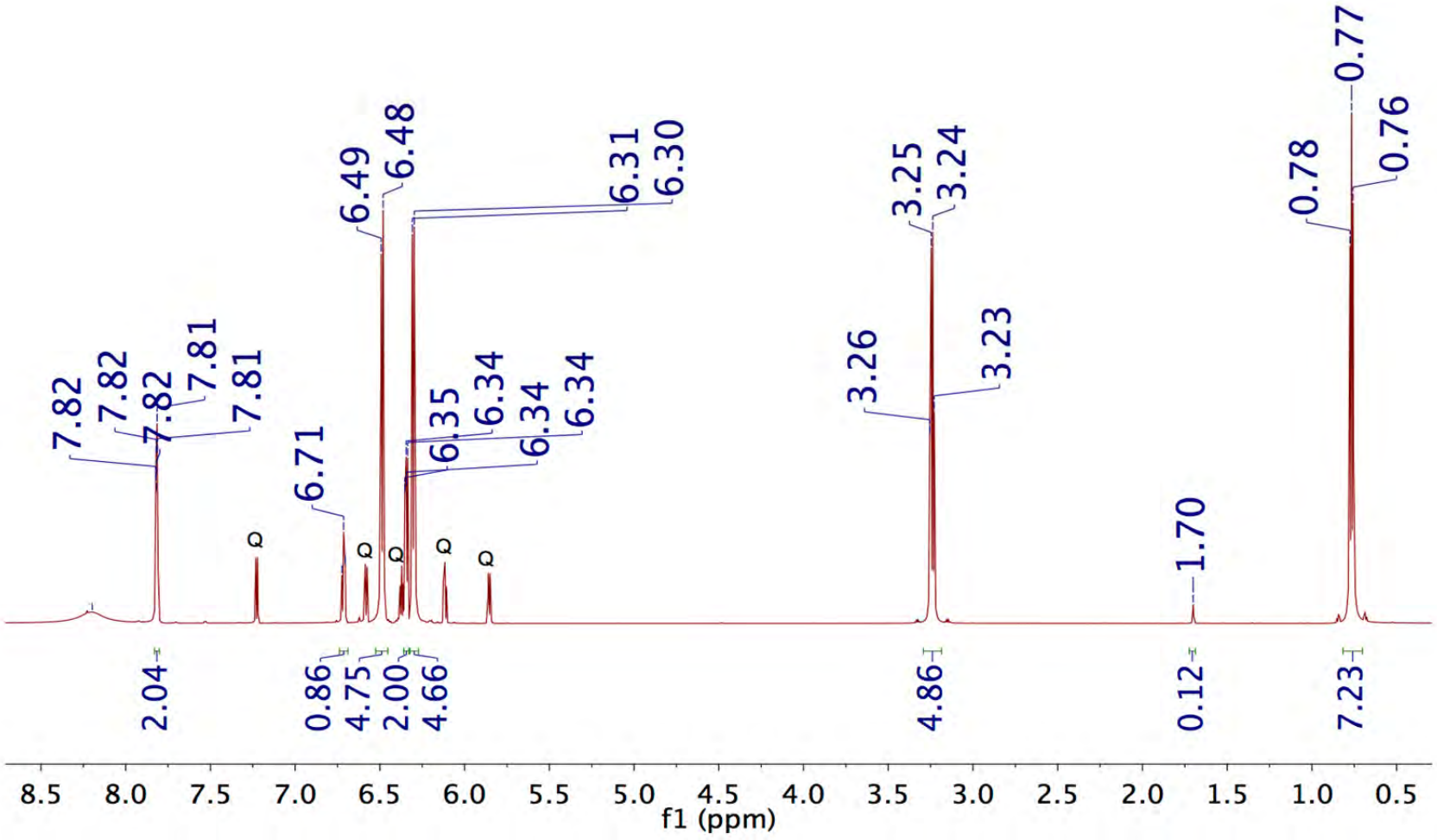

Figure S33: The 1H NMR-spectrum of pyridine mixed with 3 equivalents of 4-ethoxyphenol in toluene-*d8*. Quinoline peaks are highlighted with "Q".

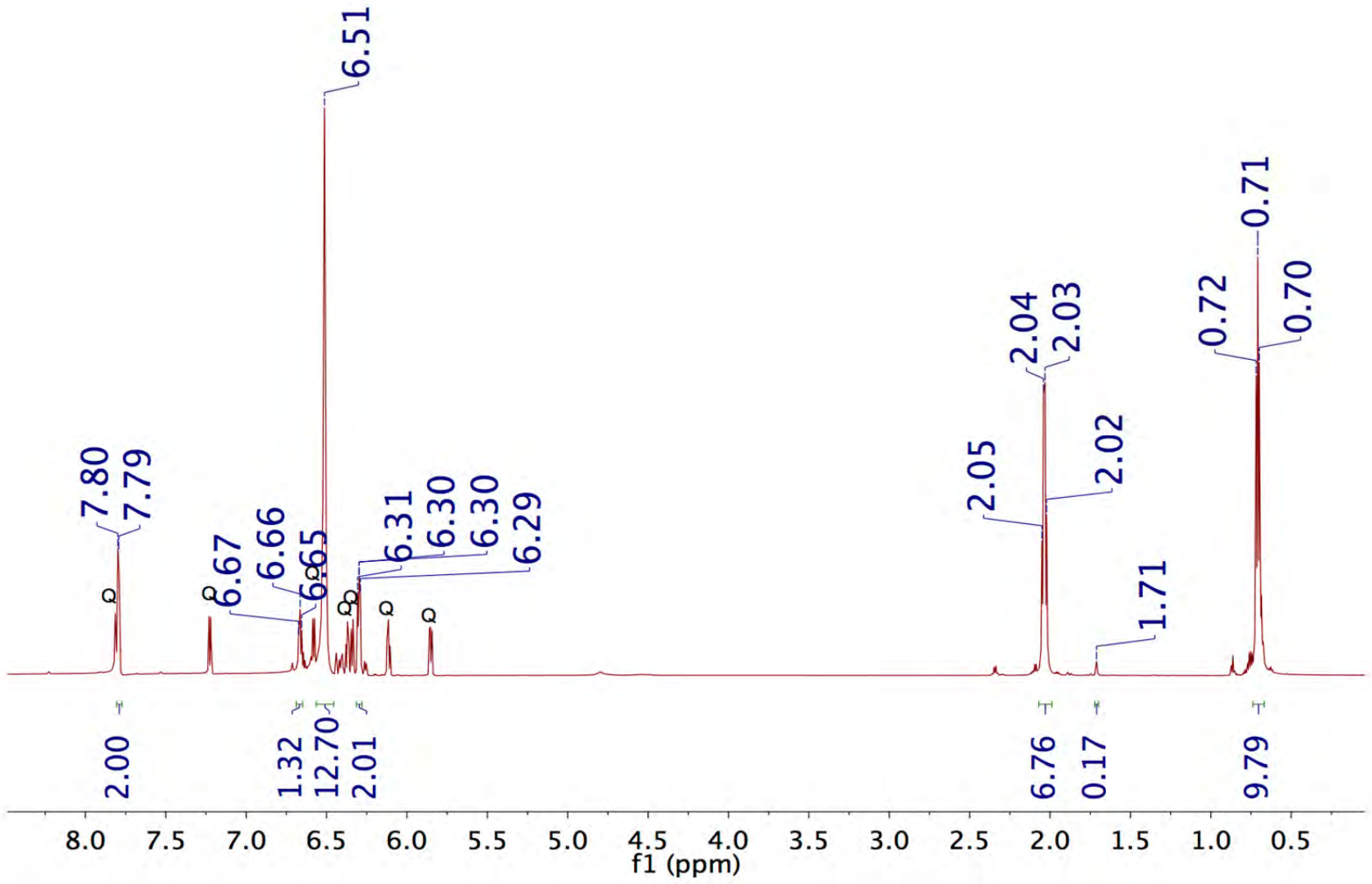

Figure S45: The 1H NMR-spectrum of pyridine mixed with 3 equivalents of 4-ethylphenol in toluene-*d8*. Quinoline peaks are highlighted with "Q".

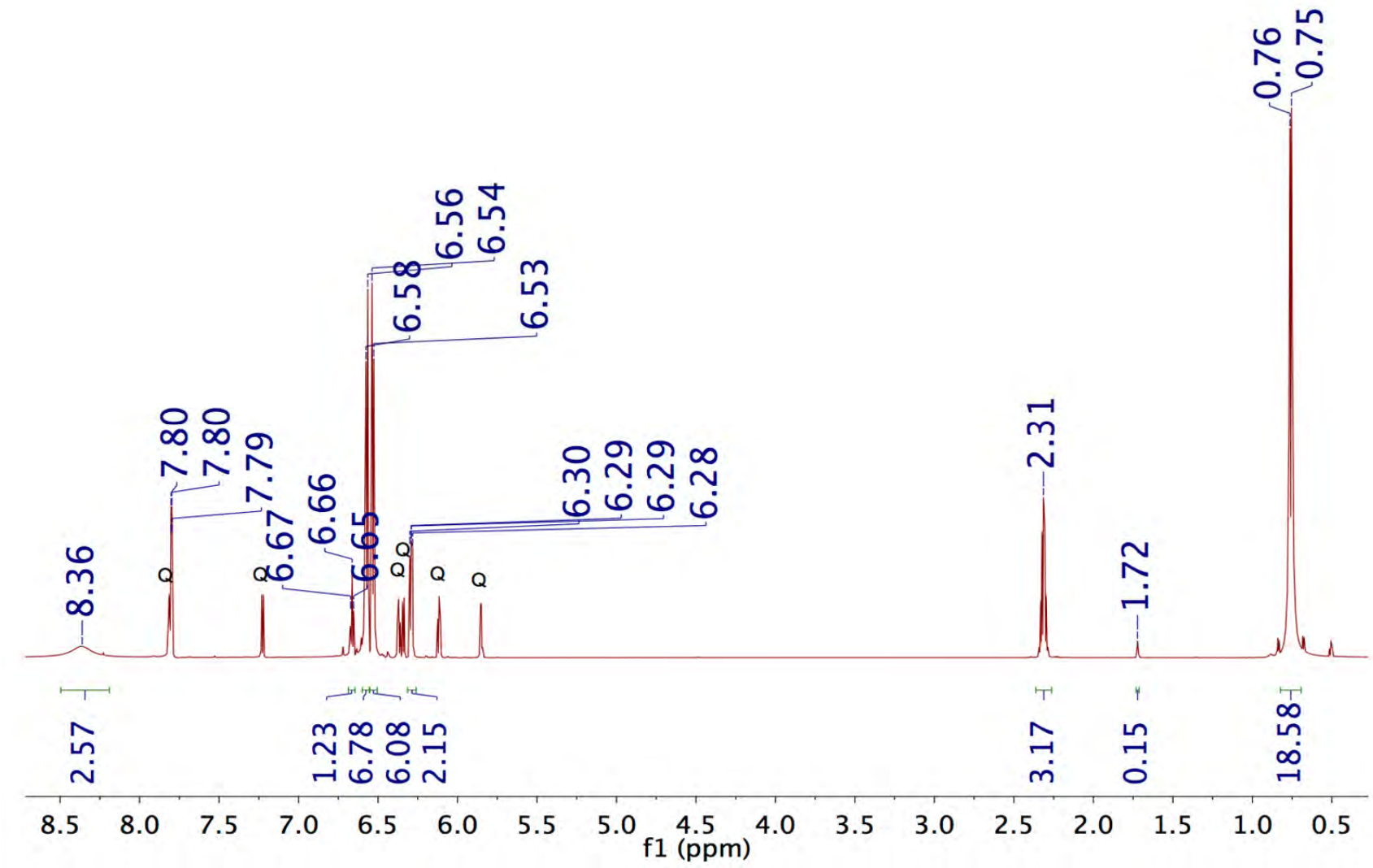

Figure S46: The 1H NMR-spectrum of pyridine mixed with 3 equivalents of 4-isopropylphenol in toluene-*d8*. Quinoline peaks are highlighted with "Q".

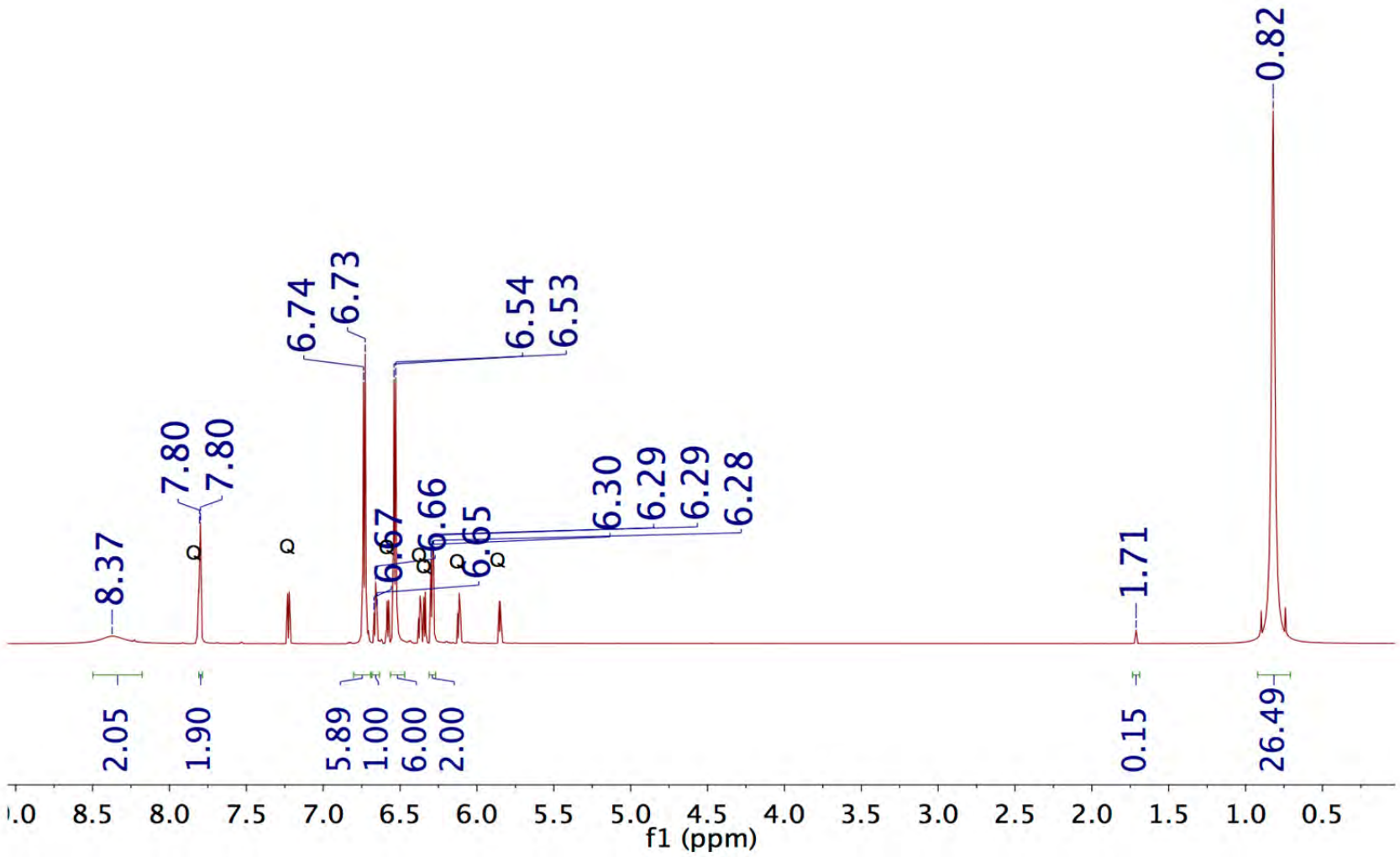

Figure S47: The 1H NMR-spectrum of pyridine mixed with 3 equivalents of 4-*tert*-butylphenol in toluene-*d8*. Quinoline peaks are highlighted with "Q".

4. Computational data

In the following, equilibrium geometries, thermochemical data, lowest vibration frequencies, data from NBO analysis, and NMR chemical shieldings for the systems investigated in this study are compiled. Energies given in Hartree units, geometries in Å, frequencies in cm^{-1}, and chemical shieldings in ppm.
Geometry optimizations and frequency calculations were performed exploiting molecular symmetry, with the corresponding standard orientation of the molecules. For the NBO analysis, the molecules were rotated into an orientation such that the π orbitals at the pyridine N atom points in *z* direction. In the following, the geometries are given for the latter orientation. Electronic energies are given for both orientations, the value in parentheses refers to the NBO calculation. Deviations between the electronic energies for different orientations are due to the different orientation of the DFT integration grids.
For some of the compounds, small imaginary lowest frequencies were observed. These imaginary frequencies are related to methyl rotations and could not be alleviated by reorienting the respective methyl group. They are supposed to be an artefact of the SCRF calculation.

Pyridine

```
================================================================================
Pyridine
--------------------------------------------------------------------------------
Energies and NBO populations
--------------------------------------------------------------------------------

Number of atoms:  11
Full point group                 C2V     NOp   4


N      0.013796   0.000000   0.000000
C      0.712997   1.142358   0.000000
C      2.107606   1.198411   0.000000
C      2.820112   0.000000   0.000000
C      2.107606  -1.198411   0.000000
C      0.712997  -1.142358   0.000000
H      0.127260   2.060220   0.000000
H      2.617005   2.157024   0.000000
H      3.906357   0.000000   0.000000
H      2.617005  -2.157025   0.000000
H      0.127260  -2.060220   0.000000

Electronic energy:                                    -248.27556669 (   -248.27555652)
Zero-point correction=                                   0.088218
Sum of electronic and zero-point Energies=            -248.187349
Sum of electronic and thermal Energies=               -248.183045
Sum of electronic and thermal Enthalpies=             -248.182100
Sum of electronic and thermal Free Energies=          -248.214115

Lowest vibration frequency:          379.1106

Summary of Natural Population Analysis:

                                     Natural Population
               Natural  -----------------------------------------------
   Atom  No    Charge         Core      Valence    Rydberg      Total
-------------------------------------------------------------------
     N    1   -0.47338      1.99946     5.45057    0.02335     7.47338
     C    2    0.04782      1.99923     3.92446    0.02849     5.95218
     C    3   -0.25026      1.99916     4.23443    0.01667     6.25026
     C    4   -0.17004      1.99918     4.15320    0.01766     6.17004
     C    5   -0.25026      1.99916     4.23443    0.01667     6.25026
     C    6    0.04782      1.99923     3.92446    0.02849     5.95218
```

```
     H    7    0.19394      0.00000     0.80473    0.00133     0.80606
     H    8    0.22127      0.00000     0.77729    0.00144     0.77873
     H    9    0.21790      0.00000     0.78078    0.00132     0.78210
     H   10    0.22127      0.00000     0.77729    0.00144     0.77873
     H   11    0.19394      0.00000     0.80473    0.00133     0.80606
=======================================================================
  * Total *    0.00000     11.99543    29.86637    0.13820    42.00000

Contributions to pi population at N atom in pyridine:
    Val( 2p)     1.17094
    Ryd( 3p)     0.00074
    Ryd( 4p)     0.00007
    Ryd( 5p)     0.00004

    Total:       1.17179

-------------------------------------------------------------------------------
NMR properties
-------------------------------------------------------------------------------
Electronic energy (NMR):                          -248.27556669

 1  N    Isotropic =   -99.6517   Anisotropy =   587.1778
 2  C    Isotropic =    21.5106   Anisotropy =   181.3627
 3  C    Isotropic =    50.9414   Anisotropy =   183.3477
 4  C    Isotropic =    37.9582   Anisotropy =   211.9098
 5  C    Isotropic =    50.9414   Anisotropy =   183.3477
 6  C    Isotropic =    21.5106   Anisotropy =   181.3627
 7  H    Isotropic =    22.5326   Anisotropy =     6.4498
 8  H    Isotropic =    23.9899   Anisotropy =     5.3831
 9  H    Isotropic =    23.5386   Anisotropy =     5.3388
10  H    Isotropic =    23.9899   Anisotropy =     5.3831
11  H    Isotropic =    22.5326   Anisotropy =     6.4498
```

Substituted halobenzenes

```
===============================================================================
X = I    R = H
-------------------------------------------------------------------------------
Energies and NBO populations
-------------------------------------------------------------------------------

Number of atoms:  12
Full point group                 C2V     NOp   4


C      0.041351   0.000000   0.000000
C      0.727635   1.217024   0.000000
C      2.125858   1.208234   0.000000
C      2.826909   0.000000   0.000000
C      2.125858  -1.208234   0.000000
C      0.727635  -1.217024   0.000000
H      0.187002   2.156972   0.000000
H      2.662148   2.152595   0.000000
H      3.912429   0.000000   0.000000
H      2.662148  -2.152595   0.000000
H      0.187002  -2.156972   0.000000
I     -2.085973   0.000000   0.000000

Electronic energy:                                -7150.87892577 (  -7150.87892577)
Zero-point correction=                               0.089394
Sum of electronic and zero-point Energies=        -7150.789532
Sum of electronic and thermal Energies=           -7150.783606
Sum of electronic and thermal Enthalpies=         -7150.782662
Sum of electronic and thermal Free Energies=      -7150.820668

Lowest vibration frequency:          148.2531

Summary of Natural Population Analysis:

                                  Natural Population
               Natural  -----------------------------------------------
   Atom  No    Charge         Core      Valence    Rydberg      Total
-------------------------------------------------------------------------
     C    1   -0.20253      1.99874     4.17700    0.02679     6.20253
     C    2   -0.23415      1.99899     4.21477    0.02039     6.23415
     C    3   -0.19333      1.99917     4.17639    0.01778     6.19333
```

C	4	-0.20798	1.99918	4.19127	0.01753	6.20798
C	5	-0.19333	1.99917	4.17639	0.01778	6.19333
C	6	-0.23415	1.99899	4.21477	0.02039	6.23415
H	7	0.22819	0.00000	0.77028	0.00154	0.77181
H	8	0.21935	0.00000	0.77928	0.00137	0.78065
H	9	0.21782	0.00000	0.78085	0.00133	0.78218
H	10	0.21935	0.00000	0.77928	0.00137	0.78065
H	11	0.22819	0.00000	0.77028	0.00154	0.77181
I	12	0.15256	45.99798	6.83003	0.01942	52.84744
* Total *		0.00000	57.99220	35.86057	0.14723	94.00000

X = I R = OCH3

Energies and NBO populations

Number of atoms: 16
Full point group CS NOp 2

C	-0.058340	0.019740	0.000000
C	-0.716327	1.247292	0.000000
C	-2.115844	1.293211	0.000000
C	-2.853733	0.102176	0.000000
C	-2.179705	-1.130230	0.000000
C	-0.789530	-1.174747	0.000000
H	-0.156157	2.175723	0.000000
H	-2.605633	2.259610	0.000000
O	-4.211342	0.036049	0.000000
H	-2.762087	-2.045952	0.000000
H	-0.283149	-2.133655	0.000000
I	2.066479	-0.040892	0.000000
C	-4.947613	1.253954	0.000000
H	-5.998807	0.965347	0.000000
H	-4.733112	1.848153	-0.896417
H	-4.733112	1.848153	0.896417

Electronic energy: -7265.40209411 (-7265.40197845)
Zero-point correction= 0.121583
Sum of electronic and zero-point Energies= -7265.280511
Sum of electronic and thermal Energies= -7265.271924
Sum of electronic and thermal Enthalpies= -7265.270979
Sum of electronic and thermal Free Energies= -7265.315926

Lowest vibration frequency: 62.8273

Summary of Natural Population Analysis:

			Natural Population			
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.23347	1.99872	4.20849	0.02626	6.23347
C	2	-0.21268	1.99900	4.19310	0.02058	6.21268
C	3	-0.28344	1.99907	4.26918	0.01519	6.28344
C	4	0.32577	1.99882	3.65229	0.02312	5.67423
C	5	-0.23310	1.99908	4.21679	0.01723	6.23310
C	6	-0.21627	1.99900	4.19713	0.02014	6.21627
H	7	0.22750	0.00000	0.77093	0.00157	0.77250
H	8	0.22590	0.00000	0.77235	0.00175	0.77410
O	9	-0.54100	1.99971	6.52363	0.01766	8.54100
H	10	0.23014	0.00000	0.76812	0.00174	0.76986
H	11	0.22875	0.00000	0.76977	0.00148	0.77125
I	12	0.14634	45.99797	6.83589	0.01980	52.85366
C	13	-0.21427	1.99927	4.19939	0.01561	6.21427
H	14	0.19773	0.00000	0.80127	0.00100	0.80227
H	15	0.17605	0.00000	0.82190	0.00205	0.82395
H	16	0.17605	0.00000	0.82190	0.00205	0.82395
* Total *		0.00000	61.99065	47.82211	0.18724	110.00000

X = I R = OCH2CH3

Energies and NBO populations

Number of atoms: 19
Full point group   CS   NOp   2

C	0.105245	-0.058393	0.000000
C	-0.758593	1.034251	0.000000
C	-2.144396	0.832402	0.000000
C	-2.661970	-0.470162	0.000000
C	-1.780334	-1.564018	0.000000
C	-0.404321	-1.362710	0.000000
H	-0.370236	2.046851	0.000000
H	-2.797647	1.696656	0.000000
O	-3.985579	-0.775657	0.000000
H	-2.191643	-2.568295	0.000000
H	0.262873	-2.217446	0.000000
I	2.209315	0.250582	0.000000
C	-4.940633	0.291966	0.000000
C	-6.327370	-0.328296	0.000000
H	-4.791010	0.917098	-0.890703
H	-4.791010	0.917098	0.890703
H	-7.084351	0.462387	0.000000
H	-6.475055	-0.948751	0.888688
H	-6.475055	-0.948751	-0.888688

Electronic energy: -7304.71769091 (-7304.71769223)
Zero-point correction=   0.149488
Sum of electronic and zero-point Energies=   -7304.568203
Sum of electronic and thermal Energies=   -7304.558195
Sum of electronic and thermal Enthalpies=   -7304.557250
Sum of electronic and thermal Free Energies=   -7304.605868

Lowest vibration frequency: 37.4409

Summary of Natural Population Analysis:

			Natural Population			
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.23337	1.99871	4.20850	0.02615	6.23337
C	2	-0.21304	1.99900	4.19359	0.02045	6.21304
C	3	-0.28319	1.99907	4.26867	0.01546	6.28319
C	4	0.32878	1.99883	3.64927	0.02312	5.67122
C	5	-0.23286	1.99908	4.21689	0.01690	6.23286
C	6	-0.21687	1.99900	4.19778	0.02008	6.21687
H	7	0.22738	0.00000	0.77104	0.00158	0.77262
H	8	0.22541	0.00000	0.77279	0.00181	0.77459
O	9	-0.55484	1.99970	6.53445	0.02069	8.55484
H	10	0.22957	0.00000	0.76874	0.00169	0.77043
H	11	0.22839	0.00000	0.77012	0.00149	0.77161
I	12	0.14482	45.99798	6.83746	0.01975	52.85518
C	13	-0.03658	1.99924	4.01887	0.01847	6.03658
C	14	-0.59441	1.99938	4.58646	0.00858	6.59441
H	15	0.17539	0.00000	0.82219	0.00242	0.82461
H	16	0.17539	0.00000	0.82219	0.00242	0.82461
H	17	0.21134	0.00000	0.78751	0.00115	0.78866
H	18	0.20934	0.00000	0.78899	0.00167	0.79066
H	19	0.20934	0.00000	0.78899	0.00167	0.79066
* Total *		0.00000	63.99000	53.80448	0.20553	118.00000

X = I   R = CH3

Energies and NBO populations

Number of atoms: 15
Full point group   CS   NOp   2

C	-0.003716	0.000886	0.000000
C	-0.693341	1.213264	0.000000
C	-2.092105	1.202649	0.000000
C	-2.814767	0.003089	0.000000

```
C     -2.092589  -1.200383   0.000000
C     -0.696800  -1.212883   0.000000
H     -0.157864   2.156174   0.000000
H     -2.623718   2.150703   0.000000
C     -4.326765  -0.003459   0.000000
H     -2.625834  -2.147952   0.000000
H     -0.161585  -2.156023   0.000000
I      2.123076  -0.001613   0.000000
H     -4.727225   1.013722   0.000000
H     -4.717711  -0.521805  -0.882753
H     -4.717711  -0.521805   0.882753

Electronic energy:                                  -7190.19304383 (  -7190.19304378)
Zero-point correction=                                  0.116324
Sum of electronic and zero-point Energies=          -7190.076720
Sum of electronic and thermal Energies=             -7190.069733
Sum of electronic and thermal Enthalpies=           -7190.068789
Sum of electronic and thermal Free Energies=        -7190.109950

Lowest vibration frequency:          -10.0416

Summary of Natural Population Analysis:

                                  Natural Population
               Natural  -----------------------------------------------
   Atom  No    Charge         Core      Valence    Rydberg      Total
------------------------------------------------------------------------
     C    1   -0.21036      1.99872     4.18534    0.02630     6.21036
     C    2   -0.22707      1.99899     4.20729    0.02079     6.22707
     C    3   -0.19620      1.99906     4.18061    0.01654     6.19620
     C    4   -0.02961      1.99907     4.01516    0.01538     6.02961
     C    5   -0.19359      1.99906     4.17791    0.01663     6.19359
     C    6   -0.22628      1.99899     4.20662    0.02067     6.22628
     H    7    0.22712      0.00000     0.77127    0.00161     0.77288
     H    8    0.21573      0.00000     0.78268    0.00160     0.78427
     C    9   -0.59774      1.99932     4.58837    0.01005     6.59774
     H   10    0.21588      0.00000     0.78257    0.00155     0.78412
     H   11    0.22701      0.00000     0.77138    0.00161     0.77299
     I   12    0.14725     45.99798     6.83509    0.01968    52.85275
     H   13    0.21126      0.00000     0.78747    0.00127     0.78874
     H   14    0.21831      0.00000     0.78037    0.00132     0.78169
     H   15    0.21831      0.00000     0.78037    0.00132     0.78169
========================================================================
  * Total *    0.00000     59.99118    41.85250    0.15632   102.00000

================================================================================================
X = I    R = CHCH32
------------------------------------------------------------------------------------------------
Energies and NBO populations
------------------------------------------------------------------------------------------------

Number of atoms:  21
Full point group                 C1      NOp   1


C     -0.066773  -0.024320   0.042338
C      0.694956   1.143132   0.094302
C      2.088164   1.043170   0.170259
C      2.736047  -0.198685   0.195410
C      1.940685  -1.354189   0.141731
C      0.548992  -1.278425   0.065623
H      0.219383   2.117668   0.076396
H      2.677518   1.955992   0.210553
C      4.255134  -0.285066   0.278508
H      2.405385  -2.336427   0.158997
H     -0.043116  -2.185934   0.025278
I     -2.187891   0.099031  -0.073676
H      4.632281   0.745440   0.307401
C      4.716170  -0.987442   1.572177
C      4.856341  -0.967557  -0.967295
H      5.809817  -0.983494   1.639606
H      4.383537  -2.031583   1.596053
H      4.316062  -0.485879   2.459280
H      4.555991  -0.451772  -1.885109
H      5.950759  -0.963620  -0.913845
H      4.529171  -2.010870  -1.044144
```

```
Electronic energy:                                  -7268.81371240 (  -7268.81372694)
Zero-point correction=                                  0.172900
Sum of electronic and zero-point Energies=          -7268.640812
Sum of electronic and thermal Energies=             -7268.630444
Sum of electronic and thermal Enthalpies=           -7268.629500
Sum of electronic and thermal Free Energies=        -7268.678721

Lowest vibration frequency:           37.3948

Summary of Natural Population Analysis:

                                    Natural Population
               Natural  -----------------------------------------------
   Atom  No    Charge         Core      Valence    Rydberg      Total
------------------------------------------------------------------------
     C    1   -0.20862      1.99872     4.18338    0.02652     6.20862
     C    2   -0.22741      1.99899     4.20779    0.02063     6.22741
     C    3   -0.19341      1.99905     4.17788    0.01649     6.19341
     C    4   -0.01576      1.99902     3.99655    0.02019     6.01576
     C    5   -0.19588      1.99904     4.18062    0.01622     6.19588
     C    6   -0.22700      1.99899     4.20726    0.02075     6.22700
     H    7    0.22735      0.00000     0.77107    0.00158     0.77265
     H    8    0.21609      0.00000     0.78221    0.00170     0.78391
     C    9   -0.24420      1.99920     4.22936    0.01564     6.24420
     H   10    0.21617      0.00000     0.78213    0.00170     0.78383
     H   11    0.22669      0.00000     0.77172    0.00159     0.77331
     I   12    0.14677     45.99798     6.83573    0.01952    52.85323
     H   13    0.19961      0.00000     0.79743    0.00295     0.80039
     C   14   -0.57024      1.99935     4.56141    0.00948     6.57024
     C   15   -0.57025      1.99935     4.56142    0.00948     6.57025
     H   16    0.20430      0.00000     0.79452    0.00119     0.79570
     H   17    0.19798      0.00000     0.80067    0.00135     0.80202
     H   18    0.20778      0.00000     0.79122    0.00100     0.79222
     H   19    0.20778      0.00000     0.79121    0.00100     0.79222
     H   20    0.20430      0.00000     0.79452    0.00119     0.79570
     H   21    0.19797      0.00000     0.80068    0.00135     0.80203
========================================================================
  * Total *    0.00000     63.98971    53.81878    0.19152   118.00000

================================================================================================
X = I    R = H
------------------------------------------------------------------------------------------------
Energies and NBO populations
------------------------------------------------------------------------------------------------

Number of atoms:  12
Full point group                 C2V     NOp   4


C     -0.018117   0.000000   0.000000
C     -0.706870   1.216023   0.000000
C     -2.104209   1.217523   0.000000
C     -2.773121   0.000000   0.000000
C     -2.104209  -1.217523   0.000000
C     -0.706870  -1.216023   0.000000
H     -0.169752   2.157436   0.000000
H     -2.664609   2.146065   0.000000
F     -4.125117   0.000000   0.000000
H     -2.664609  -2.146065   0.000000
H     -0.169752  -2.157436   0.000000
I      2.107236   0.000000   0.000000

Electronic energy:                                  -7250.12236332 (  -7250.12236332)
Zero-point correction=                                  0.081090
Sum of electronic and zero-point Energies=          -7250.041273
Sum of electronic and thermal Energies=             -7250.034503
Sum of electronic and thermal Enthalpies=           -7250.033559
Sum of electronic and thermal Free Energies=        -7250.073702

Lowest vibration frequency:           99.3474

Summary of Natural Population Analysis:

                                    Natural Population
               Natural  -----------------------------------------------
   Atom  No    Charge         Core      Valence    Rydberg      Total
------------------------------------------------------------------------
```

C	1	-0.22040	1.99874	4.19506	0.02660	6.22040
C	2	-0.21333	1.99900	4.19445	0.01987	6.21333
C	3	-0.25720	1.99905	4.24117	0.01698	6.25720
C	4	0.40924	1.99850	3.56573	0.02653	5.59076
C	5	-0.25720	1.99905	4.24117	0.01698	6.25720
C	6	-0.21333	1.99900	4.19445	0.01987	6.21333
H	7	0.23257	0.00000	0.76590	0.00153	0.76743
H	8	0.23789	0.00000	0.76058	0.00153	0.76211
F	9	-0.35126	1.99993	7.34330	0.00803	9.35126
H	10	0.23789	0.00000	0.76058	0.00153	0.76211
H	11	0.23257	0.00000	0.76590	0.00153	0.76743
I	12	0.16255	45.99798	6.81981	0.01966	52.83745
* Total *		0.00000	59.99125	41.84812	0.16063	102.00000

X = I R = Cl

Energies and NBO populations

Number of atoms: 12
Full point group C2V NOp 4

C	0.017510	0.000000	0.000000
C	-0.672835	1.214664	0.000000
C	-2.069816	1.215256	0.000000
C	-2.753001	0.000000	0.000000
C	-2.069816	-1.215256	0.000000
C	-0.672835	-1.214664	0.000000
H	-0.137820	2.157458	0.000000
H	-2.615745	2.152111	0.000000
Cl	-4.512650	0.000000	0.000000
H	-2.615745	-2.152111	0.000000
H	-0.137820	-2.157458	0.000000
I	2.140572	0.000000	0.000000

Electronic energy: -7610.44454720 (-7610.44454720)
Zero-point correction= 0.079797
Sum of electronic and zero-point Energies= -7610.364750
Sum of electronic and thermal Energies= -7610.357599
Sum of electronic and thermal Enthalpies= -7610.356655
Sum of electronic and thermal Free Energies= -7610.398106

Lowest vibration frequency: 77.9515

Summary of Natural Population Analysis:

		Natural	Natural Population			
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.20992	1.99874	4.18462	0.02657	6.20992
C	2	-0.21472	1.99899	4.19545	0.02028	6.21472
C	3	-0.21529	1.99897	4.19764	0.01868	6.21529
C	4	-0.04134	1.99860	4.01988	0.02285	6.04134
C	5	-0.21529	1.99897	4.19764	0.01868	6.21529
C	6	-0.21472	1.99899	4.19545	0.02028	6.21472
H	7	0.23363	0.00000	0.76482	0.00155	0.76637
H	8	0.23650	0.00000	0.76188	0.00162	0.76350
Cl	9	0.00264	9.99962	6.97772	0.02001	16.99736
H	10	0.23650	0.00000	0.76188	0.00162	0.76350
H	11	0.23363	0.00000	0.76482	0.00155	0.76637
I	12	0.16838	45.99797	6.81389	0.01975	52.83162
* Total *		0.00000	67.99084	41.83569	0.17347	110.00000

X = I R = OCF3

Energies and NBO populations

Number of atoms: 16
Full point group CS NOp 2

```
C     -0.089556   0.053617   0.011044
C      0.747970  -1.061816   0.029756
C      2.136476  -0.896930   0.048217
C      2.661933   0.393849   0.055099
C      1.830534   1.512830   0.037476
C      0.447325   1.344538   0.013592
H      0.336391  -2.064506   0.026571
H      2.772469  -1.772743   0.053719
O      4.026977   0.697340   0.052793
H      2.270078   2.504268   0.042994
H     -0.198345   2.215135  -0.000012
I     -2.195242  -0.212710  -0.020843
C      4.966030  -0.233952   0.312503
F      6.144175   0.384404   0.346945
F      5.028359  -1.195067  -0.632586
F      4.776899  -0.853849   1.492434

Electronic energy:                                  -7563.16097268 (  -7563.16097206)
Zero-point correction=                                  0.098069
Sum of electronic and zero-point Energies=          -7563.062904
Sum of electronic and thermal Energies=             -7563.052458
Sum of electronic and thermal Enthalpies=           -7563.051514
Sum of electronic and thermal Free Energies=        -7563.102881

Lowest vibration frequency:          14.4635

Summary of Natural Population Analysis:

                                     Natural Population
               Natural  ----------------------------------------------
   Atom  No    Charge         Core      Valence    Rydberg      Total
-----------------------------------------------------------------------
     C    1   -0.21726      1.99873     4.19189    0.02664     6.21726
     C    2   -0.20795      1.99900     4.18880    0.02015     6.20795
     C    3   -0.25135      1.99904     4.23673    0.01557     6.25135
     C    4    0.29345      1.99871     3.68542    0.02242     5.70655
     C    5   -0.22141      1.99906     4.20526    0.01708     6.22141
     C    6   -0.21051      1.99900     4.19165    0.01986     6.21051
     H    7    0.23407      0.00000     0.76442    0.00150     0.76593
     H    8    0.23959      0.00000     0.75849    0.00192     0.76041
     O    9   -0.55041      1.99964     6.53460    0.01617     8.55041
     H   10    0.23892      0.00000     0.75947    0.00160     0.76108
     H   11    0.23398      0.00000     0.76454    0.00148     0.76602
     I   12    0.16924     45.99797     6.81313    0.01967    52.83076
     C   13    1.28379      1.99965     2.64626    0.07030     4.71621
     F   14   -0.33111      1.99991     7.32489    0.00632     9.33111
     F   15   -0.35345      1.99992     7.34670    0.00684     9.35345
     F   16   -0.34959      1.99991     7.34292    0.00676     9.34959
=======================================================================
  * Total *    0.00000     67.99053    65.75518    0.25429   134.00000

================================================================================================
X = I    R = COOCH3
------------------------------------------------------------------------------------------------
Energies and NBO populations
------------------------------------------------------------------------------------------------

Number of atoms:  18
Full point group                 CS      NOp   2


C      0.042119   0.012006   0.000000
C     -0.617888   1.245227   0.000000
C     -2.011574   1.267811   0.000000
C     -2.743691   0.072699   0.000000
C     -2.066037  -1.154646   0.000000
C     -0.671625  -1.190025   0.000000
H     -0.057674   2.173297   0.000000
H     -2.544094   2.213032   0.000000
C     -4.235796   0.160397   0.000000
H     -2.627496  -2.081835   0.000000
H     -0.152689  -2.141579   0.000000
I      2.165847  -0.038424   0.000000
O     -4.820538  -1.051018   0.000000
C     -6.259561  -1.058482   0.000000
H     -6.543390  -2.110091   0.000000
```

```
H     -6.642485  -0.557046  -0.891758
H     -6.642485  -0.557046   0.891758
O     -4.857351   1.201549   0.000000

Electronic energy:                                -7378.76322051 (  -7378.76312785)
Zero-point correction=                                0.131918
Sum of electronic and zero-point Energies=        -7378.631303
Sum of electronic and thermal Energies=           -7378.620809
Sum of electronic and thermal Enthalpies=         -7378.619865
Sum of electronic and thermal Free Energies=      -7378.669884

Lowest vibration frequency:          49.4715

Summary of Natural Population Analysis:

                                  Natural Population
              Natural  -----------------------------------------------
   Atom  No    Charge         Core      Valence    Rydberg      Total
------------------------------------------------------------------------
     C    1   -0.18406      1.99875     4.15842    0.02690     6.18406
     C    2   -0.23371      1.99899     4.21449    0.02023     6.23371
     C    3   -0.14559      1.99910     4.12944    0.01705     6.14559
     C    4   -0.16080      1.99893     4.14376    0.01811     6.16080
     C    5   -0.15119      1.99910     4.13572    0.01637     6.15119
     C    6   -0.23448      1.99899     4.21527    0.02022     6.23448
     H    7    0.23247      0.00000     0.76600    0.00152     0.76753
     H    8    0.23983      0.00000     0.75856    0.00161     0.76017
     C    9    0.80370      1.99930     3.15035    0.04665     5.19630
     H   10    0.23657      0.00000     0.76189    0.00154     0.76343
     H   11    0.23181      0.00000     0.76666    0.00154     0.76819
     I   12    0.17309     45.99796     6.80953    0.01941    52.82691
     O   13   -0.54966      1.99972     6.53584    0.01410     8.54966
     C   14   -0.21740      1.99926     4.20243    0.01570     6.21740
     H   15    0.19243      0.00000     0.80650    0.00107     0.80757
     H   16    0.19049      0.00000     0.80782    0.00169     0.80951
     H   17    0.19049      0.00000     0.80782    0.00169     0.80951
     O   18   -0.61399      1.99975     6.60304    0.01120     8.61399
========================================================================
  * Total *    0.00000     65.98985    57.77356    0.23659   124.00000

================================================================================
X = I    R = COCH3
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Energies and NBO populations
--------------------------------------------------------------------------------

Number of atoms:  17
Full point group                 CS      NOp   2


C      0.000506   0.019377   0.000000
C     -0.649641   1.258950   0.000000
C     -2.041752   1.292533   0.000000
C     -2.793674   0.106421   0.000000
C     -2.118943  -1.124072   0.000000
C     -0.723978  -1.174965   0.000000
H     -0.080694   2.181809   0.000000
H     -2.566330   2.242374   0.000000
C     -4.294961   0.204747   0.000000
H     -2.670542  -2.058447   0.000000
H     -0.214468  -2.131513   0.000000
I      2.122829  -0.051840   0.000000
C     -5.109984  -1.075257   0.000000
O     -4.841699   1.294324   0.000000
H     -6.169715  -0.819096   0.000000
H     -4.881891  -1.681590   0.883636
H     -4.881891  -1.681590  -0.883636

Electronic energy:                                -7303.52753299 (  -7303.52749341)
Zero-point correction=                                0.126348
Sum of electronic and zero-point Energies=        -7303.401185
Sum of electronic and thermal Energies=           -7303.391682
Sum of electronic and thermal Enthalpies=         -7303.390738
Sum of electronic and thermal Free Energies=      -7303.438180

Lowest vibration frequency:          56.3927
```

Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.18327	1.99875	4.15746	0.02706	6.18327
C	2	-0.23198	1.99899	4.21284	0.02015	6.23198
C	3	-0.14185	1.99909	4.12470	0.01806	6.14185
C	4	-0.15529	1.99895	4.13881	0.01753	6.15529
C	5	-0.16076	1.99910	4.14620	0.01546	6.16076
C	6	-0.23475	1.99899	4.21522	0.02054	6.23475
H	7	0.23222	0.00000	0.76626	0.00153	0.76778
H	8	0.23985	0.00000	0.75828	0.00187	0.76015
C	9	0.56607	1.99931	3.39597	0.03865	5.43393
H	10	0.22324	0.00000	0.77530	0.00145	0.77676
H	11	0.23162	0.00000	0.76681	0.00156	0.76838
I	12	0.17532	45.99796	6.80730	0.01942	52.82468
C	13	-0.67871	1.99930	4.67109	0.00832	6.67871
O	14	-0.57344	1.99976	6.56006	0.01362	8.57344
H	15	0.23274	0.00000	0.76542	0.00184	0.76726
H	16	0.22949	0.00000	0.76912	0.00140	0.77051
H	17	0.22949	0.00000	0.76912	0.00140	0.77051
* Total *		0.00000	63.99019	51.79994	0.20986	116.00000

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X = I R = CF3

Energies and NBO populations

Number of atoms: 15
Full point group CS NOp 2

C	0.005904	0.001189	0.000000
C	-0.685581	1.214047	0.000000
C	-2.082804	1.205217	0.000000
C	-2.773461	-0.007806	0.000000
C	-2.071802	-1.219146	0.000000
C	-0.678468	-1.219063	0.000000
H	-0.151750	2.157383	0.000000
H	-2.624906	2.144155	0.000000
C	-4.281686	-0.043007	0.000000
H	-2.606015	-2.164120	0.000000
H	-0.137261	-2.157898	0.000000
I	2.128800	0.003031	0.000000
F	-4.830279	1.187480	0.000000
F	-4.769009	-0.693223	-1.083113
F	-4.769009	-0.693223	1.083113

Electronic energy: -7487.94206436 (-7487.94192516)
Zero-point correction= 0.093701
Sum of electronic and zero-point Energies= -7487.848363
Sum of electronic and thermal Energies= -7487.839689
Sum of electronic and thermal Enthalpies= -7487.838744
Sum of electronic and thermal Free Energies= -7487.884464

Lowest vibration frequency: -12.3412

Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.19023	1.99875	4.16428	0.02720	6.19023
C	2	-0.22455	1.99899	4.20543	0.02013	6.22455
C	3	-0.16671	1.99908	4.15089	0.01673	6.16671
C	4	-0.15263	1.99891	4.13618	0.01753	6.15263
C	5	-0.16287	1.99908	4.14669	0.01710	6.16287
C	6	-0.22376	1.99900	4.20459	0.02017	6.22376
H	7	0.23469	0.00000	0.76381	0.00149	0.76531
H	8	0.23829	0.00000	0.76014	0.00157	0.76171
C	9	1.06719	1.99913	2.87350	0.06017	4.93281
H	10	0.23432	0.00000	0.76412	0.00155	0.76568

H	11	0.23479	0.00000	0.76370	0.00152	0.76521
I	12	0.17964	45.99796	6.80299	0.01940	52.82036
F	13	-0.35426	1.99992	7.34797	0.00637	9.35426
F	14	-0.35696	1.99992	7.35051	0.00653	9.35696
F	15	-0.35696	1.99992	7.35051	0.00653	9.35696
* Total *		0.00000	65.99066	59.78532	0.22402	126.00000

X = I R = CN

Energies and NBO populations

Number of atoms: 13
Full point group C2V NOp 4

C	-0.035153	0.000000	0.000000
C	-0.723369	1.217803	0.000000
C	-2.116504	1.217079	0.000000
C	-2.818056	0.000000	0.000000
C	-2.116504	-1.217079	0.000000
C	-0.723369	-1.217803	0.000000
H	-0.184810	2.158253	0.000000
H	-2.659682	2.155953	0.000000
C	-4.251598	0.000000	0.000000
H	-2.659682	-2.155953	0.000000
H	-0.184810	-2.158253	0.000000
I	2.083774	0.000000	0.000000
N	-5.410235	0.000000	0.000000

Electronic energy: -7243.12232060 (-7243.12232060)
Zero-point correction= 0.087947
Sum of electronic and zero-point Energies= -7243.034374
Sum of electronic and thermal Energies= -7243.026645
Sum of electronic and thermal Enthalpies= -7243.025701
Sum of electronic and thermal Free Energies= -7243.068202

Lowest vibration frequency: 70.5975

Summary of Natural Population Analysis:

		Natural	Natural Population			
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.18811	1.99876	4.16205	0.02731	6.18811
C	2	-0.22564	1.99899	4.20664	0.02001	6.22564
C	3	-0.13786	1.99910	4.12320	0.01556	6.13786
C	4	-0.18695	1.99888	4.17113	0.01694	6.18695
C	5	-0.13786	1.99910	4.12320	0.01556	6.13786
C	6	-0.22564	1.99899	4.20664	0.02001	6.22564
H	7	0.23700	0.00000	0.76152	0.00148	0.76300
H	8	0.23536	0.00000	0.76338	0.00126	0.76464
C	9	0.30521	1.99927	3.66164	0.03388	5.69479
H	10	0.23536	0.00000	0.76338	0.00126	0.76464
H	11	0.23700	0.00000	0.76152	0.00148	0.76300
I	12	0.19112	45.99794	6.79153	0.01941	52.80888
N	13	-0.33900	1.99959	5.31940	0.02001	7.33900
* Total *		0.00000	61.99061	43.81523	0.19417	106.00000

X = I R = NO2

Energies and NBO populations

Number of atoms: 14
Full point group C2V NOp 4

C	0.009124	0.000000	0.000000
C	0.695773	1.219571	0.000000
C	2.089327	1.220376	0.000000
C	2.763878	0.000000	0.000000

```
C      2.089327  -1.220376   0.000000
C      0.695773  -1.219571   0.000000
H      0.156385   2.159224   0.000000
H      2.648081   2.148282   0.000000
N      4.238219   0.000000   0.000000
H      2.648081  -2.148282   0.000000
H      0.156385  -2.159224   0.000000
I     -2.109328   0.000000   0.000000
O      4.810710   1.084692   0.000000
O      4.810710  -1.084692   0.000000

Electronic energy:                                -7355.39158801 (  -7355.39158801)
Zero-point correction=                                0.091655
Sum of electronic and zero-point Energies=        -7355.299933
Sum of electronic and thermal Energies=           -7355.291422
Sum of electronic and thermal Enthalpies=         -7355.290478
Sum of electronic and thermal Free Energies=      -7355.335520

Lowest vibration frequency:          47.4789

Summary of Natural Population Analysis:

                                  Natural Population
              Natural  -----------------------------------------------
   Atom  No    Charge         Core      Valence    Rydberg      Total
------------------------------------------------------------------------
     C    1   -0.18159      1.99876     4.15540    0.02743     6.18159
     C    2   -0.22261      1.99900     4.20364    0.01997     6.22261
     C    3   -0.17062      1.99906     4.15308    0.01847     6.17062
     C    4    0.06520      1.99879     3.91514    0.02087     5.93480
     C    5   -0.17062      1.99906     4.15308    0.01847     6.17062
     C    6   -0.22261      1.99900     4.20364    0.01997     6.22261
     H    7    0.23837      0.00000     0.76018    0.00144     0.76163
     H    8    0.25466      0.00000     0.74347    0.00187     0.74534
     N    9    0.48981      1.99946     4.45564    0.05510     6.51019
     H   10    0.25466      0.00000     0.74347    0.00187     0.74534
     H   11    0.23837      0.00000     0.76018    0.00144     0.76163
     I   12    0.20045     45.99794     6.78206    0.01956    52.79955
     O   13   -0.38674      1.99980     6.37205    0.01489     8.38674
     O   14   -0.38674      1.99980     6.37205    0.01489     8.38674
========================================================================
  * Total *    0.00000     63.99066    51.77309    0.23625   116.00000

================================================================================
X = Br    R = H
--------------------------------------------------------------------------------
Energies and NBO populations
--------------------------------------------------------------------------------

Number of atoms:  12
Full point group                 C2V     NOp   4


C      0.026165   0.000000   0.015106
C      0.006109   0.000000   1.410053
C      1.221552   0.000000   2.100878
C      2.433001   0.000000   1.404694
C      2.430190   0.000000   0.007456
C      1.224196   0.000000  -0.699736
H     -0.936240   0.000000   1.946289
H      1.214481   0.000000   3.186666
H      3.372919   0.000000   1.947356
H      3.366974   0.000000  -0.541561
H      1.217415   0.000000  -1.783952
Br    -1.633754   0.000000  -0.943249

Electronic energy:                                -2805.60842779 (  -2805.60846734)
Zero-point correction=                                0.089762
Sum of electronic and zero-point Energies=        -2805.518666
Sum of electronic and thermal Energies=           -2805.512896
Sum of electronic and thermal Enthalpies=         -2805.511952
Sum of electronic and thermal Free Energies=      -2805.548950

Lowest vibration frequency:         165.4216

Summary of Natural Population Analysis:
```

			Natural Population			
		Natural				
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.10983	1.99865	4.08836	0.02281	6.10983
C	2	-0.23357	1.99897	4.21534	0.01926	6.23357
C	3	-0.19218	1.99917	4.17532	0.01769	6.19218
C	4	-0.21102	1.99918	4.19429	0.01755	6.21102
C	5	-0.19218	1.99917	4.17532	0.01769	6.19218
C	6	-0.23353	1.99897	4.21530	0.01926	6.23353
H	7	0.23021	0.00000	0.76820	0.00159	0.76979
H	8	0.21906	0.00000	0.77954	0.00140	0.78094
H	9	0.21780	0.00000	0.78089	0.00131	0.78220
H	10	0.21907	0.00000	0.77953	0.00140	0.78093
H	11	0.23022	0.00000	0.76819	0.00159	0.76978
Br	12	0.05595	27.99926	6.92540	0.01939	34.94405
* Total *		0.00000	39.99338	35.86568	0.14094	76.00000

X = Br R = OCH3

Energies and NBO populations

Number of atoms: 16
Full point group CS NOp 2

C	-0.021145	0.000000	-0.055180
C	-0.073976	0.000000	1.334325
C	1.113866	0.000000	2.075922
C	2.349902	0.000000	1.416132
C	2.385946	0.000000	0.011860
C	1.206431	0.000000	-0.724641
H	-1.028145	0.000000	1.849285
H	1.053278	0.000000	3.157552
O	3.558312	0.000000	2.039672
H	3.349305	0.000000	-0.487523
H	1.242124	0.000000	-1.808298
Br	-1.649021	0.000000	-1.067231
C	3.585599	0.000000	3.462562
H	4.640090	0.000000	3.739028
H	3.102705	-0.896540	3.869812
H	3.102705	0.896540	3.869812

Electronic energy: -2920.13113367 (-2920.13111411)
Zero-point correction= 0.121964
Sum of electronic and zero-point Energies= -2920.009170
Sum of electronic and thermal Energies= -2920.000772
Sum of electronic and thermal Enthalpies= -2919.999828
Sum of electronic and thermal Free Energies= -2920.043692

Lowest vibration frequency: 67.4077

Summary of Natural Population Analysis:

			Natural Population			
		Natural				
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.13961	1.99863	4.11858	0.02240	6.13961
C	2	-0.21228	1.99899	4.19406	0.01924	6.21228
C	3	-0.28212	1.99907	4.26794	0.01511	6.28212
C	4	0.32306	1.99882	3.65509	0.02304	5.67694
C	5	-0.23180	1.99908	4.21562	0.01709	6.23180
C	6	-0.21554	1.99899	4.19774	0.01881	6.21554
H	7	0.22950	0.00000	0.76886	0.00164	0.77050
H	8	0.22559	0.00000	0.77262	0.00179	0.77441
O	9	-0.54195	1.99971	6.52451	0.01772	8.54195
H	10	0.22983	0.00000	0.76841	0.00176	0.77017
H	11	0.23062	0.00000	0.76784	0.00154	0.76938
Br	12	0.04968	27.99927	6.93148	0.01956	34.95032
C	13	-0.21422	1.99928	4.19929	0.01565	6.21422
H	14	0.19760	0.00000	0.80140	0.00100	0.80240
H	15	0.17582	0.00000	0.82212	0.00206	0.82418
H	16	0.17582	0.00000	0.82212	0.00206	0.82418

```
=======================================================================
  * Total *    0.00000     43.99184    47.82770    0.18047    92.00000

=======================================================================================
X = Br    R = OCH2CH3
---------------------------------------------------------------------------------------
Energies and NBO populations
---------------------------------------------------------------------------------------

Number of atoms:  19
Full point group                 CS      NOp   2


C     -0.045510   0.000000  -0.114531
C     -0.125519   0.000000   1.273649
C      1.047249   0.000000   2.038886
C      2.297252   0.000000   1.404304
C      2.359501   0.000000   0.000383
C      1.194809   0.000000  -0.759732
H     -1.089740   0.000000   1.769619
H      0.964026   0.000000   3.118952
O      3.492367   0.000000   2.051477
H      3.332482   0.000000  -0.480157
H      1.252233   0.000000  -1.842510
Br    -1.653964   0.000000  -1.158330
C      3.499637   0.000000   3.483837
C      4.948791   0.000000   3.939528
H      2.972883  -0.890756   3.852099
H      2.972883   0.890756   3.852099
H      4.990954   0.000000   5.033365
H      5.470763   0.888694   3.572967
H      5.470763  -0.888694   3.572967

Electronic energy:                                -2959.44673102 (  -2959.44668799)
Zero-point correction=                                0.149913
Sum of electronic and zero-point Energies=        -2959.296818
Sum of electronic and thermal Energies=           -2959.286984
Sum of electronic and thermal Enthalpies=         -2959.286040
Sum of electronic and thermal Free Energies=      -2959.333564

Lowest vibration frequency:          43.3331

Summary of Natural Population Analysis:

                                  Natural Population
               Natural  -----------------------------------------------
   Atom  No    Charge         Core      Valence    Rydberg      Total
-----------------------------------------------------------------------
     C    1   -0.13974      1.99863     4.11878    0.02232     6.13974
     C    2   -0.21258      1.99899     4.19451    0.01908     6.21258
     C    3   -0.28190      1.99908     4.26746    0.01536     6.28190
     C    4    0.32599      1.99883     3.65216    0.02302     5.67401
     C    5   -0.23158      1.99909     4.21577    0.01673     6.23158
     C    6   -0.21612      1.99899     4.19839    0.01874     6.21612
     H    7    0.22921      0.00000     0.76914    0.00165     0.77079
     H    8    0.22511      0.00000     0.77305    0.00184     0.77489
     O    9   -0.55564      1.99970     6.53516    0.02078     8.55564
     H   10    0.22925      0.00000     0.76904    0.00171     0.77075
     H   11    0.23038      0.00000     0.76809    0.00154     0.76962
    Br   12    0.04838     27.99927     6.93282    0.01953    34.95162
     C   13   -0.03650      1.99924     4.01873    0.01852     6.03650
     C   14   -0.59441      1.99938     4.58645    0.00858     6.59441
     H   15    0.17513      0.00000     0.82244    0.00243     0.82487
     H   16    0.17513      0.00000     0.82244    0.00243     0.82487
     H   17    0.21126      0.00000     0.78759    0.00115     0.78874
     H   18    0.20931      0.00000     0.78902    0.00167     0.79069
     H   19    0.20931      0.00000     0.78902    0.00167     0.79069
=======================================================================
  * Total *    0.00000     45.99118    53.81005    0.19877   100.00000

=======================================================================================
X = Br    R = CH3
---------------------------------------------------------------------------------------
Energies and NBO populations
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Number of atoms:  15
```

Full point group CS NOp 2

C	-0.004197	0.000000	-0.001259
C	-0.019803	0.000000	1.391377
C	1.196396	0.000000	2.081792
C	2.422808	0.000000	1.405122
C	2.400371	0.000000	0.001636
C	1.198864	0.000000	-0.708350
H	-0.959566	0.000000	1.932430
H	1.182445	0.000000	3.168541
C	3.734961	0.000000	2.156354
H	3.336339	0.000000	-0.551504
H	1.199725	0.000000	-1.792748
Br	-1.661419	0.000000	-0.963865
H	3.572055	0.000000	3.237353
H	4.333208	-0.882694	1.903727
H	4.333208	0.882694	1.903727

Electronic energy: -2844.92239987 (-2844.92244554)
Zero-point correction= 0.116777
Sum of electronic and zero-point Energies= -2844.805623
Sum of electronic and thermal Energies= -2844.797921
Sum of electronic and thermal Enthalpies= -2844.796977
Sum of electronic and thermal Free Energies= -2844.839932

Lowest vibration frequency: 28.1949

Summary of Natural Population Analysis:

		Natural	Natural Population			
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.11762	1.99864	4.09654	0.02244	6.11762
C	2	-0.22655	1.99897	4.20810	0.01948	6.22655
C	3	-0.19503	1.99906	4.17952	0.01645	6.19503
C	4	-0.03275	1.99907	4.01834	0.01534	6.03275
C	5	-0.19240	1.99906	4.17679	0.01655	6.19240
C	6	-0.22556	1.99897	4.20724	0.01935	6.22556
H	7	0.22910	0.00000	0.76922	0.00168	0.77090
H	8	0.21537	0.00000	0.78300	0.00162	0.78463
C	9	-0.59744	1.99932	4.58808	0.01004	6.59744
H	10	0.21556	0.00000	0.78287	0.00157	0.78444
H	11	0.22895	0.00000	0.76937	0.00167	0.77105
Br	12	0.05141	27.99926	6.92981	0.01951	34.94859
H	13	0.21111	0.00000	0.78762	0.00128	0.78889
H	14	0.21792	0.00000	0.78075	0.00133	0.78208
H	15	0.21792	0.00000	0.78075	0.00133	0.78208
* Total *		0.00000	41.99236	41.85801	0.14963	84.00000

X = Br R = CHCH32

Energies and NBO populations

Number of atoms: 21
Full point group CS NOp 2

C	-0.067713	0.000000	-0.006790
C	-0.064865	0.000000	1.386061
C	1.161346	0.000000	2.058654
C	2.379769	0.000000	1.366803
C	2.337294	0.000000	-0.036688
C	1.125624	0.000000	-0.729789
H	-0.997169	0.000000	1.939963
H	1.162350	0.000000	3.145780
C	3.704132	0.000000	2.120596
H	3.260850	0.000000	-0.609304
H	1.111670	0.000000	-1.814054
Br	-1.738168	0.000000	-0.948665
H	3.461619	0.000000	3.191234
C	4.527208	-1.271668	1.829333
C	4.527208	1.271668	1.829333

```
H      5.444881  -1.277776   2.428074
H      4.816742  -1.323147   0.773403
H      3.956826  -2.175525   2.066716
H      5.444881   1.277776   2.428074
H      3.956826   2.175525   2.066716
H      4.816742   1.323147   0.773403

Electronic energy:                                  -2923.54302209 (  -2923.54303672)
Zero-point correction=                                  0.173214
Sum of electronic and zero-point Energies=          -2923.369808
Sum of electronic and thermal Energies=             -2923.359598
Sum of electronic and thermal Enthalpies=           -2923.358654
Sum of electronic and thermal Free Energies=        -2923.406888

Lowest vibration frequency:          38.0837

Summary of Natural Population Analysis:

                                    Natural Population
               Natural  -----------------------------------------------
   Atom  No    Charge         Core      Valence    Rydberg      Total
------------------------------------------------------------------------
     C    1   -0.11606      1.99864     4.09484    0.02258     6.11606
     C    2   -0.22690      1.99897     4.20853    0.01939     6.22690
     C    3   -0.19218      1.99906     4.17673    0.01639     6.19218
     C    4   -0.01896      1.99902     3.99983    0.02011     6.01896
     C    5   -0.19461      1.99905     4.17943    0.01614     6.19461
     C    6   -0.22609      1.99898     4.20763    0.01948     6.22609
     H    7    0.22922      0.00000     0.76914    0.00164     0.77078
     H    8    0.21567      0.00000     0.78260    0.00172     0.78433
     C    9   -0.24380      1.99920     4.22896    0.01563     6.24380
     H   10    0.21592      0.00000     0.78236    0.00173     0.78408
     H   11    0.22872      0.00000     0.76964    0.00164     0.77128
    Br   12    0.05089     27.99927     6.93044    0.01941    34.94911
     H   13    0.19934      0.00000     0.79769    0.00298     0.80066
     C   14   -0.57026      1.99935     4.56143    0.00948     6.57026
     C   15   -0.57026      1.99935     4.56143    0.00948     6.57026
     H   16    0.20411      0.00000     0.79470    0.00119     0.79589
     H   17    0.19789      0.00000     0.80076    0.00136     0.80211
     H   18    0.20769      0.00000     0.79131    0.00100     0.79231
     H   19    0.20411      0.00000     0.79470    0.00119     0.79589
     H   20    0.20769      0.00000     0.79131    0.00100     0.79231
     H   21    0.19789      0.00000     0.80076    0.00136     0.80211
========================================================================
  * Total *    0.00000     45.99089    53.82421    0.18490   100.00000

================================================================================================
X = Br    R = H
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Energies and NBO populations
------------------------------------------------------------------------------------------------

Number of atoms:  12
Full point group                 C2V     NOp   4


C      0.005801   0.000000   0.003349
C     -0.011256   0.000000   1.398757
C      1.198216   0.000000   2.097969
C      2.386344   0.000000   1.377756
C      2.416003   0.000000  -0.011299
C      1.205731   0.000000  -0.709127
H     -0.951281   0.000000   1.938440
H      1.219449   0.000000   3.182212
F      3.557232   0.000000   2.053769
H      3.365601   0.000000  -0.535032
H      1.203098   0.000000  -1.793054
Br    -1.651928   0.000000  -0.953741

Electronic energy:                                  -2904.85164392 (  -2904.85168888)
Zero-point correction=                                  0.081468
Sum of electronic and zero-point Energies=          -2904.770176
Sum of electronic and thermal Energies=             -2904.763569
Sum of electronic and thermal Enthalpies=           -2904.762625
Sum of electronic and thermal Free Energies=        -2904.801751

Lowest vibration frequency:         110.7970
```

Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.12711	1.99865	4.10596	0.02250	6.12711
C	2	-0.21243	1.99899	4.19485	0.01859	6.21243
C	3	-0.25601	1.99906	4.24012	0.01683	6.25601
C	4	0.40659	1.99850	3.56845	0.02646	5.59341
C	5	-0.25599	1.99906	4.24010	0.01683	6.25599
C	6	-0.21241	1.99899	4.19482	0.01859	6.21241
H	7	0.23463	0.00000	0.76379	0.00159	0.76537
H	8	0.23765	0.00000	0.76080	0.00156	0.76235
F	9	-0.35166	1.99993	7.34367	0.00806	9.35166
H	10	0.23765	0.00000	0.76080	0.00156	0.76235
H	11	0.23465	0.00000	0.76377	0.00158	0.76535
Br	12	0.06445	27.99926	6.91674	0.01955	34.93555
* Total *		0.00000	41.99243	41.85386	0.15371	84.00000

X = Br R = Cl

Energies and NBO populations

Number of atoms: 12
Full point group C2V NOp 4

C	-0.024354	0.000000	-0.014061
C	-0.040321	0.000000	1.380842
C	1.169481	0.000000	2.079081
C	2.368697	0.000000	1.367568
C	2.385277	0.000000	-0.026740
C	1.175684	0.000000	-0.725340
H	-0.979300	0.000000	1.922529
H	1.174046	0.000000	3.163292
Cl	3.893114	0.000000	2.247690
H	3.326514	0.000000	-0.564892
H	1.175308	0.000000	-1.809363
Br	-1.681137	0.000000	-0.970605

Electronic energy: -3265.17389558 (-3265.17394054)
Zero-point correction= 0.080164
Sum of electronic and zero-point Energies= -3265.093732
Sum of electronic and thermal Energies= -3265.086746
Sum of electronic and thermal Enthalpies= -3265.085802
Sum of electronic and thermal Free Energies= -3265.126233

Lowest vibration frequency: 87.7719

Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.11544	1.99865	4.09421	0.02258	6.11544
C	2	-0.21403	1.99897	4.19606	0.01900	6.21403
C	3	-0.21398	1.99898	4.19645	0.01856	6.21398
C	4	-0.04373	1.99861	4.02234	0.02279	6.04373
C	5	-0.21402	1.99898	4.19648	0.01856	6.21402
C	6	-0.21400	1.99897	4.19603	0.01900	6.21400
H	7	0.23587	0.00000	0.76252	0.00161	0.76413
H	8	0.23637	0.00000	0.76198	0.00165	0.76363
Cl	9	0.00171	9.99962	6.97869	0.01997	16.99829
H	10	0.23634	0.00000	0.76201	0.00166	0.76366
H	11	0.23589	0.00000	0.76250	0.00161	0.76411
Br	12	0.06901	27.99926	6.91215	0.01958	34.93099
* Total *		0.00000	49.99203	41.84141	0.16656	92.00000

X = Br R = OCF3

Energies and NBO populations

Number of atoms: 16
Full point group   C1   NOp   1

C	-0.033094	-0.073812	-0.108558
C	-0.112570	-0.064990	1.281903
C	1.055017	0.030240	2.045531
C	2.283793	0.107756	1.392269
C	2.364574	0.098531	0.000218
C	1.199465	0.009162	-0.758549
H	-1.073037	-0.127927	1.780025
H	0.979390	0.044068	3.125097
O	3.521223	0.225984	2.033573
H	3.335986	0.160737	-0.477785
H	1.255492	0.001207	-1.840839
Br	-1.636102	-0.202201	-1.142975
C	3.664457	0.003788	3.355608
F	3.215123	-1.206762	3.735477
F	4.963758	0.076144	3.634723
F	3.025032	0.918077	4.113956

Electronic energy: -3217.89105812 (-3217.89013680)
Zero-point correction=   0.098316
Sum of electronic and zero-point Energies=   -3217.792742
Sum of electronic and thermal Energies=   -3217.782463
Sum of electronic and thermal Enthalpies=   -3217.781519
Sum of electronic and thermal Free Energies=   -3217.831740

Lowest vibration frequency: 26.4590

Summary of Natural Population Analysis:

			Natural Population			
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.12310	1.99864	4.10184	0.02262	6.12310
C	2	-0.20727	1.99899	4.18941	0.01888	6.20727
C	3	-0.25000	1.99905	4.23550	0.01545	6.25000
C	4	0.29093	1.99871	3.68807	0.02230	5.70907
C	5	-0.21997	1.99907	4.20398	0.01692	6.21997
C	6	-0.20973	1.99898	4.19216	0.01858	6.20973
H	7	0.23620	0.00000	0.76224	0.00156	0.76380
H	8	0.23940	0.00000	0.75865	0.00195	0.76060
O	9	-0.55080	1.99964	6.53497	0.01619	8.55080
H	10	0.23873	0.00000	0.75965	0.00162	0.76127
H	11	0.23615	0.00000	0.76232	0.00153	0.76385
Br	12	0.07003	27.99926	6.91114	0.01958	34.92997
C	13	1.28368	1.99965	2.64633	0.07035	4.71632
F	14	-0.34955	1.99991	7.34287	0.00677	9.34955
F	15	-0.33125	1.99991	7.32502	0.00632	9.33125
F	16	-0.35343	1.99992	7.34667	0.00685	9.35343
* Total *		0.00000	49.99172	65.76080	0.24748	116.00000

X = Br   R = COOCH3

Energies and NBO populations

Number of atoms: 18
Full point group   CS   NOp   2

C	-0.047267	0.000000	-0.014245
C	-0.087120	0.000000	1.381823
C	1.113783	0.000000	2.088425
C	2.340653	0.000000	1.410256
C	2.357346	0.000000	0.008015
C	1.162510	0.000000	-0.711011
H	-1.036141	0.000000	1.905532
H	1.110555	0.000000	3.173227

```
C      3.593895   0.000000   2.224466
H      3.303158   0.000000  -0.521247
H      1.172482   0.000000  -1.794840
Br    -1.687320   0.000000  -0.995302
O      4.701003   0.000000   1.461114
C      5.954513   0.000000   2.168204
H      6.722280   0.000000   1.395597
H      6.038102  -0.891785   2.793564
H      6.038102   0.891785   2.793564
O      3.619673   0.000000   3.436858

Electronic energy:                                -3033.49273543 (  -3033.49273040)
Zero-point correction=                                0.132370
Sum of electronic and zero-point Energies=        -3033.360365
Sum of electronic and thermal Energies=           -3033.350051
Sum of electronic and thermal Enthalpies=         -3033.349107
Sum of electronic and thermal Free Energies=      -3033.398101

Lowest vibration frequency:          51.0117

Summary of Natural Population Analysis:
```

Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.09154	1.99867	4.06995	0.02292	6.09154
C	2	-0.23254	1.99897	4.21453	0.01904	6.23254
C	3	-0.14442	1.99910	4.12839	0.01693	6.14442
C	4	-0.16311	1.99893	4.14621	0.01797	6.16311
C	5	-0.15007	1.99911	4.13472	0.01624	6.15007
C	6	-0.23328	1.99897	4.21528	0.01903	6.23328
H	7	0.23456	0.00000	0.76386	0.00157	0.76544
H	8	0.23963	0.00000	0.75873	0.00164	0.76037
C	9	0.80371	1.99930	3.15028	0.04671	5.19629
H	10	0.23637	0.00000	0.76207	0.00156	0.76363
H	11	0.23391	0.00000	0.76450	0.00159	0.76609
Br	12	0.07529	27.99925	6.90597	0.01949	34.92471
O	13	-0.54962	1.99972	6.53577	0.01413	8.54962
C	14	-0.21749	1.99926	4.20251	0.01571	6.21749
H	15	0.19235	0.00000	0.80658	0.00107	0.80765
H	16	0.19050	0.00000	0.80780	0.00169	0.80950
H	17	0.19050	0.00000	0.80780	0.00169	0.80950
O	18	-0.61479	1.99975	6.60384	0.01120	8.61479
* Total *		0.00000	47.99104	57.77881	0.23016	106.00000

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================================================================================
X = Br    R = COCH3
--------------------------------------------------------------------------------
Energies and NBO populations
--------------------------------------------------------------------------------

Number of atoms:  17
Full point group                 CS      NOp   2


C     -0.015158   0.000000   0.011597
C     -0.030856   0.000000   1.409387
C      1.180461   0.000000   2.095029
C      2.402858   0.000000   1.403319
C      2.388432   0.000000  -0.000228
C      1.183041   0.000000  -0.703334
H     -0.971712   0.000000   1.948187
H      1.195251   0.000000   3.180048
C      3.679677   0.000000   2.199199
H      3.315978   0.000000  -0.563090
H      1.176598   0.000000  -1.787313
Br    -1.670167   0.000000  -0.941605
C      5.002803   0.000000   1.456125
O      3.646507   0.000000   3.417805
H      5.815988   0.000000   2.182525
H      5.088327   0.883680   0.814008
H      5.088327  -0.883680   0.814008

Electronic energy:                                -2958.25706885 (  -2958.25708368)
Zero-point correction=                                0.126577
```

Sum of electronic and zero-point Energies= -2958.130492
Sum of electronic and thermal Energies= -2958.121102
Sum of electronic and thermal Enthalpies= -2958.120158
Sum of electronic and thermal Free Energies= -2958.166790

Lowest vibration frequency: 53.8616

Summary of Natural Population Analysis:

			Natural Population			
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.09101	1.99867	4.06933	0.02302	6.09101
C	2	-0.23056	1.99897	4.21265	0.01894	6.23056
C	3	-0.14092	1.99909	4.12387	0.01796	6.14092
C	4	-0.15753	1.99895	4.14117	0.01741	6.15753
C	5	-0.15976	1.99910	4.14531	0.01534	6.15976
C	6	-0.23340	1.99898	4.21506	0.01937	6.23340
H	7	0.23425	0.00000	0.76418	0.00157	0.76575
H	8	0.23973	0.00000	0.75837	0.00190	0.76027
C	9	0.56615	1.99931	3.39587	0.03867	5.43385
H	10	0.22312	0.00000	0.77539	0.00149	0.77688
H	11	0.23375	0.00000	0.76464	0.00161	0.76625
Br	12	0.07762	27.99924	6.90361	0.01953	34.92238
C	13	-0.67866	1.99930	4.67103	0.00833	6.67866
O	14	-0.57426	1.99976	6.56085	0.01365	8.57426
H	15	0.23276	0.00000	0.76540	0.00184	0.76724
H	16	0.22936	0.00000	0.76924	0.00140	0.77064
H	17	0.22936	0.00000	0.76924	0.00140	0.77064
* Total *		0.00000	45.99138	51.80519	0.20342	98.00000

X = Br R = CF3

Energies and NBO populations

Number of atoms: 15
Full point group CS NOp 2

C	-0.012356	0.000000	-0.006527
C	-0.038468	0.000000	1.387399
C	1.169170	0.000000	2.089201
C	2.380523	0.000000	1.395107
C	2.392072	0.000000	-0.005081
C	1.192679	0.000000	-0.713573
H	-0.981439	0.000000	1.921619
H	1.159142	0.000000	3.173241
C	3.696661	0.000000	2.131480
H	3.332594	0.000000	-0.546885
H	1.195495	0.000000	-1.797227
Br	-1.659306	0.000000	-0.973623
F	3.543526	0.000000	3.469847
F	4.447552	-1.083087	1.819677
F	4.447552	1.083087	1.819677

Electronic energy: -3142.67154520 (-3142.67148747)
Zero-point correction= 0.094075
Sum of electronic and zero-point Energies= -3142.577470
Sum of electronic and thermal Energies= -3142.568961
Sum of electronic and thermal Enthalpies= -3142.568017
Sum of electronic and thermal Free Energies= -3142.612745

Lowest vibration frequency: -10.7226

Summary of Natural Population Analysis:

			Natural Population			
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.09714	1.99866	4.07535	0.02312	6.09714
C	2	-0.22346	1.99898	4.20553	0.01896	6.22346
C	3	-0.16558	1.99909	4.14986	0.01663	6.16558

C	4	-0.15510	1.99891	4.13885	0.01734	6.15510
C	5	-0.16167	1.99909	4.14560	0.01698	6.16167
C	6	-0.22247	1.99898	4.20449	0.01901	6.22247
H	7	0.23687	0.00000	0.76159	0.00155	0.76313
H	8	0.23820	0.00000	0.76020	0.00160	0.76180
C	9	1.06721	1.99913	2.87340	0.06026	4.93279
H	10	0.23424	0.00000	0.76418	0.00159	0.76576
H	11	0.23707	0.00000	0.76136	0.00156	0.76293
Br	12	0.08057	27.99925	6.90066	0.01952	34.91943
F	13	-0.35426	1.99992	7.34797	0.00638	9.35426
F	14	-0.35723	1.99992	7.35077	0.00654	9.35723
F	15	-0.35723	1.99992	7.35077	0.00654	9.35723
* Total *		0.00000	47.99185	59.79058	0.21757	108.00000

X = Br R = CN

Energies and NBO populations

Number of atoms: 13
Full point group C2V NOp 4

C	0.021815	0.000000	0.012595
C	0.003311	0.000000	1.409324
C	1.210186	0.000000	2.104506
C	2.426504	0.000000	1.400943
C	2.427649	0.000000	-0.004201
C	1.222165	0.000000	-0.701795
H	-0.937539	0.000000	1.947335
H	1.211104	0.000000	3.189073
C	3.667845	0.000000	2.117631
H	3.367370	0.000000	-0.545690
H	1.217672	0.000000	-1.785600
Br	-1.630032	0.000000	-0.941099
N	4.671303	0.000000	2.696978

Electronic energy: -2897.85188795 (-2897.85192561)
Zero-point correction= 0.088334
Sum of electronic and zero-point Energies= -2897.763554
Sum of electronic and thermal Energies= -2897.755992
Sum of electronic and thermal Enthalpies= -2897.755048
Sum of electronic and thermal Free Energies= -2897.796529

Lowest vibration frequency: 77.8866

Summary of Natural Population Analysis:

			Natural Population			
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.09323	1.99867	4.07135	0.02320	6.09323
C	2	-0.22457	1.99897	4.20672	0.01888	6.22457
C	3	-0.13659	1.99911	4.12208	0.01541	6.13659
C	4	-0.18925	1.99888	4.17346	0.01691	6.18925
C	5	-0.13657	1.99911	4.12206	0.01541	6.13657
C	6	-0.22456	1.99897	4.20671	0.01887	6.22456
H	7	0.23938	0.00000	0.75910	0.00152	0.76062
H	8	0.23538	0.00000	0.76334	0.00127	0.76462
C	9	0.30526	1.99927	3.66159	0.03388	5.69474
H	10	0.23536	0.00000	0.76336	0.00127	0.76464
H	11	0.23941	0.00000	0.75907	0.00152	0.76059
Br	12	0.08979	27.99924	6.89148	0.01949	34.91021
N	13	-0.33981	1.99959	5.32008	0.02014	7.33981
* Total *		0.00000	43.99181	43.82040	0.18779	88.00000

X = Br R = NO2

Energies and NBO populations

Number of atoms: 14

```
Full point group                 C2V     NOp   4


C     -0.000015   0.000000  -0.000009
C     -0.020401   0.000000   1.397739
C      1.185803   0.000000   2.094306
C      2.380559   0.000000   1.374416
C      2.406624   0.000000  -0.020217
C      1.200277   0.000000  -0.716537
H     -0.961575   0.000000   1.934715
H      1.206161   0.000000   3.177189
N      3.656829   0.000000   2.111271
H      3.354607   0.000000  -0.544028
H      1.194725   0.000000  -1.800106
Br    -1.649654   0.000000  -0.952428
O      3.610036   0.000000   3.337058
O      4.694995   0.000000   1.457854

Electronic energy:                                -3010.12114760 (  -3010.12117230)
Zero-point correction=                               0.092054
Sum of electronic and zero-point Energies=        -3010.029094
Sum of electronic and thermal Energies=           -3010.020755
Sum of electronic and thermal Enthalpies=         -3010.019811
Sum of electronic and thermal Free Energies=      -3010.063804

Lowest vibration frequency:          49.6593

Summary of Natural Population Analysis:

                                  Natural Population
              Natural  -----------------------------------------------
   Atom  No    Charge         Core      Valence    Rydberg      Total
------------------------------------------------------------------------
     C    1   -0.08735      1.99868     4.06541    0.02326     6.08735
     C    2   -0.22125      1.99898     4.20341    0.01886     6.22125
     C    3   -0.16933      1.99907     4.15192    0.01833     6.16933
     C    4    0.06328      1.99879     3.91714    0.02079     5.93672
     C    5   -0.16927      1.99907     4.15186    0.01833     6.16927
     C    6   -0.22124      1.99898     4.20340    0.01886     6.22124
     H    7    0.24071      0.00000     0.75780    0.00148     0.75929
     H    8    0.25463      0.00000     0.74346    0.00190     0.74537
     N    9    0.48989      1.99945     4.45559    0.05506     6.51011
     H   10    0.25465      0.00000     0.74345    0.00190     0.74535
     H   11    0.24075      0.00000     0.75776    0.00148     0.75925
    Br   12    0.09875     27.99924     6.88235    0.01967    34.90125
     O   13   -0.38715      1.99980     6.37247    0.01488     8.38715
     O   14   -0.38708      1.99980     6.37240    0.01488     8.38708
========================================================================
  * Total *    0.00000     45.99186    51.77844    0.22970    98.00000

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X = Cl    R = H
--------------------------------------------------------------------------------
Energies and NBO populations
--------------------------------------------------------------------------------

Number of atoms:  12
Full point group                 C2V     NOp   4


C     -0.043963   0.000000   0.000000
C     -0.723614   1.217682   0.000000
C     -2.121114   1.208564   0.000000
C     -2.822280   0.000000   0.000000
C     -2.121114  -1.208564   0.000000
C     -0.723614  -1.217682   0.000000
H     -0.171493   2.150993   0.000000
H     -2.657561   2.152529   0.000000
H     -3.907571   0.000000   0.000000
H     -2.657561  -2.152529   0.000000
H     -0.171493  -2.150993   0.000000
Cl     1.721378   0.000000   0.000000

Electronic energy:                                -691.80292038 (   -691.80292038)
Zero-point correction=                               0.090370
Sum of electronic and zero-point Energies=         -691.712550
Sum of electronic and thermal Energies=            -691.707015
```

Sum of electronic and thermal Enthalpies= -691.706071
Sum of electronic and thermal Free Energies= -691.741711

Lowest vibration frequency: 185.7069

Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population Core	Valence	Rydberg	Total
C	1	-0.04048	1.99861	4.01894	0.02293	6.04048
C	2	-0.23363	1.99898	4.21587	0.01878	6.23363
C	3	-0.19214	1.99918	4.17543	0.01753	6.19214
C	4	-0.21322	1.99918	4.19647	0.01758	6.21322
C	5	-0.19214	1.99918	4.17543	0.01753	6.19214
C	6	-0.23363	1.99898	4.21587	0.01878	6.23363
H	7	0.23039	0.00000	0.76799	0.00162	0.76961
H	8	0.21880	0.00000	0.77981	0.00139	0.78120
H	9	0.21762	0.00000	0.78107	0.00131	0.78238
H	10	0.21880	0.00000	0.77981	0.00139	0.78120
H	11	0.23039	0.00000	0.76799	0.00162	0.76961
Cl	12	-0.01075	9.99963	6.99138	0.01975	17.01075
* Total *		0.00000	21.99372	35.86606	0.14022	58.00000

X = Cl R = OCH3

Energies and NBO populations

Number of atoms: 16
Full point group CS NOp 2

C	-0.009832	0.000000	-0.051017
C	-0.064438	0.000000	1.337727
C	1.122586	0.000000	2.080124
C	2.358627	0.000000	1.420587
C	2.395899	0.000000	0.016550
C	1.216808	0.000000	-0.720388
H	-1.021577	0.000000	1.847479
H	1.062451	0.000000	3.161773
O	3.567429	0.000000	2.045398
H	3.359490	0.000000	-0.482146
H	1.248161	0.000000	-1.804342
Cl	-1.508824	0.000000	-0.984413
C	3.591416	0.000000	3.468291
H	4.645093	0.000000	3.747938
H	3.107249	-0.896364	3.874763
H	3.107249	0.896364	3.874763

Electronic energy: -806.32538231 (-806.32538409)
Zero-point correction= 0.122602
Sum of electronic and zero-point Energies= -806.202780
Sum of electronic and thermal Energies= -806.194650
Sum of electronic and thermal Enthalpies= -806.193706
Sum of electronic and thermal Free Energies= -806.236138

Lowest vibration frequency: 76.8919

Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population Core	Valence	Rydberg	Total
C	1	-0.06972	1.99858	4.04864	0.02251	6.06972
C	2	-0.21244	1.99900	4.19473	0.01871	6.21244
C	3	-0.28189	1.99908	4.26783	0.01498	6.28189
C	4	0.32078	1.99882	3.65745	0.02295	5.67922
C	5	-0.23164	1.99909	4.21559	0.01696	6.23164
C	6	-0.21550	1.99900	4.19827	0.01823	6.21550
H	7	0.22969	0.00000	0.76862	0.00168	0.77031
H	8	0.22542	0.00000	0.77280	0.00177	0.77458
O	9	-0.54262	1.99971	6.52520	0.01770	8.54262

H	10	0.22962	0.00000	0.76863	0.00175	0.77038
H	11	0.23082	0.00000	0.76760	0.00158	0.76918
Cl	12	-0.01692	9.99963	6.99739	0.01989	17.01692
C	13	-0.21423	1.99928	4.19927	0.01569	6.21423
H	14	0.19748	0.00000	0.80152	0.00100	0.80252
H	15	0.17557	0.00000	0.82236	0.00207	0.82443
H	16	0.17557	0.00000	0.82236	0.00207	0.82443
* Total *		0.00000	25.99218	47.82825	0.17957	74.00000

X = Cl R = OCH2CH3

Energies and NBO populations

Number of atoms: 19
Full point group CS NOp 2

C	-0.034666	0.000000	-0.113462
C	-0.118900	0.000000	1.273738
C	1.051903	0.000000	2.041550
C	2.302866	0.000000	1.409338
C	2.368906	0.000000	0.005978
C	1.205934	0.000000	-0.756242
H	-1.086722	0.000000	1.762942
H	0.968103	0.000000	3.121439
O	3.497785	0.000000	2.058307
H	3.342823	0.000000	-0.472285
H	1.260528	0.000000	-1.839264
Cl	-1.513823	0.000000	-1.078923
C	3.504983	0.000000	3.489647
C	4.954494	0.000000	3.944523
H	2.978505	-0.890537	3.859154
H	2.978505	0.890537	3.859154
H	4.997779	0.000000	5.038308
H	5.476333	0.888586	3.577485
H	5.476333	-0.888586	3.577485

Electronic energy: -845.64099789 (-845.64096100)
Zero-point correction= 0.150629
Sum of electronic and zero-point Energies= -845.490369
Sum of electronic and thermal Energies= -845.480839
Sum of electronic and thermal Enthalpies= -845.479895
Sum of electronic and thermal Free Energies= -845.525847

Lowest vibration frequency: 51.6906

Summary of Natural Population Analysis:

		Natural	Natural Population			
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.07000	1.99858	4.04899	0.02244	6.07000
C	2	-0.21272	1.99900	4.19517	0.01856	6.21272
C	3	-0.28159	1.99908	4.26726	0.01525	6.28159
C	4	0.32378	1.99883	3.65447	0.02293	5.67622
C	5	-0.23135	1.99909	4.21565	0.01661	6.23135
C	6	-0.21605	1.99900	4.19888	0.01817	6.21605
H	7	0.22939	0.00000	0.76892	0.00169	0.77061
H	8	0.22487	0.00000	0.77330	0.00183	0.77513
O	9	-0.55630	1.99970	6.53580	0.02079	8.55630
H	10	0.22904	0.00000	0.76926	0.00170	0.77096
H	11	0.23050	0.00000	0.76791	0.00158	0.76950
Cl	12	-0.01800	9.99963	6.99850	0.01987	17.01800
C	13	-0.03636	1.99924	4.01856	0.01855	6.03636
C	14	-0.59430	1.99938	4.58634	0.00859	6.59430
H	15	0.17480	0.00000	0.82276	0.00244	0.82520
H	16	0.17480	0.00000	0.82276	0.00244	0.82520
H	17	0.21109	0.00000	0.78776	0.00115	0.78891
H	18	0.20920	0.00000	0.78912	0.00168	0.79080
H	19	0.20920	0.00000	0.78912	0.00168	0.79080
* Total *		0.00000	27.99153	53.81053	0.19794	82.00000

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================================================================================
X = Cl    R = CH3
--------------------------------------------------------------------------------
Energies and NBO populations
--------------------------------------------------------------------------------

Number of atoms:  15
Full point group                 CS      NOp   2


C      0.005429   0.000000   0.004297
C     -0.010451   0.000000   1.396127
C      1.205487   0.000000   2.086858
C      2.431694   0.000000   1.410297
C      2.409357   0.000000   0.006816
C      1.207924   0.000000  -0.702722
H     -0.952627   0.000000   1.933329
H      1.190941   0.000000   3.173465
C      3.744535   0.000000   2.161958
H      3.345141   0.000000  -0.546383
H      1.203956   0.000000  -1.787305
Cl    -1.521139   0.000000  -0.882715
H      3.580571   0.000000   3.242666
H      4.342192  -0.882888   1.908822
H      4.342192   0.882888   1.908822

Electronic energy:                                -731.11682767 (   -731.11684150)
Zero-point correction=                               0.117404
Sum of electronic and zero-point Energies=        -730.999424
Sum of electronic and thermal Energies=           -730.991974
Sum of electronic and thermal Enthalpies=         -730.991030
Sum of electronic and thermal Free Energies=      -731.032574

Lowest vibration frequency:          29.6021

Summary of Natural Population Analysis:

                                  Natural Population
                Natural  -----------------------------------------------
   Atom  No     Charge          Core      Valence    Rydberg      Total
--------------------------------------------------------------------------
     C    1   -0.04820      1.99859     4.02705    0.02256     6.04820
     C    2   -0.22662      1.99898     4.20870    0.01893     6.22662
     C    3   -0.19508      1.99907     4.17971    0.01630     6.19508
     C    4   -0.03499      1.99907     4.02062    0.01530     6.03499
     C    5   -0.19244      1.99907     4.17696    0.01641     6.19244
     C    6   -0.22549      1.99898     4.20771    0.01880     6.22549
     H    7    0.22921      0.00000     0.76908    0.00171     0.77079
     H    8    0.21511      0.00000     0.78328    0.00161     0.78489
     C    9   -0.59701      1.99932     4.58769    0.01000     6.59701
     H   10    0.21531      0.00000     0.78313    0.00156     0.78469
     H   11    0.22907      0.00000     0.76922    0.00171     0.77093
    Cl   12   -0.01493      9.99963     6.99548    0.01982    17.01493
     H   13    0.21093      0.00000     0.78779    0.00127     0.78907
     H   14    0.21757      0.00000     0.78110    0.00133     0.78243
     H   15    0.21757      0.00000     0.78110    0.00133     0.78243
==========================================================================
  * Total *    0.00000     23.99270    41.85863    0.14866    66.00000

================================================================================
X = Cl    R = CHCH32
--------------------------------------------------------------------------------
Energies and NBO populations
--------------------------------------------------------------------------------

Number of atoms:  21
Full point group                 C1      NOp   1


C     -0.036137  -0.041962  -0.054017
C     -0.061056   0.003771   1.337235
C      1.151251   0.026851   2.033219
C      2.382974   0.005050   1.365562
C      2.367982  -0.041094  -0.037819
C      1.170164  -0.064759  -0.753596
H     -1.006486   0.021128   1.868307
H      1.131386   0.062585   3.119491
```

```
C      3.692176   0.030831   2.145287
H      3.302683  -0.059143  -0.591631
H      1.172519  -0.100365  -1.837548
Cl    -1.557214  -0.071564  -0.949864
H      3.428031   0.065743   3.210237
C      4.521169  -1.248909   1.912633
C      4.520737   1.292988   1.829307
H      5.426325  -1.235130   2.530051
H      4.832391  -1.334381   0.865094
H      3.945981  -2.144980   2.167336
H      3.945161   2.203570   2.024760
H      5.425830   1.320020   2.446373
H      4.831993   1.309749   0.778436

Electronic energy:                                  -809.73744491 (   -809.73745098)
Zero-point correction=                                 0.173837
Sum of electronic and zero-point Energies=          -809.563608
Sum of electronic and thermal Energies=             -809.553653
Sum of electronic and thermal Enthalpies=           -809.552709
Sum of electronic and thermal Free Energies=        -809.599625

Lowest vibration frequency:          36.1584

Summary of Natural Population Analysis:

                                     Natural Population
               Natural  -----------------------------------------------
   Atom  No    Charge         Core      Valence    Rydberg      Total
------------------------------------------------------------------------
     C    1   -0.04718      1.99859     4.02595    0.02264     6.04718
     C    2   -0.22696      1.99898     4.20907    0.01891     6.22696
     C    3   -0.19210      1.99906     4.17679    0.01624     6.19210
     C    4   -0.02135      1.99902     4.00226    0.02007     6.02135
     C    5   -0.19449      1.99906     4.17944    0.01599     6.19449
     C    6   -0.22600      1.99899     4.20803    0.01899     6.22600
     H    7    0.22931      0.00000     0.76902    0.00167     0.77069
     H    8    0.21541      0.00000     0.78287    0.00172     0.78459
     C    9   -0.24355      1.99920     4.22873    0.01562     6.24355
     H   10    0.21564      0.00000     0.78265    0.00172     0.78436
     H   11    0.22885      0.00000     0.76947    0.00167     0.77115
    Cl   12   -0.01496      9.99963     6.99552    0.01982    17.01496
     H   13    0.19921      0.00000     0.79780    0.00298     0.80079
     C   14   -0.57031      1.99935     4.56148    0.00948     6.57031
     C   15   -0.57029      1.99935     4.56145    0.00948     6.57029
     H   16    0.20398      0.00000     0.79482    0.00119     0.79602
     H   17    0.19780      0.00000     0.80084    0.00136     0.80220
     H   18    0.20760      0.00000     0.79139    0.00101     0.79240
     H   19    0.20761      0.00000     0.79138    0.00101     0.79239
     H   20    0.20399      0.00000     0.79482    0.00119     0.79601
     H   21    0.19777      0.00000     0.80087    0.00136     0.80223
========================================================================
  * Total *    0.00000     27.99123    53.82464    0.18413    82.00000

================================================================================================
X = Cl    R = H
------------------------------------------------------------------------------------------------
Energies and NBO populations
------------------------------------------------------------------------------------------------

Number of atoms:  12
Full point group                 C2V     NOp   4


C      0.017519   0.000000   0.010115
C      0.000206   0.000000   1.404975
C      1.209099   0.000000   2.104098
C      2.397635   0.000000   1.384275
C      2.426752   0.000000  -0.004938
C      1.216847   0.000000  -0.702309
H     -0.942140   0.000000   1.940761
H      1.230301   0.000000   3.188273
F      3.568753   0.000000   2.060420
H      3.376276   0.000000  -0.528665
H      1.209679   0.000000  -1.786298
Cl    -1.508109   0.000000  -0.870707

Electronic energy:                                  -791.04604457 (   -791.04605484)
```

Zero-point correction= 0.082103
Sum of electronic and zero-point Energies= -790.963942
Sum of electronic and thermal Energies= -790.957585
Sum of electronic and thermal Enthalpies= -790.956641
Sum of electronic and thermal Free Energies= -790.994402

Lowest vibration frequency: 125.8834

Summary of Natural Population Analysis:

			Natural Population			
		Natural				
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.05734	1.99860	4.03612	0.02261	6.05734
C	2	-0.21236	1.99900	4.19535	0.01802	6.21236
C	3	-0.25591	1.99906	4.24015	0.01670	6.25591
C	4	0.40466	1.99850	3.57046	0.02638	5.59534
C	5	-0.25590	1.99906	4.24013	0.01670	6.25590
C	6	-0.21233	1.99900	4.19532	0.01802	6.21233
H	7	0.23482	0.00000	0.76355	0.00163	0.76518
H	8	0.23737	0.00000	0.76108	0.00155	0.76263
F	9	-0.35201	1.99993	7.34404	0.00805	9.35201
H	10	0.23737	0.00000	0.76108	0.00155	0.76263
H	11	0.23485	0.00000	0.76352	0.00163	0.76515
Cl	12	-0.00321	9.99963	6.98367	0.01991	17.00321
* Total *		0.00000	23.99278	41.85446	0.15276	66.00000

==========

X = Cl R = Cl

Energies and NBO populations

Number of atoms: 12
Full point group D2H NOp 8

C	0.016193	0.000000	0.009349
C	0.000075	0.000000	1.403449
C	1.209411	0.000000	2.101660
C	2.408678	0.000000	1.390651
C	2.424796	0.000000	-0.003449
C	1.215460	0.000000	-0.701660
H	-0.941140	0.000000	1.941754
H	1.213833	0.000000	3.185928
Cl	3.932334	0.000000	2.270334
H	3.366011	0.000000	-0.541754
H	1.211038	0.000000	-1.785928
Cl	-1.507463	0.000000	-0.870334

Electronic energy: -1151.36836738 (-1151.36837741)
Zero-point correction= 0.080840
Sum of electronic and zero-point Energies= -1151.287527
Sum of electronic and thermal Energies= -1151.280803
Sum of electronic and thermal Enthalpies= -1151.279859
Sum of electronic and thermal Free Energies= -1151.318266

Lowest vibration frequency: 99.8754

Summary of Natural Population Analysis:

			Natural Population			
		Natural				
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.04612	1.99860	4.02477	0.02275	6.04612
C	2	-0.21378	1.99898	4.19637	0.01843	6.21378
C	3	-0.21375	1.99898	4.19634	0.01843	6.21375
C	4	-0.04612	1.99860	4.02477	0.02275	6.04612
C	5	-0.21378	1.99898	4.19637	0.01843	6.21378
C	6	-0.21375	1.99898	4.19634	0.01843	6.21375
H	7	0.23606	0.00000	0.76229	0.00165	0.76394
H	8	0.23609	0.00000	0.76226	0.00165	0.76391
Cl	9	0.00149	9.99962	6.97887	0.02002	16.99851
H	10	0.23606	0.00000	0.76229	0.00165	0.76394

```
     H   11    0.23609      0.00000     0.76226    0.00165     0.76391
    Cl   12    0.00149      9.99962     6.97887    0.02002    16.99851
=======================================================================
  * Total *    0.00000     31.99238    41.84181    0.16581    74.00000

================================================================================
X = Cl    R = OCF3
--------------------------------------------------------------------------------
Energies and NBO populations
--------------------------------------------------------------------------------

Number of atoms:  16
Full point group                 C1      NOp   1


C     -0.002621  -0.148220  -0.065928
C     -0.226654   0.260379   1.248989
C      0.866126   0.547787   2.068429
C      2.152396   0.411128   1.554185
C      2.378989   0.011456   0.240666
C      1.287633  -0.273530  -0.581403
H     -1.237651   0.358032   1.627434
H      0.719795   0.876283   3.091146
O      3.256542   0.769046   2.350018
H      3.393139  -0.070987  -0.134159
H      1.439617  -0.585996  -1.608090
Cl    -1.379317  -0.505457  -1.100886
C      3.761469  -0.168606   3.180333
F      4.174355  -1.273175   2.530513
F      4.808576   0.366145   3.806691
F      2.875920  -0.574285   4.111735

Electronic energy:                                -1104.08557295 (  -1104.08555830)
Zero-point correction=                               0.098956
Sum of electronic and zero-point Energies=        -1103.986617
Sum of electronic and thermal Energies=           -1103.976604
Sum of electronic and thermal Enthalpies=         -1103.975660
Sum of electronic and thermal Free Energies=      -1104.024480

Lowest vibration frequency:          27.3433

Summary of Natural Population Analysis:

                                  Natural Population
              Natural  -----------------------------------------------
   Atom  No    Charge         Core      Valence    Rydberg      Total
-------------------------------------------------------------------------
     C    1   -0.04125      1.99861     4.01987    0.02277     6.04125
     C    2   -0.21523      1.99899     4.19805    0.01819     6.21523
     C    3   -0.21417      1.99904     4.19838    0.01675     6.21417
     C    4    0.26322      1.99869     3.71487    0.02323     5.73678
     C    5   -0.21174      1.99904     4.19574    0.01696     6.21174
     C    6   -0.21534      1.99899     4.19819    0.01817     6.21534
     H    7    0.23709      0.00000     0.76128    0.00163     0.76291
     H    8    0.23945      0.00000     0.75886    0.00169     0.76055
     O    9   -0.56341      1.99965     6.54659    0.01717     8.56341
     H   10    0.23880      0.00000     0.75953    0.00166     0.76120
     H   11    0.23707      0.00000     0.76130    0.00163     0.76293
    Cl   12    0.00556      9.99962     6.97484    0.01998    16.99444
     C   13    1.28126      1.99965     2.64811    0.07099     4.71874
     F   14   -0.35225      1.99991     7.34570    0.00663     9.35225
     F   15   -0.33497      1.99991     7.32871    0.00635     9.33497
     F   16   -0.35409      1.99991     7.34756    0.00662     9.35409
=========================================================================
  * Total *    0.00000     31.99201    65.75757    0.25042    98.00000

================================================================================
X = Cl    R = COOCH3
--------------------------------------------------------------------------------
Energies and NBO populations
--------------------------------------------------------------------------------

Number of atoms:  18
Full point group                 CS      NOp   2


C     -0.039050   0.000000  -0.009127
```

C	-0.078630	0.000000	1.386324
C	1.122050	0.000000	2.092146
C	2.348604	0.000000	1.413218
C	2.364279	0.000000	0.010715
C	1.169310	0.000000	-0.707259
H	-1.029741	0.000000	1.906310
H	1.119929	0.000000	3.176865
C	3.601397	0.000000	2.227445
H	3.309701	0.000000	-0.519124
H	1.173601	0.000000	-1.791264
Cl	-1.549217	0.000000	-0.909991
O	4.709269	0.000000	1.465087
C	5.961590	0.000000	2.173139
H	6.730556	0.000000	1.401737
H	6.044775	-0.891609	2.798894
H	6.044775	0.891609	2.798894
O	3.626818	0.000000	3.439990

Electronic energy: -919.68734883 (-919.68735257)
Zero-point correction= 0.132933
Sum of electronic and zero-point Energies= -919.554416
Sum of electronic and thermal Energies= -919.544331
Sum of electronic and thermal Enthalpies= -919.543387
Sum of electronic and thermal Free Energies= -919.591177

Lowest vibration frequency: 49.2247

Summary of Natural Population Analysis:

			Natural Population			
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.02131	1.99862	3.99961	0.02308	6.02131
C	2	-0.23225	1.99898	4.21472	0.01855	6.23225
C	3	-0.14417	1.99911	4.12826	0.01680	6.14417
C	4	-0.16519	1.99893	4.14834	0.01791	6.16519
C	5	-0.14983	1.99911	4.13461	0.01612	6.14983
C	6	-0.23301	1.99898	4.21549	0.01854	6.23301
H	7	0.23482	0.00000	0.76357	0.00161	0.76518
H	8	0.23951	0.00000	0.75886	0.00164	0.76049
C	9	0.80371	1.99930	3.15028	0.04671	5.19629
H	10	0.23615	0.00000	0.76230	0.00155	0.76385
H	11	0.23423	0.00000	0.76414	0.00162	0.76577
Cl	12	0.00683	9.99961	6.97362	0.01994	16.99317
O	13	-0.54967	1.99972	6.53582	0.01414	8.54967
C	14	-0.21753	1.99926	4.20252	0.01575	6.21753
H	15	0.19227	0.00000	0.80666	0.00107	0.80773
H	16	0.19042	0.00000	0.80789	0.00169	0.80958
H	17	0.19042	0.00000	0.80789	0.00169	0.80958
O	18	-0.61538	1.99975	6.60442	0.01121	8.61538
* Total *		0.00000	29.99138	57.77901	0.22961	88.00000

X = Cl R = COCH3

Energies and NBO populations

Number of atoms: 17
Full point group CS NOp 2

C	-0.006401	0.000000	0.018023
C	-0.022356	0.000000	1.415217
C	1.188737	0.000000	2.099921
C	2.410732	0.000000	1.406673
C	2.395530	0.000000	0.003296
C	1.189714	0.000000	-0.698767
H	-0.965472	0.000000	1.950135
H	1.205214	0.000000	3.184738
C	3.686978	0.000000	2.202184
H	3.322813	0.000000	-0.559575
H	1.177787	0.000000	-1.782788
Cl	-1.530833	0.000000	-0.857236
C	5.011528	0.000000	1.459421

```
O      3.653925   0.000000   3.420773
H      5.823480   0.000000   2.187235
H      5.097393   0.884250   0.818210
H      5.097393  -0.884250   0.818210

Electronic energy:                                  -844.45170183 (   -844.45169824)
Zero-point correction=                                 0.127149
Sum of electronic and zero-point Energies=          -844.324553
Sum of electronic and thermal Energies=             -844.315389
Sum of electronic and thermal Enthalpies=           -844.314445
Sum of electronic and thermal Free Energies=        -844.359858

Lowest vibration frequency:          50.6968

Summary of Natural Population Analysis:

                                     Natural Population
              Natural  -----------------------------------------------
   Atom  No    Charge         Core      Valence    Rydberg      Total
------------------------------------------------------------------------
     C    1   -0.02033      1.99862     3.99854    0.02317     6.02033
     C    2   -0.23028      1.99898     4.21287    0.01843     6.23028
     C    3   -0.14052      1.99910     4.12359    0.01783     6.14052
     C    4   -0.15975      1.99895     4.14345    0.01735     6.15975
     C    5   -0.15929      1.99911     4.14498    0.01521     6.15929
     C    6   -0.23322      1.99898     4.21533    0.01890     6.23322
     H    7    0.23458      0.00000     0.76381    0.00161     0.76542
     H    8    0.23962      0.00000     0.75848    0.00190     0.76038
     C    9    0.56619      1.99931     3.39582    0.03868     5.43381
     H   10    0.22297      0.00000     0.77555    0.00148     0.77703
     H   11    0.23415      0.00000     0.76420    0.00165     0.76585
    Cl   12    0.00842      9.99961     6.97201    0.01996    16.99158
     C   13   -0.67846      1.99930     4.67085    0.00832     6.67846
     O   14   -0.57501      1.99976     6.56157    0.01367     8.57501
     H   15    0.23263      0.00000     0.76552    0.00185     0.76737
     H   16    0.22914      0.00000     0.76946    0.00140     0.77086
     H   17    0.22914      0.00000     0.76946    0.00140     0.77086
========================================================================
  * Total *    0.00000     27.99173    51.80548    0.20279    80.00000

================================================================================
X = Cl    R = CF3
--------------------------------------------------------------------------------
Energies and NBO populations
--------------------------------------------------------------------------------

Number of atoms:  15
Full point group                 CS      NOp   2


C     -0.001878   0.000000  -0.000952
C     -0.029438   0.000000   1.392249
C      1.177294   0.000000   2.094578
C      2.388806   0.000000   1.400616
C      2.400897   0.000000   0.000483
C      1.202296   0.000000  -0.708311
H     -0.975184   0.000000   1.921561
H      1.166733   0.000000   3.178534
C      3.705379   0.000000   2.136025
H      3.341979   0.000000  -0.540003
H      1.200398   0.000000  -1.792130
Cl    -1.517307   0.000000  -0.890808
F      3.552827   0.000000   3.474794
F      4.456201  -1.082838   1.823849
F      4.456201   1.082838   1.823849

Electronic energy:                                 -1028.86611429 (  -1028.86608880)
Zero-point correction=                                 0.094740
Sum of electronic and zero-point Energies=         -1028.771374
Sum of electronic and thermal Energies=            -1028.763127
Sum of electronic and thermal Enthalpies=          -1028.762183
Sum of electronic and thermal Free Energies=       -1028.805566

Lowest vibration frequency:         -19.4527

Summary of Natural Population Analysis:
```

			Natural Population			
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.02660	1.99862	4.00473	0.02325	6.02660
C	2	-0.22327	1.99898	4.20581	0.01848	6.22327
C	3	-0.16541	1.99909	4.14979	0.01653	6.16541
C	4	-0.15705	1.99891	4.14086	0.01728	6.15705
C	5	-0.16153	1.99910	4.14556	0.01687	6.16153
C	6	-0.22213	1.99899	4.20460	0.01854	6.22213
H	7	0.23719	0.00000	0.76123	0.00158	0.76281
H	8	0.23808	0.00000	0.76033	0.00160	0.76192
C	9	1.06722	1.99913	2.87336	0.06028	4.93278
H	10	0.23404	0.00000	0.76437	0.00159	0.76596
H	11	0.23748	0.00000	0.76092	0.00160	0.76252
Cl	12	0.01109	9.99962	6.96935	0.01995	16.98891
F	13	-0.35452	1.99992	7.34823	0.00637	9.35452
F	14	-0.35730	1.99992	7.35084	0.00654	9.35730
F	15	-0.35730	1.99992	7.35084	0.00654	9.35730
* Total *		0.00000	29.99219	59.79082	0.21699	90.00000

X = Cl R = CN

Energies and NBO populations

Number of atoms: 13
Full point group C2V NOp 4

C	0.033602	0.000000	0.019400
C	0.013558	0.000000	1.415520
C	1.219937	0.000000	2.110422
C	2.436206	0.000000	1.406544
C	2.437647	0.000000	0.001285
C	1.232656	0.000000	-0.696019
H	-0.929812	0.000000	1.949204
H	1.221767	0.000000	3.194902
C	3.677551	0.000000	2.123235
H	3.377750	0.000000	-0.539370
H	1.223154	0.000000	-1.779843
Cl	-1.485739	0.000000	-0.857792
N	4.680886	0.000000	2.702511

Electronic energy: -784.04652810 (-784.04653071)
Zero-point correction= 0.088996
Sum of electronic and zero-point Energies= -783.957532
Sum of electronic and thermal Energies= -783.950226
Sum of electronic and thermal Enthalpies= -783.949282
Sum of electronic and thermal Free Energies= -783.989401

Lowest vibration frequency: 88.0705

Summary of Natural Population Analysis:

			Natural Population			
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.02209	1.99863	4.00010	0.02336	6.02209
C	2	-0.22427	1.99898	4.20687	0.01842	6.22427
C	3	-0.13636	1.99911	4.12195	0.01529	6.13636
C	4	-0.19100	1.99888	4.17530	0.01682	6.19100
C	5	-0.13633	1.99911	4.12193	0.01529	6.13633
C	6	-0.22425	1.99898	4.20685	0.01842	6.22425
H	7	0.23984	0.00000	0.75861	0.00156	0.76016
H	8	0.23529	0.00000	0.76345	0.00127	0.76471
C	9	0.30533	1.99927	3.66151	0.03390	5.69467
H	10	0.23527	0.00000	0.76347	0.00127	0.76473
H	11	0.23988	0.00000	0.75856	0.00156	0.76012
Cl	12	0.01930	9.99961	6.96110	0.02000	16.98070
N	13	-0.34059	1.99959	5.32080	0.02020	7.34059
* Total *		0.00000	25.99216	43.82048	0.18736	70.00000

```
================================================================================
X = Cl    R = NO2
--------------------------------------------------------------------------------
Energies and NBO populations
--------------------------------------------------------------------------------

Number of atoms:  14
Full point group                 C2V     NOp   4


C      0.010495   0.000000   0.006059
C     -0.010524   0.000000   1.403377
C      1.195016   0.000000   2.099604
C      2.390304   0.000000   1.380042
C      2.415818   0.000000  -0.014888
C      1.210098   0.000000  -0.710803
H     -0.954045   0.000000   1.936393
H      1.215257   0.000000   3.182413
N      3.665594   0.000000   2.116332
H      3.363679   0.000000  -0.538763
H      1.199943   0.000000  -1.794424
Cl    -1.506067   0.000000  -0.869528
O      3.619163   0.000000   3.342242
O      4.704048   0.000000   1.463166

Electronic energy:                                  -896.31581271 (   -896.31580214)
Zero-point correction=                                 0.092727
Sum of electronic and zero-point Energies=          -896.223086
Sum of electronic and thermal Energies=             -896.215012
Sum of electronic and thermal Enthalpies=           -896.214068
Sum of electronic and thermal Free Energies=        -896.256697

Lowest vibration frequency:           49.2593

Summary of Natural Population Analysis:

                                     Natural Population
              Natural  -----------------------------------------------
   Atom  No    Charge         Core      Valence    Rydberg      Total
-------------------------------------------------------------------------
     C    1   -0.01596      1.99864     3.99385    0.02347     6.01596
     C    2   -0.22087      1.99899     4.20350    0.01838     6.22087
     C    3   -0.16877      1.99908     4.15148    0.01821     6.16877
     C    4    0.06151      1.99879     3.91900    0.02070     5.93849
     C    5   -0.16871      1.99908     4.15142    0.01821     6.16871
     C    6   -0.22085      1.99899     4.20348    0.01837     6.22085
     H    7    0.24114      0.00000     0.75734    0.00152     0.75886
     H    8    0.25449      0.00000     0.74361    0.00190     0.74551
     N    9    0.48985      1.99945     4.45566    0.05503     6.51015
     H   10    0.25450      0.00000     0.74360    0.00190     0.74550
     H   11    0.24119      0.00000     0.75729    0.00152     0.75881
    Cl   12    0.02762      9.99961     6.95261    0.02016    16.97238
     O   13   -0.38761      1.99980     6.37293    0.01488     8.38761
     O   14   -0.38753      1.99980     6.37286    0.01488     8.38753
=========================================================================
  * Total *    0.00000     27.99222    51.77863    0.22915    80.00000
```

Substituted halobenzenes complexed with pyridine

```
================================================================================
X = I    R = H
--------------------------------------------------------------------------------
Energies and NBO populations
--------------------------------------------------------------------------------

Number of atoms:  23
Full point group                 C2V     NOp   4


C      0.000000  -0.562419   0.000000
C      0.000000  -1.257290   1.214244
C      0.000000  -2.655555   1.207955
C      0.000000  -3.357632   0.000000
C      0.000000  -2.655555  -1.207955
C      0.000000  -1.257290  -1.214244
H      0.000000  -0.717817   2.155519
```

```
H      0.000000  -3.192575   2.152060
H      0.000000  -4.443259   0.000000
H      0.000000  -3.192575  -2.152060
H      0.000000  -0.717817  -2.155519
I      0.000000   1.571499   0.000000
N      0.000000   4.682508   0.000000
C     -1.146506   5.375047   0.000000
C     -1.200285   6.770506   0.000000
C      0.000000   7.482636   0.000000
C      1.200285   6.770506   0.000000
C      1.146506   5.375047   0.000000
H     -2.060542   4.785097   0.000000
H     -2.158500   7.279550   0.000000
H      0.000000   8.568443   0.000000
H      2.158500   7.279550   0.000000
H      2.060542   4.785097   0.000000

Electronic energy:                                -7399.15920688 (  -7399.15920688)
Zero-point correction=                                0.178216
Sum of electronic and zero-point Energies=        -7398.980991
Sum of electronic and thermal Energies=           -7398.968439
Sum of electronic and thermal Enthalpies=         -7398.967495
Sum of electronic and thermal Free Energies=      -7399.026576

Lowest vibration frequency:          10.0685

Counterpoise: BSSE energy =       0.000678761722

Summary of Natural Population Analysis:

                                     Natural Population
               Natural  -----------------------------------------------
   Atom  No    Charge         Core      Valence    Rydberg      Total
------------------------------------------------------------------------
     C    1   -0.22464      1.99876     4.19852    0.02736     6.22464
     C    2   -0.23569      1.99900     4.21616    0.02054     6.23569
     C    3   -0.19788      1.99917     4.18081    0.01791     6.19788
     C    4   -0.21348      1.99918     4.19662    0.01768     6.21348
     C    5   -0.19788      1.99917     4.18081    0.01791     6.19788
     C    6   -0.23569      1.99900     4.21616    0.02054     6.23569
     H    7    0.22365      0.00000     0.77479    0.00157     0.77635
     H    8    0.21613      0.00000     0.78247    0.00140     0.78387
     H    9    0.21502      0.00000     0.78362    0.00136     0.78498
     H   10    0.21613      0.00000     0.78247    0.00140     0.78387
     H   11    0.22365      0.00000     0.77479    0.00157     0.77635
     I   12    0.18056     45.99809     6.79853    0.02282    52.81944
     N   13   -0.48138      1.99942     5.45954    0.02242     7.48138
     C   14    0.05479      1.99923     3.91942    0.02657     5.94521
     C   15   -0.24634      1.99917     4.23087    0.01630     6.24634
     C   16   -0.16663      1.99918     4.15010    0.01735     6.16663
     C   17   -0.24634      1.99917     4.23087    0.01630     6.24634
     C   18    0.05479      1.99923     3.91942    0.02657     5.94521
     H   19    0.19826      0.00000     0.80026    0.00148     0.80174
     H   20    0.22277      0.00000     0.77574    0.00149     0.77723
     H   21    0.21921      0.00000     0.77952    0.00128     0.78079
     H   22    0.22277      0.00000     0.77574    0.00149     0.77723
     H   23    0.19826      0.00000     0.80026    0.00148     0.80174
========================================================================
  * Total *    0.00000     69.98774    65.72749    0.28477   136.00000

Contributions to pi population at N atom in pyridine:
    Val( 2p)     1.19091
    Ryd( 3p)     0.00080
    Ryd( 4p)     0.00038
    Ryd( 5p)     0.00002

    Total:       1.19211

-------------------------------------------------------------------------------
NMR properties
-------------------------------------------------------------------------------
Electronic energy (NMR):                          -7399.15920688

 1  C    Isotropic =    35.2211   Anisotropy =   142.1813
 2  C    Isotropic =    36.1974   Anisotropy =   164.8949
 3  C    Isotropic =    44.3749   Anisotropy =   185.5380
 4  C    Isotropic =    46.9259   Anisotropy =   192.7416
```

```
 5  C    Isotropic =    44.3749   Anisotropy =   185.5380
 6  C    Isotropic =    36.1974   Anisotropy =   164.8949
 7  H    Isotropic =    23.6405   Anisotropy =    11.9992
 8  H    Isotropic =    23.9781   Anisotropy =     5.1795
 9  H    Isotropic =    24.0016   Anisotropy =     4.0698
10  H    Isotropic =    23.9781   Anisotropy =     5.1795
11  H    Isotropic =    23.6405   Anisotropy =    11.9992
12  I    Isotropic =  3194.3713   Anisotropy =  3144.1720
13  N    Isotropic =   -95.7897   Anisotropy =   564.2350
14  C    Isotropic =    22.8215   Anisotropy =   180.9776
15  C    Isotropic =    50.3616   Anisotropy =   183.7978
16  C    Isotropic =    37.0154   Anisotropy =   212.7685
17  C    Isotropic =    50.3616   Anisotropy =   183.7978
18  C    Isotropic =    22.8215   Anisotropy =   180.9776
19  H    Isotropic =    22.5871   Anisotropy =    10.6447
20  H    Isotropic =    23.9449   Anisotropy =     5.3530
21  H    Isotropic =    23.5092   Anisotropy =     4.8547
22  H    Isotropic =    23.9449   Anisotropy =     5.3530
23  H    Isotropic =    22.5871   Anisotropy =    10.6447

================================================================================
X = I    R = OCH3
--------------------------------------------------------------------------------
Energies and NBO populations
--------------------------------------------------------------------------------

Number of atoms:  27
Full point group                 CS      NOp   2


C      0.000000  -0.507423   0.034652
C      0.000000  -1.249893   1.214800
C      0.000000  -2.650139   1.173800
C      0.000000  -3.311152  -0.061016
C      0.000000  -2.560242  -1.247361
C      0.000000  -1.169829  -1.200957
H      0.000000  -0.751063   2.178321
H      0.000000  -3.201949   2.106510
O      0.000000  -4.664367  -0.212911
H      0.000000  -3.083496  -2.198325
H      0.000000  -0.605004  -2.127286
I      0.000000   1.622910   0.104425
C      0.000000  -5.472710   0.957598
H      0.000000  -6.504929   0.606683
H     -0.896000  -5.294464   1.564418
H      0.896000  -5.294464   1.564418
N      0.000000   4.748081   0.176765
C      1.146436   5.440648   0.176765
C      1.200348   6.836179   0.176784
C      0.000000   7.548333   0.176683
C     -1.200348   6.836179   0.176784
C     -1.146436   5.440648   0.176765
H      2.060496   4.850650   0.176267
H      2.158638   7.345124   0.176498
H      0.000000   8.634167   0.176327
H     -2.158638   7.345124   0.176498
H     -2.060496   4.850650   0.176267

Electronic energy:                                -7513.68201593 (  -7513.68201594)
Zero-point correction=                                0.210550
Sum of electronic and zero-point Energies=        -7513.471466
Sum of electronic and thermal Energies=           -7513.456307
Sum of electronic and thermal Enthalpies=         -7513.455362
Sum of electronic and thermal Free Energies=      -7513.520539

Lowest vibration frequency:          12.7347

Counterpoise: BSSE energy =       0.000662309277

Summary of Natural Population Analysis:

                                     Natural Population
               Natural  -----------------------------------------------
   Atom  No    Charge         Core      Valence    Rydberg      Total
-------------------------------------------------------------------------
     C    1   -0.25516      1.99874     4.22952    0.02690     6.25516
     C    2   -0.21401      1.99901     4.19428    0.02072     6.21401
```

```
     C    3   -0.28726      1.99907     4.27294    0.01526     6.28726
     C    4    0.32103      1.99881     3.65707    0.02308     5.67897
     C    5   -0.23753      1.99908     4.22113    0.01732     6.23753
     C    6   -0.21690      1.99901     4.19767    0.02022     6.21690
     H    7    0.22328      0.00000     0.77512    0.00160     0.77672
     H    8    0.22319      0.00000     0.77503    0.00179     0.77681
     O    9   -0.54396      1.99971     6.52648    0.01777     8.54396
     H   10    0.22726      0.00000     0.77098    0.00177     0.77274
     H   11    0.22442      0.00000     0.77407    0.00151     0.77558
     I   12    0.17458     45.99808     6.80430    0.02304    52.82542
     C   13   -0.21367      1.99928     4.19871    0.01568     6.21367
     H   14    0.19622      0.00000     0.80276    0.00101     0.80378
     H   15    0.17499      0.00000     0.82291    0.00210     0.82501
     H   16    0.17499      0.00000     0.82291    0.00210     0.82501
     N   17   -0.48053      1.99942     5.45860    0.02251     7.48053
     C   18    0.05449      1.99923     3.91962    0.02666     5.94551
     C   19   -0.24664      1.99917     4.23116    0.01631     6.24664
     C   20   -0.16706      1.99918     4.15052    0.01736     6.16706
     C   21   -0.24664      1.99917     4.23116    0.01631     6.24664
     C   22    0.05449      1.99923     3.91962    0.02666     5.94551
     H   23    0.19816      0.00000     0.80036    0.00149     0.80184
     H   24    0.22256      0.00000     0.77595    0.00149     0.77744
     H   25    0.21901      0.00000     0.77972    0.00128     0.78099
     H   26    0.22256      0.00000     0.77595    0.00149     0.77744
     H   27    0.19816      0.00000     0.80036    0.00149     0.80184
=======================================================================
  * Total *    0.00000     73.98617    77.68892    0.32491   152.00000

Contributions to pi population at N atom in pyridine:
    Val( 2p)     1.18960
    Ryd( 3p)     0.00080
    Ryd( 4p)     0.00037
    Ryd( 5p)     0.00002

    Total:       1.19079

-------------------------------------------------------------------------------
NMR properties
-------------------------------------------------------------------------------
Electronic energy (NMR):                          -7513.68201593

 1  C    Isotropic =    49.6286   Anisotropy =   121.3590
 2  C    Isotropic =    35.6841   Anisotropy =   162.8120
 3  C    Isotropic =    65.2034   Anisotropy =   159.4900
 4  C    Isotropic =    11.5499   Anisotropy =   148.0149
 5  C    Isotropic =    55.9970   Anisotropy =   148.8774
 6  C    Isotropic =    35.4107   Anisotropy =   161.8443
 7  H    Isotropic =    23.7675   Anisotropy =    11.9335
 8  H    Isotropic =    24.5772   Anisotropy =     7.8242
 9  O    Isotropic =   222.8598   Anisotropy =    84.4183
10  H    Isotropic =    24.4112   Anisotropy =     5.9833
11  H    Isotropic =    23.8426   Anisotropy =    11.5354
12  I    Isotropic =  3259.7586   Anisotropy =  3105.4221
13  C    Isotropic =   124.6639   Anisotropy =    75.4529
14  H    Isotropic =    27.5012   Anisotropy =     8.5082
15  H    Isotropic =    27.9001   Anisotropy =     8.0508
16  H    Isotropic =    27.9001   Anisotropy =     8.0508
17  N    Isotropic =   -96.3123   Anisotropy =   565.9891
18  C    Isotropic =    22.7399   Anisotropy =   180.8905
19  C    Isotropic =    50.4278   Anisotropy =   183.6736
20  C    Isotropic =    37.0851   Anisotropy =   212.5243
21  C    Isotropic =    50.4278   Anisotropy =   183.6736
22  C    Isotropic =    22.7399   Anisotropy =   180.8905
23  H    Isotropic =    22.5921   Anisotropy =    10.7105
24  H    Isotropic =    23.9566   Anisotropy =     5.3717
25  H    Isotropic =    23.5212   Anisotropy =     4.8402
26  H    Isotropic =    23.9566   Anisotropy =     5.3717
27  H    Isotropic =    22.5921   Anisotropy =    10.7105

===============================================================================
X = I    R = OCH2CH3
-------------------------------------------------------------------------------
Energies and NBO populations
-------------------------------------------------------------------------------

Number of atoms:  30
Full point group                 CS      NOp   2
```

C	0.000000	-0.305755	-0.054597
C	0.000000	-1.042804	1.128943
C	0.000000	-2.443236	1.094838
C	0.000000	-3.111533	-0.136813
C	0.000000	-2.364765	-1.326313
C	0.000000	-0.974151	-1.286851
H	0.000000	-0.539440	2.090145
H	0.000000	-2.989903	2.030447
O	0.000000	-4.464373	-0.283558
H	0.000000	-2.892173	-2.275024
H	0.000000	-0.413965	-2.216019
I	0.000000	1.824792	0.004116
C	0.000000	-5.282803	0.890386
C	0.000000	-6.734669	0.442095
H	-0.890258	-5.059231	1.493601
H	0.890258	-5.059231	1.493601
H	0.000000	-7.391386	1.317932
H	0.889067	-6.955323	-0.156428
H	-0.889067	-6.955323	-0.156428
N	0.000000	4.953759	0.055085
C	1.146385	5.646241	0.055085
C	1.200485	7.041772	0.055208
C	0.000000	7.754075	0.055199
C	-1.200485	7.041772	0.055208
C	-1.146385	5.646241	0.055085
H	2.060383	5.056132	0.054471
H	2.158853	7.550582	0.054933
H	0.000000	8.839915	0.054959
H	-2.158853	7.550582	0.054933
H	-2.060383	5.056132	0.054471

Electronic energy:	-7552.99755110 (	-7552.99755118)
Zero-point correction=	0.238492	
Sum of electronic and zero-point Energies=	-7552.759059	
Sum of electronic and thermal Energies=	-7552.742474	
Sum of electronic and thermal Enthalpies=	-7552.741530	
Sum of electronic and thermal Free Energies=	-7552.810152	

Lowest vibration frequency: 12.5858

Counterpoise: BSSE energy = 0.000660112364

Summary of Natural Population Analysis:

			Natural Population			
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.25553	1.99874	4.23001	0.02678	6.25553
C	2	-0.21423	1.99901	4.19464	0.02058	6.21423
C	3	-0.28691	1.99907	4.27232	0.01552	6.28691
C	4	0.32405	1.99882	3.65405	0.02308	5.67595
C	5	-0.23721	1.99908	4.22116	0.01697	6.23721
C	6	-0.21737	1.99901	4.19819	0.02017	6.21737
H	7	0.22300	0.00000	0.77539	0.00161	0.77700
H	8	0.22264	0.00000	0.77552	0.00184	0.77736
O	9	-0.55751	1.99970	6.53702	0.02078	8.55751
H	10	0.22669	0.00000	0.77160	0.00172	0.77331
H	11	0.22415	0.00000	0.77434	0.00152	0.77585
I	12	0.17359	45.99808	6.80532	0.02302	52.82641
C	13	-0.03608	1.99924	4.01825	0.01859	6.03608
C	14	-0.59419	1.99938	4.58625	0.00856	6.59419
H	15	0.17436	0.00000	0.82318	0.00246	0.82564
H	16	0.17436	0.00000	0.82318	0.00246	0.82564
H	17	0.21036	0.00000	0.78848	0.00116	0.78964
H	18	0.20880	0.00000	0.78952	0.00169	0.79120
H	19	0.20880	0.00000	0.78952	0.00169	0.79120
N	20	-0.48033	1.99942	5.45839	0.02252	7.48033
C	21	0.05443	1.99923	3.91968	0.02667	5.94557
C	22	-0.24672	1.99917	4.23123	0.01631	6.24672
C	23	-0.16711	1.99918	4.15058	0.01735	6.16711
C	24	-0.24672	1.99917	4.23123	0.01631	6.24672
C	25	0.05443	1.99923	3.91968	0.02667	5.94557
H	26	0.19812	0.00000	0.80039	0.00149	0.80188
H	27	0.22252	0.00000	0.77599	0.00149	0.77748

```
     H   28    0.21897      0.00000     0.77976    0.00128     0.78103
     H   29    0.22252      0.00000     0.77599    0.00149     0.77748
     H   30    0.19812      0.00000     0.80039    0.00149     0.80188
=======================================================================
  * Total *    0.00000     75.98552    83.67122    0.34326   160.00000

Contributions to pi population at N atom in pyridine:
    Val( 2p)     1.18932
    Ryd( 3p)     0.00080
    Ryd( 4p)     0.00037
    Ryd( 5p)     0.00002

    Total:       1.19051

-------------------------------------------------------------------------------
NMR properties
-------------------------------------------------------------------------------
Electronic energy (NMR):                          -7552.99755110

 1  C    Isotropic =    49.9653   Anisotropy =   120.4776
 2  C    Isotropic =    35.7204   Anisotropy =   162.3232
 3  C    Isotropic =    64.6013   Anisotropy =   157.4116
 4  C    Isotropic =    11.9341   Anisotropy =   147.3212
 5  C    Isotropic =    55.9670   Anisotropy =   147.8607
 6  C    Isotropic =    35.4161   Anisotropy =   161.5224
 7  H    Isotropic =    23.7987   Anisotropy =    11.9557
 8  H    Isotropic =    24.6185   Anisotropy =     8.4346
 9  O    Isotropic =   192.8679   Anisotropy =    69.7989
10  H    Isotropic =    24.3987   Anisotropy =     6.4715
11  H    Isotropic =    23.8436   Anisotropy =    11.5412
12  I    Isotropic =  3262.6606   Anisotropy =  3102.9789
13  C    Isotropic =   113.6376   Anisotropy =    63.1547
14  C    Isotropic =   165.9159   Anisotropy =    25.7178
15  H    Isotropic =    27.6511   Anisotropy =     5.3576
16  H    Isotropic =    27.6511   Anisotropy =     5.3576
17  H    Isotropic =    30.2647   Anisotropy =    10.1316
18  H    Isotropic =    30.0311   Anisotropy =     8.2201
19  H    Isotropic =    30.0311   Anisotropy =     8.2201
20  N    Isotropic =   -96.3388   Anisotropy =   566.3019
21  C    Isotropic =    22.7350   Anisotropy =   180.8412
22  C    Isotropic =    50.4245   Anisotropy =   183.6693
23  C    Isotropic =    37.0499   Anisotropy =   212.4983
24  C    Isotropic =    50.4245   Anisotropy =   183.6693
25  C    Isotropic =    22.7350   Anisotropy =   180.8412
26  H    Isotropic =    22.5918   Anisotropy =    10.7381
27  H    Isotropic =    23.9572   Anisotropy =     5.3804
28  H    Isotropic =    23.5217   Anisotropy =     4.8329
29  H    Isotropic =    23.9572   Anisotropy =     5.3804
30  H    Isotropic =    22.5918   Anisotropy =    10.7381

===============================================================================
X = I    R = CH3
-------------------------------------------------------------------------------
Energies and NBO populations
-------------------------------------------------------------------------------

Number of atoms:  26
Full point group                 CS      NOp   2


C      0.000000  -0.469356  -0.008260
C      0.000000  -1.147834   1.212332
C      0.000000  -2.546711   1.226595
C      0.000000  -3.289516   0.039371
C      0.000000  -2.586006  -1.175073
C      0.000000  -1.190391  -1.207559
H      0.000000  -0.598449   2.148022
H      0.000000  -3.063694   2.183012
C      0.000000  -4.801864   0.057229
H      0.000000  -3.134913  -2.113962
H      0.000000  -0.671770  -2.160663
I      0.000000   1.662931  -0.043976
H      0.000000  -5.185615   1.081043
H     -0.882455  -5.202453  -0.454276
H      0.882455  -5.202453  -0.454276
N      0.000000   4.788135  -0.069128
C      1.146420   5.480648  -0.069128
```

```
C      1.200372   6.876171  -0.069121
C      0.000000   7.588360  -0.069087
C     -1.200372   6.876171  -0.069121
C     -1.146420   5.480648  -0.069128
H      2.060498   4.890666  -0.068793
H      2.158666   7.385096  -0.068959
H      0.000000   8.674186  -0.068926
H     -2.158666   7.385096  -0.068959
H     -2.060498   4.890666  -0.068793

Electronic energy:                                -7438.47308046 (  -7438.47308046)
Zero-point correction=                                0.205160
Sum of electronic and zero-point Energies=        -7438.267920
Sum of electronic and thermal Energies=           -7438.254314
Sum of electronic and thermal Enthalpies=         -7438.253370
Sum of electronic and thermal Free Energies=      -7438.315201

Lowest vibration frequency:          -18.7009

Counterpoise: BSSE energy =       0.000655306574

Summary of Natural Population Analysis:

                                     Natural Population
               Natural  -----------------------------------------------
   Atom  No    Charge         Core      Valence    Rydberg      Total
------------------------------------------------------------------------
     C    1   -0.23238      1.99874     4.20673    0.02691     6.23238
     C    2   -0.22855      1.99900     4.20862    0.02093     6.22855
     C    3   -0.20026      1.99906     4.18456    0.01664     6.20026
     C    4   -0.03500      1.99907     4.02049    0.01544     6.03500
     C    5   -0.19784      1.99906     4.18206    0.01672     6.19784
     C    6   -0.22738      1.99900     4.20758    0.02080     6.22738
     H    7    0.22274      0.00000     0.77561    0.00165     0.77726
     H    8    0.21268      0.00000     0.78569    0.00163     0.78732
     C    9   -0.59692      1.99932     4.58760    0.01000     6.59692
     H   10    0.21281      0.00000     0.78561    0.00158     0.78719
     H   11    0.22263      0.00000     0.77573    0.00164     0.77737
     I   12    0.17570     45.99808     6.80319    0.02303    52.82430
     H   13    0.20999      0.00000     0.78872    0.00129     0.79001
     H   14    0.21650      0.00000     0.78216    0.00134     0.78350
     H   15    0.21650      0.00000     0.78216    0.00134     0.78350
     N   16   -0.48061      1.99942     5.45874    0.02246     7.48061
     C   17    0.05453      1.99923     3.91961    0.02663     5.94547
     C   18   -0.24659      1.99917     4.23111    0.01631     6.24659
     C   19   -0.16699      1.99918     4.15046    0.01735     6.16699
     C   20   -0.24659      1.99917     4.23111    0.01631     6.24659
     C   21    0.05453      1.99923     3.91961    0.02663     5.94547
     H   22    0.19814      0.00000     0.80038    0.00148     0.80186
     H   23    0.22259      0.00000     0.77592    0.00149     0.77741
     H   24    0.21903      0.00000     0.77969    0.00128     0.78097
     H   25    0.22259      0.00000     0.77592    0.00149     0.77741
     H   26    0.19814      0.00000     0.80038    0.00148     0.80186
========================================================================
  * Total *    0.00000     71.98671    71.71945    0.29384   144.00000

Contributions to pi population at N atom in pyridine:
    Val( 2p)     1.18974
    Ryd( 3p)     0.00080
    Ryd( 4p)     0.00037
    Ryd( 5p)     0.00002

    Total:       1.19093

-------------------------------------------------------------------------------
NMR properties
-------------------------------------------------------------------------------
Electronic energy (NMR):                          -7438.47308046

 1  C    Isotropic =    40.4880   Anisotropy =   134.3040
 2  C    Isotropic =    36.4073   Anisotropy =   161.0137
 3  C    Isotropic =    43.4759   Anisotropy =   160.2570
 4  C    Isotropic =    33.9686   Anisotropy =   206.9717
 5  C    Isotropic =    43.4497   Anisotropy =   171.1440
 6  C    Isotropic =    36.6850   Anisotropy =   161.4147
 7  H    Isotropic =    23.8228   Anisotropy =    11.8107
 8  H    Isotropic =    24.1970   Anisotropy =     6.7157
```

```
 9  C    Isotropic =   159.6141   Anisotropy =    41.6860
10  H    Isotropic =    24.0732   Anisotropy =     7.2358
11  H    Isotropic =    23.7758   Anisotropy =    11.8221
12  I    Isotropic =  3232.0591   Anisotropy =  3113.2495
13  H    Isotropic =    29.5226   Anisotropy =     7.6382
14  H    Isotropic =    28.9901   Anisotropy =     8.6033
15  H    Isotropic =    28.9901   Anisotropy =     8.6033
16  N    Isotropic =   -96.1964   Anisotropy =   565.6524
17  C    Isotropic =    22.7710   Anisotropy =   180.9132
18  C    Isotropic =    50.4044   Anisotropy =   183.7083
19  C    Isotropic =    37.0622   Anisotropy =   212.5981
20  C    Isotropic =    50.4044   Anisotropy =   183.7083
21  C    Isotropic =    22.7710   Anisotropy =   180.9132
22  H    Isotropic =    22.5932   Anisotropy =    10.6783
23  H    Isotropic =    23.9548   Anisotropy =     5.3661
24  H    Isotropic =    23.5186   Anisotropy =     4.8464
25  H    Isotropic =    23.9548   Anisotropy =     5.3661
26  H    Isotropic =    22.5932   Anisotropy =    10.6783

================================================================================
X = I    R = CHCH32
--------------------------------------------------------------------------------
Energies and NBO populations
--------------------------------------------------------------------------------

Number of atoms:  32
Full point group                 C1      NOp   1


C     -0.007974  -0.313207  -0.068934
C     -0.380435  -0.949786   1.116951
C     -0.463483  -2.345481   1.154638
C     -0.181069  -3.128145   0.027483
C      0.192462  -2.464958  -1.152263
C      0.280077  -1.072436  -1.208204
H     -0.605687  -0.370167   2.006134
H     -0.755046  -2.830603   2.083317
C     -0.278250  -4.647814   0.090852
H      0.419949  -3.036262  -2.048752
H      0.569881  -0.585582  -2.133613
I      0.116302   1.814874  -0.143626
H     -0.593936  -4.903682   1.110775
C     -1.346503  -5.193742  -0.878461
C      1.088495  -5.318892  -0.155424
H     -1.441071  -6.280296  -0.771635
H     -1.080743  -4.982051  -1.920583
H     -2.324966  -4.743233  -0.682569
H      1.840816  -4.954665   0.551671
H      1.007114  -6.405746  -0.041045
H      1.452667  -5.115839  -1.169133
N      0.226534   4.939401  -0.215029
C      1.372925   5.632276  -0.215029
C      1.426691   7.027832  -0.215055
C      0.226385   7.739927  -0.215349
C     -0.973851   7.027778  -0.215422
C     -0.919863   5.632274  -0.215029
H      2.287337   5.042883  -0.214537
H      2.384938   7.536894  -0.214761
H      0.226407   8.825761  -0.215274
H     -1.932218   7.536618  -0.215521
H     -1.834311   5.042808  -0.213953

Electronic energy:                                -7517.09363449 (  -7517.09365451)
Zero-point correction=                                0.261707
Sum of electronic and zero-point Energies=        -7516.831927
Sum of electronic and thermal Energies=           -7516.814932
Sum of electronic and thermal Enthalpies=         -7516.813988
Sum of electronic and thermal Free Energies=      -7516.884324

Lowest vibration frequency:           6.6128

Counterpoise: BSSE energy =       0.000575744854

Summary of Natural Population Analysis:

                                 Natural Population
              Natural  -----------------------------------------------
```

Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.23088	1.99874	4.20502	0.02712	6.23088
C	2	-0.22887	1.99900	4.20912	0.02076	6.22887
C	3	-0.19736	1.99905	4.18174	0.01658	6.19736
C	4	-0.02117	1.99902	4.00195	0.02020	6.02117
C	5	-0.19996	1.99905	4.18462	0.01629	6.19996
C	6	-0.22804	1.99900	4.20817	0.02086	6.22804
H	7	0.22284	0.00000	0.77554	0.00162	0.77716
H	8	0.21305	0.00000	0.78522	0.00173	0.78695
C	9	-0.24351	1.99920	4.22863	0.01568	6.24351
H	10	0.21334	0.00000	0.78494	0.00173	0.78666
H	11	0.22244	0.00000	0.77595	0.00161	0.77756
I	12	0.17565	45.99808	6.80338	0.02290	52.82435
H	13	0.19836	0.00000	0.79865	0.00299	0.80164
C	14	-0.57025	1.99935	4.56144	0.00946	6.57025
C	15	-0.57010	1.99935	4.56130	0.00945	6.57010
H	16	0.20292	0.00000	0.79587	0.00120	0.79708
H	17	0.19768	0.00000	0.80096	0.00137	0.80232
H	18	0.20735	0.00000	0.79163	0.00101	0.79265
H	19	0.20736	0.00000	0.79163	0.00102	0.79264
H	20	0.20283	0.00000	0.79597	0.00121	0.79717
H	21	0.19774	0.00000	0.80090	0.00137	0.80226
N	22	-0.48052	1.99942	5.45867	0.02244	7.48052
C	23	0.05470	1.99923	3.91944	0.02664	5.94530
C	24	-0.24669	1.99917	4.23121	0.01631	6.24669
C	25	-0.16700	1.99918	4.15047	0.01736	6.16700
C	26	-0.24657	1.99917	4.23109	0.01631	6.24657
C	27	0.05433	1.99922	3.91983	0.02662	5.94567
H	28	0.19801	0.00000	0.80053	0.00145	0.80199
H	29	0.22256	0.00000	0.77595	0.00149	0.77744
H	30	0.21901	0.00000	0.77971	0.00128	0.78099
H	31	0.22258	0.00000	0.77593	0.00149	0.77742
H	32	0.19818	0.00000	0.80031	0.00151	0.80182
* Total *		0.00000	75.98524	83.68572	0.32905	160.00000

Contributions to pi population at N atom in pyridine:

Val(2p)	1.18963
Ryd(3p)	0.00081
Ryd(4p)	0.00038
Ryd(5p)	0.00002
Total:	1.19084

NMR properties

Electronic energy (NMR): -7517.09363449

1	C	Isotropic =	39.7539	Anisotropy =	133.3445
2	C	Isotropic =	36.3021	Anisotropy =	160.3427
3	C	Isotropic =	44.3931	Anisotropy =	154.7170
4	C	Isotropic =	22.2269	Anisotropy =	215.9476
5	C	Isotropic =	47.0963	Anisotropy =	183.8068
6	C	Isotropic =	36.2478	Anisotropy =	161.9927
7	H	Isotropic =	23.8122	Anisotropy =	11.6856
8	H	Isotropic =	24.1956	Anisotropy =	7.3744
9	C	Isotropic =	139.5764	Anisotropy =	24.8615
10	H	Isotropic =	24.0372	Anisotropy =	9.6800
11	H	Isotropic =	23.7229	Anisotropy =	12.0042
12	I	Isotropic =	3228.3591	Anisotropy =	3117.3709
13	H	Isotropic =	28.7570	Anisotropy =	6.8543
14	C	Isotropic =	155.8020	Anisotropy =	36.7633
15	C	Isotropic =	155.7741	Anisotropy =	36.8192
16	H	Isotropic =	30.2875	Anisotropy =	10.2732
17	H	Isotropic =	30.3108	Anisotropy =	6.4795
18	H	Isotropic =	30.2959	Anisotropy =	8.3954
19	H	Isotropic =	30.3303	Anisotropy =	8.3932
20	H	Isotropic =	30.2690	Anisotropy =	10.2949
21	H	Isotropic =	30.3388	Anisotropy =	6.5646
22	N	Isotropic =	-96.5561	Anisotropy =	565.1519
23	C	Isotropic =	22.8281	Anisotropy =	180.9213
24	C	Isotropic =	50.4037	Anisotropy =	183.3566
25	C	Isotropic =	37.2471	Anisotropy =	212.9671
26	C	Isotropic =	50.3728	Anisotropy =	183.4464
27	C	Isotropic =	22.8033	Anisotropy =	181.4146

```
28  H    Isotropic =    22.6039   Anisotropy =    10.5111
29  H    Isotropic =    23.9572   Anisotropy =     5.3316
30  H    Isotropic =    23.5122   Anisotropy =     4.8359
31  H    Isotropic =    23.9534   Anisotropy =     5.4322
32  H    Isotropic =    22.5843   Anisotropy =    10.9688

================================================================================
X = I    R = H
--------------------------------------------------------------------------------
Energies and NBO populations
--------------------------------------------------------------------------------

Number of atoms:  23
Full point group                 C2V     NOp   4


C      0.000000  -0.525753   0.000000
C      0.000000  -1.223880   1.212723
C      0.000000  -2.621398   1.216732
C      0.000000  -3.291435   0.000000
C      0.000000  -2.621398  -1.216732
C      0.000000  -1.223880  -1.212723
H      0.000000  -0.688501   2.155942
H      0.000000  -3.181463   2.145729
F      0.000000  -4.645207   0.000000
H      0.000000  -3.181463  -2.145729
H      0.000000  -0.688501  -2.155942
I      0.000000   1.605928   0.000000
N      0.000000   4.690377   0.000000
C      1.146782   5.382637   0.000000
C      1.200337   6.777975   0.000000
C      0.000000   7.490019   0.000000
C     -1.200337   6.777975   0.000000
C     -1.146782   5.382637   0.000000
H      2.060700   4.792534   0.000000
H      2.158534   7.287022   0.000000
H      0.000000   8.575809   0.000000
H     -2.158534   7.287022   0.000000
H     -2.060700   4.792534   0.000000

Electronic energy:                                  -7498.40323600 (  -7498.40323600)
Zero-point correction=                                  0.169980
Sum of electronic and zero-point Energies=          -7498.233256
Sum of electronic and thermal Energies=             -7498.219893
Sum of electronic and thermal Enthalpies=           -7498.218949
Sum of electronic and thermal Free Energies=        -7498.279570

Lowest vibration frequency:          11.1323

Counterpoise: BSSE energy =       0.000705938760

Summary of Natural Population Analysis:

                                     Natural Population
              Natural  -----------------------------------------------
   Atom  No    Charge         Core      Valence    Rydberg      Total
--------------------------------------------------------------------
     C    1   -0.24366      1.99876     4.21775    0.02715     6.24366
     C    2   -0.21463      1.99901     4.19564    0.01997     6.21463
     C    3   -0.26223      1.99905     4.24613    0.01705     6.26223
     C    4    0.40460      1.99849     3.57039    0.02652     5.59540
     C    5   -0.26223      1.99905     4.24613    0.01705     6.26223
     C    6   -0.21463      1.99901     4.19564    0.01997     6.21463
     H    7    0.22784      0.00000     0.77060    0.00156     0.77216
     H    8    0.23464      0.00000     0.76380    0.00156     0.76536
     F    9   -0.35494      1.99993     7.34701    0.00800     9.35494
     H   10    0.23464      0.00000     0.76380    0.00156     0.76536
     H   11    0.22784      0.00000     0.77060    0.00156     0.77216
     I   12    0.18998     45.99810     6.78873    0.02319    52.81002
     N   13   -0.48308      1.99941     5.46117    0.02249     7.48308
     C   14    0.05518      1.99922     3.91907    0.02652     5.94482
     C   15   -0.24582      1.99917     4.23037    0.01629     6.24582
     C   16   -0.16585      1.99918     4.14933    0.01733     6.16585
     C   17   -0.24582      1.99917     4.23037    0.01629     6.24582
     C   18    0.05518      1.99922     3.91907    0.02652     5.94482
     H   19    0.19852      0.00000     0.80000    0.00148     0.80148
     H   20    0.22316      0.00000     0.77536    0.00148     0.77684
```

```
     H   21    0.21958      0.00000     0.77914    0.00127     0.78042
     H   22    0.22316      0.00000     0.77536    0.00148     0.77684
     H   23    0.19852      0.00000     0.80000    0.00148     0.80148
=======================================================================
  * Total *    0.00000     71.98679    71.71546    0.29775   144.00000

Contributions to pi population at N atom in pyridine:
    Val( 2p)     1.19334
    Ryd( 3p)     0.00081
    Ryd( 4p)     0.00038
    Ryd( 5p)     0.00002

    Total:       1.19455

-------------------------------------------------------------------------------
NMR properties
-------------------------------------------------------------------------------
Electronic energy (NMR):                          -7498.40323600

 1  C    Isotropic =    42.3971   Anisotropy =   137.4914
 2  C    Isotropic =    34.8483   Anisotropy =   163.9808
 3  C    Isotropic =    58.2884   Anisotropy =   152.3919
 4  C    Isotropic =     6.4124   Anisotropy =   108.1165
 5  C    Isotropic =    58.2884   Anisotropy =   152.3919
 6  C    Isotropic =    34.8483   Anisotropy =   163.9808
 7  H    Isotropic =    23.7140   Anisotropy =    11.5719
 8  H    Isotropic =    24.3110   Anisotropy =     4.7880
 9  F    Isotropic =   294.0431   Anisotropy =    97.3839
10  H    Isotropic =    24.3110   Anisotropy =     4.7880
11  H    Isotropic =    23.7140   Anisotropy =    11.5719
12  I    Isotropic =  3202.7053   Anisotropy =  3155.9798
13  N    Isotropic =   -94.8637   Anisotropy =   561.5538
14  C    Isotropic =    22.9406   Anisotropy =   180.8756
15  C    Isotropic =    50.2887   Anisotropy =   183.9685
16  C    Isotropic =    36.8846   Anisotropy =   213.0350
17  C    Isotropic =    50.2887   Anisotropy =   183.9685
18  C    Isotropic =    22.9406   Anisotropy =   180.8756
19  H    Isotropic =    22.6071   Anisotropy =    10.7080
20  H    Isotropic =    23.9423   Anisotropy =     5.3590
21  H    Isotropic =    23.5055   Anisotropy =     4.8533
22  H    Isotropic =    23.9423   Anisotropy =     5.3590
23  H    Isotropic =    22.6071   Anisotropy =    10.7080

===============================================================================
X = I    R = Cl
-------------------------------------------------------------------------------
Energies and NBO populations
-------------------------------------------------------------------------------

Number of atoms:  23
Full point group                 C2V     NOp   4


C      0.000000  -0.487592   0.000000
C      0.000000  -1.186437   1.211671
C      0.000000  -2.583736   1.214941
C      0.000000  -3.267011   0.000000
C      0.000000  -2.583736  -1.214941
C      0.000000  -1.186437  -1.211671
H      0.000000  -0.652840   2.156049
H      0.000000  -3.130133   2.151722
Cl     0.000000  -5.029181   0.000000
H      0.000000  -3.130133  -2.151722
H      0.000000  -0.652840  -2.156049
I      0.000000   1.643142   0.000000
N      0.000000   4.720311   0.000000
C      1.146952   5.412338   0.000000
C      1.200413   6.807678   0.000000
C      0.000000   7.519591   0.000000
C     -1.200413   6.807678   0.000000
C     -1.146952   5.412338   0.000000
H      2.060879   4.822253   0.000000
H      2.158595   7.316704   0.000000
H      0.000000   8.605376   0.000000
H     -2.158595   7.316704   0.000000
H     -2.060879   4.822253   0.000000
```

Electronic energy: -7858.72558324 (-7858.72558324)
Zero-point correction= 0.168677
Sum of electronic and zero-point Energies= -7858.556906
Sum of electronic and thermal Energies= -7858.543161
Sum of electronic and thermal Enthalpies= -7858.542217
Sum of electronic and thermal Free Energies= -7858.604047

Lowest vibration frequency: 11.3387

Counterpoise: BSSE energy = 0.000705924157

Summary of Natural Population Analysis:

			Natural Population			
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.23217	1.99876	4.20628	0.02714	6.23217
C	2	-0.21619	1.99900	4.19683	0.02037	6.21619
C	3	-0.21998	1.99897	4.20226	0.01875	6.21998
C	4	-0.04387	1.99860	4.02256	0.02271	6.04387
C	5	-0.21998	1.99897	4.20226	0.01875	6.21998
C	6	-0.21619	1.99900	4.19683	0.02037	6.21619
H	7	0.22905	0.00000	0.76937	0.00158	0.77095
H	8	0.23349	0.00000	0.76486	0.00165	0.76651
Cl	9	-0.00552	9.99962	6.98593	0.01997	17.00552
H	10	0.23349	0.00000	0.76486	0.00165	0.76651
H	11	0.22905	0.00000	0.76937	0.00158	0.77095
I	12	0.19522	45.99810	6.78340	0.02329	52.80478
N	13	-0.48370	1.99941	5.46182	0.02247	7.48370
C	14	0.05535	1.99922	3.91894	0.02648	5.94465
C	15	-0.24561	1.99917	4.23017	0.01628	6.24561
C	16	-0.16562	1.99918	4.14911	0.01733	6.16562
C	17	-0.24561	1.99917	4.23017	0.01628	6.24561
C	18	0.05535	1.99922	3.91894	0.02648	5.94465
H	19	0.19860	0.00000	0.79992	0.00148	0.80140
H	20	0.22328	0.00000	0.77523	0.00148	0.77672
H	21	0.21969	0.00000	0.77904	0.00127	0.78031
H	22	0.22328	0.00000	0.77523	0.00148	0.77672
H	23	0.19860	0.00000	0.79992	0.00148	0.80140
* Total *		0.00000	79.98639	71.70331	0.31030	152.00000

Contributions to pi population at N atom in pyridine:
Val(2p) 1.19414
Ryd(3p) 0.00081
Ryd(4p) 0.00038
Ryd(5p) 0.00002

Total: 1.19535

NMR properties

Electronic energy (NMR): -7858.72558324

1	C	Isotropic =	37.2790	Anisotropy =	146.5006
2	C	Isotropic =	35.3379	Anisotropy =	161.4783
3	C	Isotropic =	44.2592	Anisotropy =	157.1247
4	C	Isotropic =	31.3266	Anisotropy =	123.1087
5	C	Isotropic =	44.2592	Anisotropy =	157.1247
6	C	Isotropic =	35.3379	Anisotropy =	161.4783
7	H	Isotropic =	23.7477	Anisotropy =	11.6351
8	H	Isotropic =	24.0417	Anisotropy =	7.4124
9	Cl	Isotropic =	686.8649	Anisotropy =	501.5431
10	H	Isotropic =	24.0417	Anisotropy =	7.4124
11	H	Isotropic =	23.7477	Anisotropy =	11.6351
12	I	Isotropic =	3183.4077	Anisotropy =	3141.3335
13	N	Isotropic =	-94.4717	Anisotropy =	560.5017
14	C	Isotropic =	22.9814	Anisotropy =	180.8153
15	C	Isotropic =	50.2504	Anisotropy =	184.0500
16	C	Isotropic =	36.8299	Anisotropy =	213.1007
17	C	Isotropic =	50.2504	Anisotropy =	184.0500
18	C	Isotropic =	22.9814	Anisotropy =	180.8153
19	H	Isotropic =	22.6135	Anisotropy =	10.7543
20	H	Isotropic =	23.9406	Anisotropy =	5.3714
21	H	Isotropic =	23.5046	Anisotropy =	4.8489

```
22  H    Isotropic =    23.9406   Anisotropy =     5.3714
23  H    Isotropic =    22.6135   Anisotropy =    10.7543

================================================================================
X = I    R = OCF3
--------------------------------------------------------------------------------
Energies and NBO populations
--------------------------------------------------------------------------------

Number of atoms:  27
Full point group                 C1      NOp   1


C      0.004787  -0.346961   0.065111
C      0.093874  -1.039194  -1.144838
C      0.103264  -2.437658  -1.165469
C      0.010407  -3.127606   0.041465
C     -0.080474  -2.450614   1.256091
C     -0.080432  -1.056342   1.268479
H      0.162019  -0.500271  -2.083475
H      0.185650  -2.955827  -2.112600
O      0.039532  -4.524004   0.160559
H     -0.150144  -3.017436   2.178305
H     -0.150913  -0.531552   2.214907
I     -0.002023   1.784020   0.075795
C     -0.257999  -5.329484  -0.876549
F     -0.309234  -6.578016  -0.414036
F      0.670309  -5.291908  -1.856757
F     -1.441948  -5.038652  -1.446437
N     -0.012639   4.855820   0.072622
C     -1.159687   5.547801   0.072622
C     -1.213059   6.943091   0.072637
C     -0.012679   7.655009   0.072905
C      1.187777   6.943201   0.072734
C      1.134340   5.547814   0.072622
H     -2.073732   4.957924   0.072650
H     -2.171232   7.452123   0.072635
H     -0.012749   8.740793   0.073269
H      2.145929   7.452268   0.072790
H      2.048249   4.957713   0.072523

Electronic energy:                                -7811.44200808 (  -7811.44194046)
Zero-point correction=                                0.186987
Sum of electronic and zero-point Energies=        -7811.255021
Sum of electronic and thermal Energies=           -7811.238035
Sum of electronic and thermal Enthalpies=         -7811.237091
Sum of electronic and thermal Free Energies=      -7811.307596

Lowest vibration frequency:          11.8355

Counterpoise: BSSE energy =       0.000671572644

Summary of Natural Population Analysis:

                                     Natural Population
                Natural  -----------------------------------------------
   Atom  No     Charge         Core      Valence    Rydberg      Total
-------------------------------------------------------------------------
     C    1   -0.23854      1.99875     4.21256    0.02723     6.23854
     C    2   -0.20993      1.99901     4.19069    0.02023     6.20993
     C    3   -0.25417      1.99904     4.23937    0.01576     6.25417
     C    4    0.28687      1.99870     3.69196    0.02247     5.71313
     C    5   -0.22548      1.99906     4.20930    0.01713     6.22548
     C    6   -0.21222      1.99901     4.19329    0.01992     6.21222
     H    7    0.22939      0.00000     0.76907    0.00153     0.77061
     H    8    0.23718      0.00000     0.76092    0.00190     0.76282
     O    9   -0.55297      1.99964     6.53713    0.01620     8.55297
     H   10    0.23586      0.00000     0.76251    0.00163     0.76414
     H   11    0.22941      0.00000     0.76908    0.00151     0.77059
     I   12    0.19578     45.99810     6.78292    0.02320    52.80422
     C   13    1.28354      1.99965     2.64649    0.07031     4.71646
     F   14   -0.33353      1.99991     7.32731    0.00632     9.33353
     F   15   -0.35570      1.99992     7.34893    0.00685     9.35570
     F   16   -0.34964      1.99991     7.34299    0.00673     9.34964
     N   17   -0.48396      1.99941     5.46207    0.02249     7.48396
     C   18    0.05545      1.99922     3.91885    0.02647     5.94455
     C   19   -0.24551      1.99917     4.23007    0.01627     6.24551
```

```
     C   20   -0.16548      1.99918     4.14897    0.01733     6.16548
     C   21   -0.24551      1.99917     4.23006    0.01627     6.24551
     C   22    0.05540      1.99922     3.91891    0.02647     5.94460
     H   23    0.19867      0.00000     0.79986    0.00147     0.80133
     H   24    0.22335      0.00000     0.77517    0.00148     0.77665
     H   25    0.21976      0.00000     0.77897    0.00127     0.78024
     H   26    0.22335      0.00000     0.77516    0.00148     0.77665
     H   27    0.19863      0.00000     0.79989    0.00148     0.80137
=======================================================================
  * Total *    0.00000     79.98607    95.62250    0.39142   176.00000

Contributions to pi population at N atom in pyridine:
    Val( 2p)     1.19459
    Ryd( 3p)     0.00081
    Ryd( 4p)     0.00038
    Ryd( 5p)     0.00002

    Total:       1.19580

-------------------------------------------------------------------------------
NMR properties
-------------------------------------------------------------------------------
Electronic energy (NMR):                          -7811.44200808

 1  C    Isotropic =    40.0252   Anisotropy =   141.9064
 2  C    Isotropic =    35.5102   Anisotropy =   164.6885
 3  C    Isotropic =    58.9082   Anisotropy =   159.6043
 4  C    Isotropic =    20.9675   Anisotropy =   119.7546
 5  C    Isotropic =    55.0788   Anisotropy =   155.4456
 6  C    Isotropic =    34.6864   Anisotropy =   165.3147
 7  H    Isotropic =    23.6696   Anisotropy =    11.9798
 8  H    Isotropic =    24.0978   Anisotropy =     9.6473
 9  O    Isotropic =   156.6522   Anisotropy =    41.9549
10  H    Isotropic =    24.2879   Anisotropy =     6.2964
11  H    Isotropic =    23.6664   Anisotropy =    11.4372
12  I    Isotropic =  3186.5554   Anisotropy =  3159.7843
13  C    Isotropic =    47.0420   Anisotropy =     9.7578
14  F    Isotropic =   236.1858   Anisotropy =   177.1019
15  F    Isotropic =   231.0784   Anisotropy =   167.1652
16  F    Isotropic =   245.6397   Anisotropy =   168.5918
17  N    Isotropic =   -94.3032   Anisotropy =   560.3131
18  C    Isotropic =    22.9956   Anisotropy =   180.7874
19  C    Isotropic =    50.2466   Anisotropy =   184.0423
20  C    Isotropic =    36.8264   Anisotropy =   213.1414
21  C    Isotropic =    50.2342   Anisotropy =   184.0982
22  C    Isotropic =    22.9639   Anisotropy =   180.7720
23  H    Isotropic =    22.6083   Anisotropy =    10.7850
24  H    Isotropic =    23.9420   Anisotropy =     5.3667
25  H    Isotropic =    23.5013   Anisotropy =     4.8254
26  H    Isotropic =    23.9300   Anisotropy =     5.3870
27  H    Isotropic =    22.6041   Anisotropy =    10.8383

===============================================================================
X = I    R = COOCH3
-------------------------------------------------------------------------------
Energies and NBO populations
-------------------------------------------------------------------------------

Number of atoms:  29
Full point group                 CS      NOp   2


C      0.000000  -0.356497   0.015723
C      0.000000  -1.065449   1.223487
C      0.000000  -2.458901   1.203960
C      0.000000  -3.154107  -0.013554
C      0.000000  -2.435388  -1.217981
C      0.000000  -1.040670  -1.205697
H      0.000000  -0.537254   2.170789
H      0.000000  -3.020828   2.132204
C      0.000000  -4.646712   0.027732
H      0.000000  -2.965740  -2.163456
H      0.000000  -0.492619  -2.141695
I      0.000000   1.772640   0.035205
O      0.000000  -5.195492  -1.201297
C      0.000000  -6.633077  -1.248897
H      0.000000  -6.888004  -2.307967
```

H	-0.891393	-7.030417	-0.757967
H	0.891393	-7.030417	-0.757967
O	0.000000	-5.303506	1.047880
N	0.000000	4.851533	0.048233
C	1.146915	5.543603	0.048233
C	1.200414	6.938927	0.048174
C	0.000000	7.650894	0.048119
C	-1.200414	6.938927	0.048174
C	-1.146915	5.543603	0.048233
H	2.060869	4.953558	0.048231
H	2.158618	7.447910	0.048180
H	0.000000	8.736676	0.048047
H	-2.158618	7.447910	0.048180
H	-2.060869	4.953558	0.048231

Electronic energy: -7627.04416581 (-7627.04416579)
Zero-point correction= 0.220793
Sum of electronic and zero-point Energies= -7626.823373
Sum of electronic and thermal Energies= -7626.806286
Sum of electronic and thermal Enthalpies= -7626.805341
Sum of electronic and thermal Free Energies= -7626.875390

Lowest vibration frequency: 11.7425

Counterpoise: BSSE energy = 0.000680913739

Summary of Natural Population Analysis:

			Natural Population			
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.20682	1.99877	4.18066	0.02738	6.20682
C	2	-0.23552	1.99900	4.21620	0.02032	6.23552
C	3	-0.14897	1.99910	4.13275	0.01712	6.14897
C	4	-0.16680	1.99893	4.14981	0.01806	6.16680
C	5	-0.15469	1.99910	4.13915	0.01644	6.15469
C	6	-0.23627	1.99900	4.21695	0.02032	6.23627
H	7	0.22777	0.00000	0.77068	0.00155	0.77223
H	8	0.23663	0.00000	0.76174	0.00163	0.76337
C	9	0.80358	1.99930	3.15045	0.04667	5.19642
H	10	0.23337	0.00000	0.76508	0.00155	0.76663
H	11	0.22714	0.00000	0.77129	0.00157	0.77286
I	12	0.20239	45.99807	6.77633	0.02320	52.79761
O	13	-0.55068	1.99972	6.53677	0.01420	8.55068
C	14	-0.21746	1.99926	4.20242	0.01577	6.21746
H	15	0.19151	0.00000	0.80741	0.00108	0.80849
H	16	0.18973	0.00000	0.80856	0.00171	0.81027
H	17	0.18973	0.00000	0.80856	0.00171	0.81027
O	18	-0.61821	1.99975	6.60723	0.01123	8.61821
N	19	-0.48395	1.99941	5.46209	0.02244	7.48395
C	20	0.05535	1.99922	3.91895	0.02647	5.94465
C	21	-0.24556	1.99917	4.23012	0.01627	6.24556
C	22	-0.16554	1.99918	4.14903	0.01733	6.16554
C	23	-0.24556	1.99917	4.23012	0.01627	6.24556
C	24	0.05535	1.99922	3.91895	0.02647	5.94465
H	25	0.19857	0.00000	0.79996	0.00147	0.80143
H	26	0.22331	0.00000	0.77521	0.00148	0.77669
H	27	0.21971	0.00000	0.77902	0.00127	0.78029
H	28	0.22331	0.00000	0.77521	0.00148	0.77669
H	29	0.19857	0.00000	0.79996	0.00147	0.80143
* Total *		0.00000	77.98539	87.64066	0.37395	166.00000

Contributions to pi population at N atom in pyridine:
Val(2p) 1.19422
Ryd(3p) 0.00081
Ryd(4p) 0.00038
Ryd(5p) 0.00002

Total: 1.19543

NMR properties

Electronic energy (NMR): -7627.04416581

```
 1  C    Isotropic =    25.9984   Anisotropy =   158.2798
 2  C    Isotropic =    36.5210   Anisotropy =   163.9242
 3  C    Isotropic =    42.2466   Anisotropy =   192.5237
 4  C    Isotropic =    44.6939   Anisotropy =   167.2227
 5  C    Isotropic =    43.7275   Anisotropy =   187.3074
 6  C    Isotropic =    36.9932   Anisotropy =   163.2878
 7  H    Isotropic =    23.5543   Anisotropy =    12.0425
 8  H    Isotropic =    23.1291   Anisotropy =     7.8667
 9  C    Isotropic =     6.1051   Anisotropy =    85.7470
10  H    Isotropic =    23.3346   Anisotropy =     8.8208
11  H    Isotropic =    23.6084   Anisotropy =    12.1824
12  I    Isotropic =  3139.1645   Anisotropy =  3098.8820
13  O    Isotropic =   145.4559   Anisotropy =   141.8150
14  C    Isotropic =   126.7688   Anisotropy =    73.1295
15  H    Isotropic =    27.7780   Anisotropy =     7.6484
16  H    Isotropic =    27.6141   Anisotropy =     8.5179
17  H    Isotropic =    27.6141   Anisotropy =     8.5179
18  O    Isotropic =   -65.9414   Anisotropy =   603.4103
19  N    Isotropic =   -94.3236   Anisotropy =   560.4446
20  C    Isotropic =    22.9686   Anisotropy =   180.8228
21  C    Isotropic =    50.2321   Anisotropy =   184.1228
22  C    Isotropic =    36.7838   Anisotropy =   213.1060
23  C    Isotropic =    50.2321   Anisotropy =   184.1228
24  C    Isotropic =    22.9686   Anisotropy =   180.8228
25  H    Isotropic =    22.5988   Anisotropy =    10.7448
26  H    Isotropic =    23.9311   Anisotropy =     5.3667
27  H    Isotropic =    23.4971   Anisotropy =     4.8320
28  H    Isotropic =    23.9311   Anisotropy =     5.3667
29  H    Isotropic =    22.5988   Anisotropy =    10.7448

================================================================================
X = I    R = COCH3
--------------------------------------------------------------------------------
Energies and NBO populations
--------------------------------------------------------------------------------

Number of atoms:  28
Full point group                 CS      NOp   2


C      0.000000  -0.410150  -0.002704
C      0.000000  -1.069407   1.234387
C      0.000000  -2.460848   1.272499
C      0.000000  -3.215238   0.087354
C      0.000000  -2.539935  -1.143369
C      0.000000  -1.144943  -1.193048
H      0.000000  -0.501015   2.158359
H      0.000000  -2.984273   2.223137
C      0.000000  -4.714264   0.186448
H      0.000000  -3.092812  -2.077201
H      0.000000  -0.637783  -2.151812
I      0.000000   1.717835  -0.068150
C      0.000000  -5.531142  -1.093917
O      0.000000  -5.263941   1.275406
H      0.000000  -6.590592  -0.836035
H      0.883548  -5.303998  -1.700251
H     -0.883548  -5.303998  -1.700251
N      0.000000   4.792325  -0.131973
C      1.147089   5.484446  -0.131973
C      1.200320   6.879788  -0.132131
C      0.000000   7.591481  -0.132161
C     -1.200320   6.879788  -0.132131
C     -1.147089   5.484446  -0.131973
H      2.061145   4.894573  -0.131274
H      2.158410   7.388963  -0.131782
H      0.000000   8.677268  -0.131868
H     -2.158410   7.388963  -0.131782
H     -2.061145   4.894573  -0.131274

Electronic energy:                                -7551.80861151 (  -7551.80861158)
Zero-point correction=                                0.215117
Sum of electronic and zero-point Energies=        -7551.593495
Sum of electronic and thermal Energies=           -7551.577344
Sum of electronic and thermal Enthalpies=         -7551.576400
Sum of electronic and thermal Free Energies=      -7551.644139

Lowest vibration frequency:          11.9137
```

Counterpoise: BSSE energy =   0.000669636196

Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population Core	Valence	Rydberg	Total
C	1	-0.20575	1.99877	4.17942	0.02755	6.20575
C	2	-0.23369	1.99900	4.21446	0.02023	6.23369
C	3	-0.14535	1.99909	4.12812	0.01814	6.14535
C	4	-0.16126	1.99895	4.14484	0.01747	6.16126
C	5	-0.16395	1.99910	4.14931	0.01554	6.16395
C	6	-0.23675	1.99900	4.21709	0.02066	6.23675
H	7	0.22744	0.00000	0.77100	0.00156	0.77256
H	8	0.23677	0.00000	0.76135	0.00188	0.76323
C	9	0.56535	1.99931	3.39663	0.03870	5.43465
H	10	0.22018	0.00000	0.77834	0.00148	0.77982
H	11	0.22698	0.00000	0.77142	0.00160	0.77302
I	12	0.20454	45.99807	6.77416	0.02322	52.79546
C	13	-0.67809	1.99930	4.67047	0.00832	6.67809
O	14	-0.57861	1.99976	6.56514	0.01370	8.57861
H	15	0.23114	0.00000	0.76698	0.00188	0.76886
H	16	0.22854	0.00000	0.77005	0.00141	0.77146
H	17	0.22854	0.00000	0.77005	0.00141	0.77146
N	18	-0.48433	1.99941	5.46248	0.02244	7.48433
C	19	0.05541	1.99922	3.91891	0.02645	5.94459
C	20	-0.24543	1.99917	4.22999	0.01627	6.24543
C	21	-0.16542	1.99918	4.14891	0.01733	6.16542
C	22	-0.24543	1.99917	4.22999	0.01627	6.24543
C	23	0.05541	1.99922	3.91891	0.02645	5.94459
H	24	0.19859	0.00000	0.79994	0.00147	0.80141
H	25	0.22339	0.00000	0.77513	0.00148	0.77661
H	26	0.21980	0.00000	0.77893	0.00127	0.78020
H	27	0.22339	0.00000	0.77513	0.00148	0.77661
H	28	0.19859	0.00000	0.79994	0.00147	0.80141
* Total *		0.00000	75.98574	81.66712	0.34714	158.00000

Contributions to pi population at N atom in pyridine:

Val(2p)	1.19466
Ryd(3p)	0.00081
Ryd(4p)	0.00038
Ryd(5p)	0.00002
Total:	1.19587

NMR properties

Electronic energy (NMR):   -7551.80861151

1	C	Isotropic =	25.2543	Anisotropy =	159.1643
2	C	Isotropic =	36.1183	Anisotropy =	163.5639
3	C	Isotropic =	45.4630	Anisotropy =	196.4004
4	C	Isotropic =	38.1239	Anisotropy =	180.3063
5	C	Isotropic =	43.2512	Anisotropy =	181.6166
6	C	Isotropic =	37.1010	Anisotropy =	162.8520
7	H	Isotropic =	23.5510	Anisotropy =	12.1352
8	H	Isotropic =	23.1541	Anisotropy =	7.0652
9	C	Isotropic =	-26.0274	Anisotropy =	173.8296
10	H	Isotropic =	23.4624	Anisotropy =	8.5816
11	H	Isotropic =	23.5655	Anisotropy =	12.2120
12	I	Isotropic =	3133.6217	Anisotropy =	3089.6734
13	C	Isotropic =	153.8732	Anisotropy =	46.4303
14	O	Isotropic =	-290.7385	Anisotropy =	967.7174
15	H	Isotropic =	29.3605	Anisotropy =	7.0408
16	H	Isotropic =	28.7365	Anisotropy =	4.6607
17	H	Isotropic =	28.7365	Anisotropy =	4.6607
18	N	Isotropic =	-94.3101	Anisotropy =	560.0627
19	C	Isotropic =	22.9695	Anisotropy =	180.8706
20	C	Isotropic =	50.2234	Anisotropy =	184.1533
21	C	Isotropic =	36.8134	Anisotropy =	213.1478
22	C	Isotropic =	50.2234	Anisotropy =	184.1533
23	C	Isotropic =	22.9695	Anisotropy =	180.8706
24	H	Isotropic =	22.5988	Anisotropy =	10.7143

```
25  H    Isotropic =    23.9290   Anisotropy =     5.3582
26  H    Isotropic =    23.4959   Anisotropy =     4.8406
27  H    Isotropic =    23.9290   Anisotropy =     5.3582
28  H    Isotropic =    22.5988   Anisotropy =    10.7143

================================================================================
X = I    R = CF3
--------------------------------------------------------------------------------
Energies and NBO populations
--------------------------------------------------------------------------------

Number of atoms:  26
Full point group                 CS      NOp   2


C      0.000281  -0.430734  -0.015907
C      0.000127  -1.088714   1.217430
C     -0.000344  -2.485032   1.260827
C     -0.000609  -3.218929   0.073242
C     -0.000428  -2.559180  -1.161576
C      0.000020  -1.166369  -1.208105
H      0.000353  -0.523425   2.142891
H     -0.000487  -2.993703   2.218308
C     -0.001647  -4.725748   0.092002
H     -0.000528  -3.127435  -2.086622
H      0.000198  -0.659787  -2.166944
I      0.000927   1.698059  -0.081613
F      0.002130  -5.231818   1.341122
F     -1.087197  -5.238673  -0.536779
F      1.078794  -5.240271  -0.544097
N      0.001442   4.757427  -0.142844
C      1.148616   5.449172  -0.142844
C      1.201909   6.844455  -0.142652
C      0.001440   7.556261  -0.142495
C     -1.199027   6.844454  -0.142647
C     -1.145731   5.449173  -0.142844
H      2.062524   4.859111  -0.142584
H      2.160040   7.353513  -0.142422
H      0.001443   8.642032  -0.142198
H     -2.157161   7.353509  -0.142434
H     -2.059642   4.859114  -0.142586

Electronic energy:                                -7736.22341853 (  -7736.22343597)
Zero-point correction=                                0.182513
Sum of electronic and zero-point Energies=        -7736.040906
Sum of electronic and thermal Energies=           -7736.025626
Sum of electronic and thermal Enthalpies=         -7736.024681
Sum of electronic and thermal Free Energies=      -7736.090498

Lowest vibration frequency:          -22.8678

Counterpoise: BSSE energy =       0.000704977204

Summary of Natural Population Analysis:

                                     Natural Population
                Natural  -----------------------------------------------
   Atom  No     Charge         Core      Valence    Rydberg      Total
--------------------------------------------------------------------------
     C    1   -0.21305      1.99877     4.18663    0.02765     6.21305
     C    2   -0.22668      1.99900     4.20746    0.02023     6.22668
     C    3   -0.17059      1.99908     4.15470    0.01681     6.17059
     C    4   -0.15913      1.99891     4.14277    0.01745     6.15913
     C    5   -0.16695      1.99909     4.15070    0.01716     6.16695
     C    6   -0.22548      1.99901     4.20623    0.02024     6.22548
     H    7    0.22972      0.00000     0.76875    0.00153     0.77028
     H    8    0.23502      0.00000     0.76339    0.00159     0.76498
     C    9    1.06722      1.99912     2.87356    0.06009     4.93278
     H   10    0.23103      0.00000     0.76739    0.00158     0.76897
     H   11    0.23005      0.00000     0.76840    0.00155     0.76995
     I   12    0.20672     45.99809     6.77195    0.02324    52.79328
     F   13   -0.35566      1.99992     7.34937    0.00638     9.35566
     F   14   -0.35899      1.99992     7.35255    0.00653     9.35899
     F   15   -0.35898      1.99992     7.35253    0.00653     9.35898
     N   16   -0.48513      1.99941     5.46327    0.02245     7.48513
     C   17    0.05567      1.99922     3.91869    0.02641     5.94433
     C   18   -0.24512      1.99917     4.22969    0.01626     6.24512
```

```
     C   19   -0.16496      1.99918     4.14846    0.01732     6.16496
     C   20   -0.24512      1.99917     4.22969    0.01626     6.24512
     C   21    0.05567      1.99922     3.91870    0.02641     5.94433
     H   22    0.19876      0.00000     0.79977    0.00147     0.80124
     H   23    0.22362      0.00000     0.77490    0.00148     0.77638
     H   24    0.22001      0.00000     0.77873    0.00127     0.77999
     H   25    0.22362      0.00000     0.77490    0.00148     0.77638
     H   26    0.19876      0.00000     0.79977    0.00147     0.80124
=======================================================================
  * Total *    0.00000     77.98621    89.65296    0.36084   168.00000

Contributions to pi population at N atom in pyridine:
    Val( 2p)     1.19610
    Ryd( 3p)     0.00082
    Ryd( 4p)     0.00038
    Ryd( 5p)     0.00002

    Total:       1.19732

-------------------------------------------------------------------------------
NMR properties
-------------------------------------------------------------------------------
Electronic energy (NMR):                          -7736.22341853

 1  C    Isotropic =    28.0395   Anisotropy =   158.9877
 2  C    Isotropic =    36.6836   Anisotropy =   166.6052
 3  C    Isotropic =    48.4892   Anisotropy =   184.3964
 4  C    Isotropic =    42.4941   Anisotropy =   166.9481
 5  C    Isotropic =    46.4282   Anisotropy =   186.3705
 6  C    Isotropic =    35.9429   Anisotropy =   168.0859
 7  H    Isotropic =    23.5457   Anisotropy =    11.9150
 8  H    Isotropic =    23.6874   Anisotropy =     8.5717
 9  C    Isotropic =    43.1080   Anisotropy =    10.6489
10  H    Isotropic =    23.7493   Anisotropy =     8.0971
11  H    Isotropic =    23.5044   Anisotropy =    11.8923
12  I    Isotropic =  3133.0780   Anisotropy =  3153.0123
13  F    Isotropic =   261.0141   Anisotropy =   114.4206
14  F    Isotropic =   232.4075   Anisotropy =   148.7354
15  F    Isotropic =   232.6172   Anisotropy =   148.6238
16  N    Isotropic =   -93.6587   Anisotropy =   558.3359
17  C    Isotropic =    23.0600   Anisotropy =   180.7629
18  C    Isotropic =    50.1589   Anisotropy =   184.2541
19  C    Isotropic =    36.6918   Anisotropy =   213.3203
20  C    Isotropic =    50.1591   Anisotropy =   184.2534
21  C    Isotropic =    23.0602   Anisotropy =   180.7656
22  H    Isotropic =    22.6050   Anisotropy =    10.7852
23  H    Isotropic =    23.9240   Anisotropy =     5.3704
24  H    Isotropic =    23.4900   Anisotropy =     4.8363
25  H    Isotropic =    23.9242   Anisotropy =     5.3706
26  H    Isotropic =    22.6049   Anisotropy =    10.7873

===============================================================================
X = I    R = CN
-------------------------------------------------------------------------------
Energies and NBO populations
-------------------------------------------------------------------------------

Number of atoms:  24
Full point group                 C2V     NOp   4


C      0.000000  -0.503559   0.000000
C      0.000000  -1.200815   1.214823
C      0.000000  -2.593817   1.216830
C      0.000000  -3.296618   0.000000
C      0.000000  -2.593817  -1.216830
C      0.000000  -1.200815  -1.214823
H      0.000000  -0.663448   2.156748
H      0.000000  -3.137523   2.155609
C      0.000000  -4.729802   0.000000
H      0.000000  -3.137523  -2.155609
H      0.000000  -0.663448  -2.156748
I      0.000000   1.624639   0.000000
N      0.000000  -5.888669   0.000000
N      0.000000   4.667512   0.000000
C      1.147356   5.359101   0.000000
C      1.200490   6.754271   0.000000
```

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C      0.000000   7.466042   0.000000
C     -1.200490   6.754271   0.000000
C     -1.147356   5.359101   0.000000
H      2.061216   4.769007   0.000000
H      2.158608   7.263314   0.000000
H      0.000000   8.551787   0.000000
H     -2.158608   7.263314   0.000000
H     -2.061216   4.769007   0.000000

Electronic energy:                                  -7491.40422390 (  -7491.40422390)
Zero-point correction=                                  0.176882
Sum of electronic and zero-point Energies=          -7491.227342
Sum of electronic and thermal Energies=             -7491.213051
Sum of electronic and thermal Enthalpies=           -7491.212107
Sum of electronic and thermal Free Energies=        -7491.274551

Lowest vibration frequency:          12.6196

Counterpoise: BSSE energy =       0.000697647821

Summary of Natural Population Analysis:

                                     Natural Population
               Natural  -----------------------------------------------
   Atom  No    Charge         Core      Valence    Rydberg      Total
------------------------------------------------------------------------
     C    1   -0.20958      1.99878     4.18304    0.02776     6.20958
     C    2   -0.22797      1.99900     4.20889    0.02008     6.22797
     C    3   -0.14188      1.99910     4.12714    0.01564     6.14188
     C    4   -0.19350      1.99888     4.17757    0.01705     6.19350
     C    5   -0.14188      1.99910     4.12714    0.01564     6.14188
     C    6   -0.22797      1.99900     4.20889    0.02008     6.22797
     H    7    0.23216      0.00000     0.76633    0.00151     0.76784
     H    8    0.23201      0.00000     0.76671    0.00128     0.76799
     C    9    0.30785      1.99927     3.65885    0.03403     5.69215
     H   10    0.23201      0.00000     0.76671    0.00128     0.76799
     H   11    0.23216      0.00000     0.76633    0.00151     0.76784
     I   12    0.21701     45.99809     6.76161    0.02329    52.78299
     N   13   -0.34827      1.99959     5.32846    0.02022     7.34827
     N   14   -0.48653      1.99941     5.46467    0.02246     7.48653
     C   15    0.05598      1.99922     3.91845    0.02635     5.94402
     C   16   -0.24468      1.99917     4.22926    0.01625     6.24468
     C   17   -0.16429      1.99918     4.14780    0.01731     6.16429
     C   18   -0.24468      1.99917     4.22926    0.01625     6.24468
     C   19    0.05598      1.99922     3.91845    0.02635     5.94402
     H   20    0.19892      0.00000     0.79961    0.00147     0.80108
     H   21    0.22395      0.00000     0.77458    0.00148     0.77605
     H   22    0.22033      0.00000     0.77840    0.00126     0.77967
     H   23    0.22395      0.00000     0.77458    0.00148     0.77605
     H   24    0.19892      0.00000     0.79961    0.00147     0.80108
========================================================================
  * Total *    0.00000     73.98618    73.68235    0.33148   148.00000

Contributions to pi population at N atom in pyridine:
    Val( 2p)     1.19804
    Ryd( 3p)     0.00082
    Ryd( 4p)     0.00039
    Ryd( 5p)     0.00002

    Total:       1.19927

-------------------------------------------------------------------------------
NMR properties
-------------------------------------------------------------------------------
Electronic energy (NMR):                            -7491.40422390

 1  C    Isotropic =    25.0253   Anisotropy =   166.4518
 2  C    Isotropic =    35.9882   Anisotropy =   169.0891
 3  C    Isotropic =    39.9301   Anisotropy =   187.0703
 4  C    Isotropic =    63.5325   Anisotropy =   151.0618
 5  C    Isotropic =    39.9301   Anisotropy =   187.0703
 6  C    Isotropic =    35.9882   Anisotropy =   169.0891
 7  H    Isotropic =    23.5507   Anisotropy =    11.8377
 8  H    Isotropic =    23.7459   Anisotropy =     6.3628
 9  C    Isotropic =    55.3911   Anisotropy =   353.1877
10  H    Isotropic =    23.7459   Anisotropy =     6.3628
11  H    Isotropic =    23.5507   Anisotropy =    11.8377
```

```
12  I    Isotropic =  3085.3909   Anisotropy =  3129.1333
13  N    Isotropic =   -43.0783   Anisotropy =   417.4651
14  N    Isotropic =   -92.8231   Anisotropy =   555.7247
15  C    Isotropic =    23.1796   Anisotropy =   180.7567
16  C    Isotropic =    50.0684   Anisotropy =   184.4227
17  C    Isotropic =    36.5759   Anisotropy =   213.6631
18  C    Isotropic =    50.0684   Anisotropy =   184.4227
19  C    Isotropic =    23.1796   Anisotropy =   180.7567
20  H    Isotropic =    22.6192   Anisotropy =    10.7435
21  H    Isotropic =    23.9175   Anisotropy =     5.3645
22  H    Isotropic =    23.4812   Anisotropy =     4.8570
23  H    Isotropic =    23.9175   Anisotropy =     5.3645
24  H    Isotropic =    22.6192   Anisotropy =    10.7435

===============================================================================
X = I    R = NO2
-------------------------------------------------------------------------------
Energies and NBO populations
-------------------------------------------------------------------------------

Number of atoms:  25
Full point group                 C2V     NOp   4


C      0.000000  -0.450351   0.000000
C      0.000000  -1.147316   1.216275
C      0.000000  -2.540412   1.220080
C      0.000000  -3.217085   0.000000
C      0.000000  -2.540412  -1.220080
C      0.000000  -1.147316  -1.216275
H      0.000000  -0.609487   2.157701
H      0.000000  -3.098819   2.148274
N      0.000000  -4.688947   0.000000
H      0.000000  -3.098819  -2.148274
H      0.000000  -0.609487  -2.157701
I      0.000000   1.676189   0.000000
O      0.000000  -5.263610   1.084693
O      0.000000  -5.263610  -1.084693
N      0.000000   4.703519   0.000000
C      1.147544   5.394844   0.000000
C      1.200540   6.789960   0.000000
C      0.000000   7.501641   0.000000
C     -1.200540   6.789960   0.000000
C     -1.147544   5.394844   0.000000
H      2.061356   4.804722   0.000000
H      2.158618   7.299028   0.000000
H      0.000000   8.587374   0.000000
H     -2.158618   7.299028   0.000000
H     -2.061356   4.804722   0.000000

Electronic energy:                                -7603.67386110 (  -7603.67386110)
Zero-point correction=                                0.180566
Sum of electronic and zero-point Energies=        -7603.493295
Sum of electronic and thermal Energies=           -7603.478201
Sum of electronic and thermal Enthalpies=         -7603.477257
Sum of electronic and thermal Free Energies=      -7603.542469

Lowest vibration frequency:          12.5144

Counterpoise: BSSE energy =       0.000715535538

Summary of Natural Population Analysis:

                                     Natural Population
               Natural  -----------------------------------------------
   Atom  No    Charge         Core      Valence    Rydberg      Total
-------------------------------------------------------------------------
     C    1   -0.20371      1.99879     4.17709    0.02783     6.20371
     C    2   -0.22506      1.99901     4.20603    0.02003     6.22506
     C    3   -0.17426      1.99907     4.15669    0.01851     6.17426
     C    4    0.06044      1.99879     3.91993    0.02084     5.93956
     C    5   -0.17426      1.99907     4.15669    0.01851     6.17426
     C    6   -0.22506      1.99901     4.20603    0.02003     6.22506
     H    7    0.23335      0.00000     0.76518    0.00147     0.76665
     H    8    0.25133      0.00000     0.74678    0.00188     0.74867
     N    9    0.48921      1.99945     4.45637    0.05498     6.51079
     H   10    0.25133      0.00000     0.74678    0.00188     0.74867
```

```
     H   11    0.23335      0.00000     0.76518    0.00147     0.76665
     I   12    0.22758     45.99809     6.75074    0.02360    52.77242
     O   13   -0.39197      1.99980     6.37723    0.01494     8.39197
     O   14   -0.39197      1.99980     6.37723    0.01494     8.39197
     N   15   -0.48774      1.99941     5.46587    0.02246     7.48774
     C   16    0.05631      1.99922     3.91817    0.02629     5.94369
     C   17   -0.24429      1.99917     4.22889    0.01623     6.24429
     C   18   -0.16377      1.99918     4.14729    0.01730     6.16377
     C   19   -0.24429      1.99917     4.22889    0.01623     6.24429
     C   20    0.05631      1.99922     3.91817    0.02629     5.94369
     H   21    0.19909      0.00000     0.79945    0.00146     0.80091
     H   22    0.22421      0.00000     0.77432    0.00147     0.77579
     H   23    0.22057      0.00000     0.77816    0.00126     0.77943
     H   24    0.22421      0.00000     0.77432    0.00147     0.77579
     H   25    0.19909      0.00000     0.79945    0.00146     0.80091
=======================================================================
  * Total *    0.00000     75.98624    81.64092    0.37285   158.00000

Contributions to pi population at N atom in pyridine:
    Val( 2p)     1.19971
    Ryd( 3p)     0.00083
    Ryd( 4p)     0.00039
    Ryd( 5p)     0.00002

    Total:       1.20095

-------------------------------------------------------------------------------
NMR properties
-------------------------------------------------------------------------------
Electronic energy (NMR):                          -7603.67386110

 1  C    Isotropic =    19.7682   Anisotropy =   173.6822
 2  C    Isotropic =    36.2578   Anisotropy =   165.0509
 3  C    Isotropic =    49.7180   Anisotropy =   182.1551
 4  C    Isotropic =    25.0905   Anisotropy =   117.4083
 5  C    Isotropic =    49.7180   Anisotropy =   182.1551
 6  C    Isotropic =    36.2578   Anisotropy =   165.0509
 7  H    Isotropic =    23.4942   Anisotropy =    11.9803
 8  H    Isotropic =    23.0071   Anisotropy =     6.0738
 9  N    Isotropic =  -155.0186   Anisotropy =   291.6879
10  H    Isotropic =    23.0071   Anisotropy =     6.0738
11  H    Isotropic =    23.4942   Anisotropy =    11.9803
12  I    Isotropic =  3067.4532   Anisotropy =  3075.1417
13  O    Isotropic =  -307.6753   Anisotropy =   723.9530
14  O    Isotropic =  -307.6753   Anisotropy =   723.9530
15  N    Isotropic =   -92.1983   Anisotropy =   554.0301
16  C    Isotropic =    23.2568   Anisotropy =   180.7688
17  C    Isotropic =    50.0021   Anisotropy =   184.6005
18  C    Isotropic =    36.4737   Anisotropy =   213.8564
19  C    Isotropic =    50.0021   Anisotropy =   184.6005
20  C    Isotropic =    23.2568   Anisotropy =   180.7688
21  H    Isotropic =    22.6154   Anisotropy =    10.7242
22  H    Isotropic =    23.9062   Anisotropy =     5.3473
23  H    Isotropic =    23.4713   Anisotropy =     4.8519
24  H    Isotropic =    23.9062   Anisotropy =     5.3473
25  H    Isotropic =    22.6154   Anisotropy =    10.7242

===============================================================================
X = Br    R = H
-------------------------------------------------------------------------------
Energies and NBO populations
-------------------------------------------------------------------------------

Number of atoms:  23
Full point group                 C2V     NOp   4


C      0.000000  -0.568430   0.000000
C      0.000000  -1.255166   1.216061
C      0.000000  -2.653139   1.208412
C      0.000000  -3.354816   0.000000
C      0.000000  -2.653139  -1.208412
C      0.000000  -1.255166  -1.216061
H      0.000000  -0.708191   2.152621
H      0.000000  -3.190401   2.152157
H      0.000000  -4.440314   0.000000
H      0.000000  -3.190401  -2.152157
```

```
H      0.000000  -0.708191  -2.152621
Br     0.000000   1.349170   0.000000
N      0.000000   4.496990   0.000000
C      1.144942   5.192448   0.000000
C      1.199851   6.588363   0.000000
C      0.000000   7.301117   0.000000
C     -1.199851   6.588363   0.000000
C     -1.144942   5.192448   0.000000
H      2.060403   4.604414   0.000000
H      2.158409   7.097040   0.000000
H      0.000000   8.387014   0.000000
H     -2.158409   7.097040   0.000000
H     -2.060403   4.604414   0.000000

Electronic energy:                                  -3053.88644195 (  -3053.88644195)
Zero-point correction=                                 0.178365
Sum of electronic and zero-point Energies=          -3053.708077
Sum of electronic and thermal Energies=             -3053.696487
Sum of electronic and thermal Enthalpies=           -3053.695543
Sum of electronic and thermal Free Energies=        -3053.751489

Lowest vibration frequency:           -2.0199

Counterpoise: BSSE energy =       0.000457795755

Summary of Natural Population Analysis:

                                     Natural Population
                Natural  -----------------------------------------------
   Atom  No     Charge         Core      Valence    Rydberg      Total
------------------------------------------------------------------------
     C    1   -0.12216      1.99867     4.10029    0.02319     6.12216
     C    2   -0.23490      1.99898     4.21652    0.01941     6.23490
     C    3   -0.19539      1.99917     4.17849    0.01773     6.19539
     C    4   -0.21535      1.99918     4.19851    0.01767     6.21535
     C    5   -0.19539      1.99917     4.17849    0.01773     6.19539
     C    6   -0.23490      1.99898     4.21652    0.01941     6.23490
     H    7    0.22718      0.00000     0.77121    0.00161     0.77282
     H    8    0.21674      0.00000     0.78184    0.00142     0.78326
     H    9    0.21567      0.00000     0.78300    0.00133     0.78433
     H   10    0.21674      0.00000     0.78184    0.00142     0.78326
     H   11    0.22718      0.00000     0.77121    0.00161     0.77282
    Br   12    0.07950     27.99929     6.89911    0.02211    34.92050
     N   13   -0.47447      1.99944     5.45263    0.02241     7.47447
     C   14    0.05160      1.99923     3.92199    0.02718     5.94840
     C   15   -0.24863      1.99917     4.23302    0.01644     6.24863
     C   16   -0.16948      1.99918     4.15287    0.01744     6.16948
     C   17   -0.24863      1.99917     4.23302    0.01644     6.24863
     C   18    0.05160      1.99923     3.92199    0.02718     5.94840
     H   19    0.19606      0.00000     0.80248    0.00146     0.80394
     H   20    0.22143      0.00000     0.77708    0.00149     0.77857
     H   21    0.21812      0.00000     0.78059    0.00129     0.78188
     H   22    0.22143      0.00000     0.77708    0.00149     0.77857
     H   23    0.19606      0.00000     0.80248    0.00146     0.80394
========================================================================
  * Total *    0.00000     51.98884    65.73225    0.27891   118.00000

Contributions to pi population at N atom in pyridine:
    Val( 2p)     1.17833
    Ryd( 3p)     0.00073
    Ryd( 4p)     0.00034
    Ryd( 5p)     0.00002

    Total:       1.17942

-------------------------------------------------------------------------------
NMR properties
-------------------------------------------------------------------------------
Electronic energy (NMR):                            -3053.88644195

 1  C    Isotropic =    29.0803   Anisotropy =   133.8628
 2  C    Isotropic =    41.2152   Anisotropy =   163.5715
 3  C    Isotropic =    44.1792   Anisotropy =   187.0894
 4  C    Isotropic =    47.6054   Anisotropy =   191.9693
 5  C    Isotropic =    44.1792   Anisotropy =   187.0894
 6  C    Isotropic =    41.2152   Anisotropy =   163.5715
 7  H    Isotropic =    23.7302   Anisotropy =     9.8219
```

```
 8  H    Isotropic =    23.9203   Anisotropy =     5.0113
 9  H    Isotropic =    23.9892   Anisotropy =     4.1870
10  H    Isotropic =    23.9203   Anisotropy =     5.0113
11  H    Isotropic =    23.7302   Anisotropy =     9.8219
12  Br   Isotropic =  1939.1207   Anisotropy =  1467.8390
13  N    Isotropic =   -99.5788   Anisotropy =   578.6408
14  C    Isotropic =    21.8922   Anisotropy =   180.9487
15  C    Isotropic =    50.6225   Anisotropy =   183.4124
16  C    Isotropic =    37.5102   Anisotropy =   211.8561
17  C    Isotropic =    50.6225   Anisotropy =   183.4124
18  C    Isotropic =    21.8922   Anisotropy =   180.9487
19  H    Isotropic =    22.5018   Anisotropy =     9.4377
20  H    Isotropic =    23.9486   Anisotropy =     5.3271
21  H    Isotropic =    23.5209   Anisotropy =     4.9419
22  H    Isotropic =    23.9486   Anisotropy =     5.3271
23  H    Isotropic =    22.5018   Anisotropy =     9.4377

================================================================================
X = Br    R = OCH3
--------------------------------------------------------------------------------
Energies and NBO populations
--------------------------------------------------------------------------------

Number of atoms:  27
Full point group                 CS      NOp   2


C      0.000000  -0.414219  -0.024155
C      0.000000  -1.158280   1.152084
C      0.000000  -2.557858   1.098366
C      0.000000  -3.208408  -0.142203
C      0.000000  -2.448188  -1.322856
C      0.000000  -1.058364  -1.266519
H      0.000000  -0.659549   2.115329
H      0.000000  -3.117316   2.026333
O      0.000000  -4.560453  -0.305409
H      0.000000  -2.963953  -2.277721
H      0.000000  -0.478958  -2.183419
Br     0.000000   1.501625   0.054654
C      0.000000  -5.378357   0.858375
H      0.000000  -6.407658   0.499034
H     -0.896132  -5.205061   1.466634
H      0.896132  -5.205061   1.466634
N      0.000000   4.659423   0.169458
C      1.144871   5.354957   0.169458
C      1.199836   6.750906   0.169758
C      0.000000   7.463689   0.169889
C     -1.199836   6.750906   0.169758
C     -1.144871   5.354957   0.169458
H      2.060313   4.766881   0.168909
H      2.158406   7.259589   0.169581
H      0.000000   8.549595   0.169888
H     -2.158406   7.259589   0.169581
H     -2.060313   4.766881   0.168909

Electronic energy:                                  -3168.40894100 (  -3168.40894108)
Zero-point correction=                                  0.210768
Sum of electronic and zero-point Energies=          -3168.198173
Sum of electronic and thermal Energies=             -3168.183089
Sum of electronic and thermal Enthalpies=           -3168.182144
Sum of electronic and thermal Free Energies=        -3168.248143

Lowest vibration frequency:           4.7384

Counterpoise: BSSE energy =       0.000453931277

Summary of Natural Population Analysis:

                                     Natural Population
                Natural  -----------------------------------------------
   Atom  No     Charge         Core      Valence    Rydberg      Total
-------------------------------------------------------------------------
     C    1   -0.15140      1.99865     4.13000    0.02275     6.15140
     C    2   -0.21354      1.99899     4.19514    0.01940     6.21354
     C    3   -0.28474      1.99907     4.27057    0.01509     6.28474
     C    4    0.31920      1.99881     3.65899    0.02300     5.68080
     C    5   -0.23496      1.99908     4.21876    0.01712     6.23496
```

C	6	-0.21625	1.99899	4.19834	0.01892	6.21625
H	7	0.22670	0.00000	0.77164	0.00166	0.77330
H	8	0.22366	0.00000	0.77454	0.00181	0.77634
O	9	-0.54411	1.99971	6.52659	0.01780	8.54411
H	10	0.22775	0.00000	0.77048	0.00178	0.77225
H	11	0.22780	0.00000	0.77064	0.00156	0.77220
Br	12	0.07289	27.99929	6.90555	0.02227	34.92711
C	13	-0.21371	1.99928	4.19871	0.01572	6.21371
H	14	0.19642	0.00000	0.80256	0.00101	0.80358
H	15	0.17497	0.00000	0.82293	0.00210	0.82503
H	16	0.17497	0.00000	0.82293	0.00210	0.82503
N	17	-0.47376	1.99944	5.45185	0.02247	7.47376
C	18	0.05147	1.99923	3.92206	0.02724	5.94853
C	19	-0.24884	1.99917	4.23322	0.01645	6.24884
C	20	-0.16976	1.99918	4.15314	0.01744	6.16976
C	21	-0.24884	1.99917	4.23322	0.01645	6.24884
C	22	0.05147	1.99923	3.92206	0.02724	5.94853
H	23	0.19604	0.00000	0.80250	0.00146	0.80396
H	24	0.22128	0.00000	0.77723	0.00149	0.77872
H	25	0.21797	0.00000	0.78073	0.00129	0.78203
H	26	0.22128	0.00000	0.77723	0.00149	0.77872
H	27	0.19604	0.00000	0.80250	0.00146	0.80396
* Total *		0.00000	55.98729	77.69413	0.31857	134.00000

Contributions to pi population at N atom in pyridine:

Val(2p)	1.17756
Ryd(3p)	0.00073
Ryd(4p)	0.00033
Ryd(5p)	0.00002
Total:	1.17864

NMR properties

Electronic energy (NMR): -3168.40894100

1	C	Isotropic =	41.2234	Anisotropy =	115.6101
2	C	Isotropic =	40.7702	Anisotropy =	161.7672
3	C	Isotropic =	65.5272	Anisotropy =	160.4591
4	C	Isotropic =	12.3273	Anisotropy =	146.3826
5	C	Isotropic =	56.1651	Anisotropy =	149.9131
6	C	Isotropic =	40.2763	Anisotropy =	161.2150
7	H	Isotropic =	23.8453	Anisotropy =	9.7712
8	H	Isotropic =	24.5539	Anisotropy =	7.6159
9	O	Isotropic =	223.2488	Anisotropy =	84.6280
10	H	Isotropic =	24.3837	Anisotropy =	5.8321
11	H	Isotropic =	23.9160	Anisotropy =	9.3721
12	Br	Isotropic =	1982.9693	Anisotropy =	1452.3829
13	C	Isotropic =	124.5430	Anisotropy =	75.5031
14	H	Isotropic =	27.4854	Anisotropy =	8.4007
15	H	Isotropic =	27.8837	Anisotropy =	8.0317
16	H	Isotropic =	27.8837	Anisotropy =	8.0317
17	N	Isotropic =	-99.9298	Anisotropy =	579.7036
18	C	Isotropic =	21.8408	Anisotropy =	180.8837
19	C	Isotropic =	50.6866	Anisotropy =	183.3014
20	C	Isotropic =	37.5617	Anisotropy =	211.6456
21	C	Isotropic =	50.6866	Anisotropy =	183.3014
22	C	Isotropic =	21.8408	Anisotropy =	180.8837
23	H	Isotropic =	22.5118	Anisotropy =	9.5107
24	H	Isotropic =	23.9606	Anisotropy =	5.3449
25	H	Isotropic =	23.5329	Anisotropy =	4.9292
26	H	Isotropic =	23.9606	Anisotropy =	5.3449
27	H	Isotropic =	22.5118	Anisotropy =	9.5107

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X = Br R = OCH2CH3

Energies and NBO populations

Number of atoms: 30

Full point group CS NOp 2

C 0.000000 -0.312698 -0.053010

C	0.000000	-1.058061	1.122391
C	0.000000	-2.457599	1.067582
C	0.000000	-3.108252	-0.173640
C	0.000000	-2.345501	-1.353152
C	0.000000	-0.955671	-1.295840
H	0.000000	-0.560273	2.086149
H	0.000000	-3.017111	1.995376
O	0.000000	-4.459225	-0.339247
H	0.000000	-2.860057	-2.308709
H	0.000000	-0.375542	-2.212301
Br	0.000000	1.603396	0.027688
C	0.000000	-5.293293	0.823453
C	0.000000	-6.739035	0.355852
H	-0.890389	-5.077746	1.429736
H	0.890389	-5.077746	1.429736
H	0.000000	-7.407316	1.222870
H	0.888631	-6.951787	-0.245576
H	-0.888631	-6.951787	-0.245576
N	0.000000	4.763546	0.143309
C	1.144879	5.459034	0.143309
C	1.199856	6.855016	0.143491
C	0.000000	7.567771	0.143568
C	-1.199856	6.855016	0.143491
C	-1.144879	5.459034	0.143309
H	2.060348	4.871007	0.142822
H	2.158403	7.363731	0.143292
H	0.000000	8.653684	0.143533
H	-2.158403	7.363731	0.143292
H	-2.060348	4.871007	0.142822

Electronic energy: -3207.72448027 (-3207.72446349)
Zero-point correction= 0.238755
Sum of electronic and zero-point Energies= -3207.485725
Sum of electronic and thermal Energies= -3207.469220
Sum of electronic and thermal Enthalpies= -3207.468276
Sum of electronic and thermal Free Energies= -3207.537645

Lowest vibration frequency: 5.3586

Counterpoise: BSSE energy = 0.000442848601

Summary of Natural Population Analysis:

			Natural Population			
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.15163	1.99864	4.13033	0.02266	6.15163
C	2	-0.21383	1.99899	4.19555	0.01928	6.21383
C	3	-0.28435	1.99907	4.26997	0.01530	6.28435
C	4	0.32217	1.99882	3.65604	0.02297	5.67783
C	5	-0.23463	1.99909	4.21878	0.01676	6.23463
C	6	-0.21676	1.99899	4.19891	0.01886	6.21676
H	7	0.22643	0.00000	0.77191	0.00166	0.77357
H	8	0.22313	0.00000	0.77501	0.00186	0.77687
O	9	-0.55778	1.99970	6.53721	0.02087	8.55778
H	10	0.22718	0.00000	0.77110	0.00173	0.77282
H	11	0.22753	0.00000	0.77091	0.00156	0.77247
Br	12	0.07182	27.99929	6.90665	0.02224	34.92818
C	13	-0.03610	1.99925	4.01823	0.01862	6.03610
C	14	-0.59417	1.99938	4.58622	0.00857	6.59417
H	15	0.17432	0.00000	0.82322	0.00246	0.82568
H	16	0.17432	0.00000	0.82322	0.00246	0.82568
H	17	0.21047	0.00000	0.78838	0.00115	0.78953
H	18	0.20883	0.00000	0.78949	0.00169	0.79117
H	19	0.20883	0.00000	0.78949	0.00169	0.79117
N	20	-0.47361	1.99944	5.45171	0.02246	7.47361
C	21	0.05146	1.99923	3.92207	0.02724	5.94854
C	22	-0.24888	1.99917	4.23325	0.01646	6.24888
C	23	-0.16984	1.99918	4.15322	0.01744	6.16984
C	24	-0.24888	1.99917	4.23325	0.01646	6.24888
C	25	0.05146	1.99923	3.92207	0.02724	5.94854
H	26	0.19604	0.00000	0.80250	0.00146	0.80396
H	27	0.22124	0.00000	0.77726	0.00150	0.77876
H	28	0.21794	0.00000	0.78077	0.00129	0.78206
H	29	0.22124	0.00000	0.77726	0.00150	0.77876
H	30	0.19604	0.00000	0.80250	0.00146	0.80396

```
================================================================================
  * Total *    0.00000     57.98664    83.67647    0.33689   142.00000

Contributions to pi population at N atom in pyridine:
    Val( 2p)     1.17740
    Ryd( 3p)     0.00073
    Ryd( 4p)     0.00033
    Ryd( 5p)     0.00002

    Total:       1.17848

--------------------------------------------------------------------------------
NMR properties
--------------------------------------------------------------------------------
Electronic energy (NMR):                          -3207.72448027

 1  C    Isotropic =    41.4395   Anisotropy =   114.8869
 2  C    Isotropic =    40.8045   Anisotropy =   161.2611
 3  C    Isotropic =    64.9359   Anisotropy =   158.4218
 4  C    Isotropic =    12.7025   Anisotropy =   145.7050
 5  C    Isotropic =    56.1547   Anisotropy =   148.8789
 6  C    Isotropic =    40.3110   Anisotropy =   160.9023
 7  H    Isotropic =    23.8745   Anisotropy =     9.7997
 8  H    Isotropic =    24.5952   Anisotropy =     8.2315
 9  O    Isotropic =   193.3481   Anisotropy =    70.2450
10  H    Isotropic =    24.3710   Anisotropy =     6.3233
11  H    Isotropic =    23.9169   Anisotropy =     9.3768
12  Br   Isotropic =  1983.7882   Anisotropy =  1452.9244
13  C    Isotropic =   113.5093   Anisotropy =    63.1869
14  C    Isotropic =   165.9502   Anisotropy =    25.6620
15  H    Isotropic =    27.6335   Anisotropy =     5.3802
16  H    Isotropic =    27.6335   Anisotropy =     5.3802
17  H    Isotropic =    30.2564   Anisotropy =    10.0870
18  H    Isotropic =    30.0324   Anisotropy =     8.2204
19  H    Isotropic =    30.0324   Anisotropy =     8.2204
20  N    Isotropic =   -99.9801   Anisotropy =   579.9339
21  C    Isotropic =    21.8279   Anisotropy =   180.8523
22  C    Isotropic =    50.6950   Anisotropy =   183.2913
23  C    Isotropic =    37.5633   Anisotropy =   211.5787
24  C    Isotropic =    50.6950   Anisotropy =   183.2913
25  C    Isotropic =    21.8279   Anisotropy =   180.8523
26  H    Isotropic =    22.5117   Anisotropy =     9.5410
27  H    Isotropic =    23.9620   Anisotropy =     5.3525
28  H    Isotropic =    23.5352   Anisotropy =     4.9212
29  H    Isotropic =    23.9620   Anisotropy =     5.3525
30  H    Isotropic =    22.5117   Anisotropy =     9.5410

================================================================================
X = Br    R = CH3
--------------------------------------------------------------------------------
Energies and NBO populations
--------------------------------------------------------------------------------

Number of atoms:  26
Full point group                 CS      NOp   2


C      0.000000  -0.477013  -0.007327
C      0.000000  -1.111407   1.234037
C      0.000000  -2.509052   1.287760
C      0.000000  -3.285847   0.122256
C      0.000000  -2.618554  -1.112743
C      0.000000  -1.224866  -1.187215
H      0.000000  -0.527730   2.148336
H      0.000000  -2.997923   2.258599
C      0.000000  -4.797133   0.183878
H      0.000000  -3.194796  -2.034886
H      0.000000  -0.726538  -2.150746
Br     0.000000   1.438743  -0.096918
H      0.000000  -5.151161   1.218329
H     -0.882698  -5.212372  -0.315637
H      0.882698  -5.212372  -0.315637
N      0.000000   4.597416  -0.218676
C      1.144873   5.292968  -0.218676
C      1.199835   6.688912  -0.218835
C      0.000000   7.401694  -0.218884
C     -1.199835   6.688912  -0.218835
```

```
C     -1.144873   5.292968  -0.218676
H      2.060344   4.704939  -0.218271
H      2.158404   7.197591  -0.218697
H      0.000000   8.487599  -0.218816
H     -2.158404   7.197591  -0.218697
H     -2.060344   4.704939  -0.218271

Electronic energy:                                  -3093.20023672 (  -3093.20023677)
Zero-point correction=                                 0.205418
Sum of electronic and zero-point Energies=          -3092.994819
Sum of electronic and thermal Energies=             -3092.981325
Sum of electronic and thermal Enthalpies=           -3092.980381
Sum of electronic and thermal Free Energies=        -3093.041703

Lowest vibration frequency:           -3.6078

Counterpoise: BSSE energy =       0.000418767595

Summary of Natural Population Analysis:

                                     Natural Population
                Natural  -----------------------------------------------
   Atom  No     Charge         Core      Valence    Rydberg      Total
------------------------------------------------------------------------
     C    1   -0.12937      1.99865     4.10793    0.02278     6.12937
     C    2   -0.22793      1.99898     4.20932    0.01962     6.22793
     C    3   -0.19788      1.99906     4.18234    0.01648     6.19788
     C    4   -0.03695      1.99907     4.02253    0.01535     6.03695
     C    5   -0.19536      1.99906     4.17972    0.01658     6.19536
     C    6   -0.22671      1.99898     4.20823    0.01949     6.22671
     H    7    0.22620      0.00000     0.77210    0.00170     0.77380
     H    8    0.21323      0.00000     0.78513    0.00164     0.78677
     C    9   -0.59682      1.99932     4.58751    0.00999     6.59682
     H   10    0.21335      0.00000     0.78506    0.00159     0.78665
     H   11    0.22610      0.00000     0.77220    0.00170     0.77390
    Br   12    0.07446     27.99929     6.90405    0.02221    34.92554
     H   13    0.21019      0.00000     0.78852    0.00129     0.78981
     H   14    0.21652      0.00000     0.78214    0.00134     0.78348
     H   15    0.21652      0.00000     0.78214    0.00134     0.78348
     N   16   -0.47386      1.99944     5.45201    0.02241     7.47386
     C   17    0.05150      1.99923     3.92206    0.02721     5.94850
     C   18   -0.24881      1.99917     4.23319    0.01645     6.24881
     C   19   -0.16972      1.99918     4.15310    0.01744     6.16972
     C   20   -0.24881      1.99917     4.23319    0.01645     6.24881
     C   21    0.05150      1.99923     3.92206    0.02721     5.94850
     H   22    0.19602      0.00000     0.80252    0.00146     0.80398
     H   23    0.22130      0.00000     0.77721    0.00149     0.77870
     H   24    0.21799      0.00000     0.78071    0.00129     0.78201
     H   25    0.22130      0.00000     0.77721    0.00149     0.77870
     H   26    0.19602      0.00000     0.80252    0.00146     0.80398
========================================================================
  * Total *    0.00000     53.98782    71.72469    0.28749   126.00000

Contributions to pi population at N atom in pyridine:
    Val( 2p)     1.17764
    Ryd( 3p)     0.00073
    Ryd( 4p)     0.00034
    Ryd( 5p)     0.00002

    Total:       1.17873

-------------------------------------------------------------------------------
NMR properties
-------------------------------------------------------------------------------
Electronic energy (NMR):                            -3093.20023672

 1  C    Isotropic =    33.3237   Anisotropy =   126.8832
 2  C    Isotropic =    41.5298   Anisotropy =   159.8372
 3  C    Isotropic =    43.4765   Anisotropy =   161.4204
 4  C    Isotropic =    34.6683   Anisotropy =   205.6111
 5  C    Isotropic =    43.3582   Anisotropy =   172.3976
 6  C    Isotropic =    41.6428   Anisotropy =   160.3252
 7  H    Isotropic =    23.9176   Anisotropy =     9.6356
 8  H    Isotropic =    24.1539   Anisotropy =     6.5537
 9  C    Isotropic =   159.6196   Anisotropy =    41.4511
10  H    Isotropic =    24.0187   Anisotropy =     7.0995
11  H    Isotropic =    23.8509   Anisotropy =     9.6567
```

```
12  Br   Isotropic =  1961.5294   Anisotropy =  1456.3923
13  H    Isotropic =    29.4927   Anisotropy =     7.5849
14  H    Isotropic =    28.9639   Anisotropy =     8.5394
15  H    Isotropic =    28.9639   Anisotropy =     8.5394
16  N    Isotropic =   -99.8518   Anisotropy =   579.4807
17  C    Isotropic =    21.8530   Anisotropy =   180.9160
18  C    Isotropic =    50.6709   Anisotropy =   183.3253
19  C    Isotropic =    37.5556   Anisotropy =   211.7053
20  C    Isotropic =    50.6709   Anisotropy =   183.3253
21  C    Isotropic =    21.8530   Anisotropy =   180.9160
22  H    Isotropic =    22.5126   Anisotropy =     9.4731
23  H    Isotropic =    23.9595   Anisotropy =     5.3396
24  H    Isotropic =    23.5311   Anisotropy =     4.9359
25  H    Isotropic =    23.9595   Anisotropy =     5.3396
26  H    Isotropic =    22.5126   Anisotropy =     9.4731

================================================================================
X = Br    R = CHCH32
--------------------------------------------------------------------------------
Energies and NBO populations
--------------------------------------------------------------------------------

Number of atoms:  32
Full point group                 CS      NOp   2


C      0.000000  -0.330631   0.048206
C      0.000000  -1.071106   1.229488
C      0.000000  -2.467901   1.159121
C      0.000000  -3.141782  -0.069240
C      0.000000  -2.367707  -1.240688
C      0.000000  -0.972665  -1.192131
H      0.000000  -0.569834   2.191491
H      0.000000  -3.040493   2.083525
C      0.000000  -4.664920  -0.123211
H      0.000000  -2.853207  -2.213072
H      0.000000  -0.391696  -2.108266
Br     0.000000   1.585759   0.123981
H      0.000000  -5.020519   0.915481
C     -1.271447  -5.212984  -0.803214
C      1.271447  -5.212984  -0.803214
H     -1.278515  -6.308482  -0.775156
H     -1.322423  -4.905046  -1.853989
H     -2.175185  -4.851188  -0.302170
H      1.278515  -6.308482  -0.775156
H      2.175185  -4.851188  -0.302170
H      1.322423  -4.905046  -1.853989
N      0.000000   4.747277   0.212694
C      1.144857   5.442869   0.212694
C      1.199820   6.838823   0.212793
C      0.000000   7.551627   0.212946
C     -1.199820   6.838823   0.212793
C     -1.144857   5.442869   0.212694
H      2.060340   4.854868   0.212402
H      2.158405   7.347484   0.212670
H      0.000000   8.637530   0.213070
H     -2.158405   7.347484   0.212670
H     -2.060340   4.854868   0.212402

Electronic energy:                                -3171.82081334 (  -3171.82082070)
Zero-point correction=                                0.261873
Sum of electronic and zero-point Energies=        -3171.558940
Sum of electronic and thermal Energies=           -3171.542949
Sum of electronic and thermal Enthalpies=         -3171.542004
Sum of electronic and thermal Free Energies=      -3171.607753

Lowest vibration frequency:           -7.3245

Counterpoise: BSSE energy =       0.000410560388

Summary of Natural Population Analysis:

                                  Natural Population
              Natural  -----------------------------------------------
   Atom  No    Charge         Core      Valence    Rydberg      Total
-----------------------------------------------------------------------
     C    1   -0.12827      1.99865     4.10671    0.02291     6.12827
```

C	2	-0.22815	1.99898	4.20966	0.01951	6.22815
C	3	-0.19496	1.99906	4.17947	0.01643	6.19496
C	4	-0.02320	1.99902	4.00408	0.02010	6.02320
C	5	-0.19749	1.99905	4.18227	0.01617	6.19749
C	6	-0.22714	1.99898	4.20855	0.01961	6.22714
H	7	0.22631	0.00000	0.77203	0.00166	0.77369
H	8	0.21352	0.00000	0.78474	0.00174	0.78648
C	9	-0.24333	1.99920	4.22846	0.01567	6.24333
H	10	0.21371	0.00000	0.78455	0.00174	0.78629
H	11	0.22583	0.00000	0.77251	0.00166	0.77417
Br	12	0.07461	27.99929	6.90395	0.02216	34.92539
H	13	0.19852	0.00000	0.79847	0.00301	0.80148
C	14	-0.57022	1.99935	4.56140	0.00947	6.57022
C	15	-0.57022	1.99935	4.56140	0.00947	6.57022
H	16	0.20305	0.00000	0.79575	0.00120	0.79695
H	17	0.19763	0.00000	0.80101	0.00137	0.80237
H	18	0.20739	0.00000	0.79159	0.00101	0.79261
H	19	0.20305	0.00000	0.79575	0.00120	0.79695
H	20	0.20739	0.00000	0.79159	0.00101	0.79261
H	21	0.19763	0.00000	0.80101	0.00137	0.80237
N	22	-0.47378	1.99944	5.45193	0.02241	7.47378
C	23	0.05146	1.99923	3.92208	0.02723	5.94854
C	24	-0.24882	1.99917	4.23320	0.01645	6.24882
C	25	-0.16974	1.99918	4.15312	0.01744	6.16974
C	26	-0.24882	1.99917	4.23320	0.01645	6.24882
C	27	0.05146	1.99923	3.92208	0.02723	5.94854
H	28	0.19602	0.00000	0.80252	0.00146	0.80398
H	29	0.22129	0.00000	0.77722	0.00149	0.77871
H	30	0.21799	0.00000	0.78072	0.00129	0.78201
H	31	0.22129	0.00000	0.77722	0.00149	0.77871
H	32	0.19602	0.00000	0.80252	0.00146	0.80398
* Total *		0.00000	57.98635	83.69079	0.32287	142.00000

Contributions to pi population at N atom in pyridine:

Val(2p)	1.17756
Ryd(3p)	0.00073
Ryd(4p)	0.00034
Ryd(5p)	0.00002
Total:	1.17865

NMR properties

Electronic energy (NMR): -3171.82081334

1	C	Isotropic =	32.8472	Anisotropy =	125.8137
2	C	Isotropic =	41.4597	Anisotropy =	159.2673
3	C	Isotropic =	44.5323	Anisotropy =	156.1379
4	C	Isotropic =	22.9064	Anisotropy =	214.5764
5	C	Isotropic =	47.1852	Anisotropy =	185.3806
6	C	Isotropic =	41.2384	Anisotropy =	160.9324
7	H	Isotropic =	23.8975	Anisotropy =	9.4498
8	H	Isotropic =	24.1485	Anisotropy =	7.2185
9	C	Isotropic =	139.6199	Anisotropy =	24.5509
10	H	Isotropic =	23.9925	Anisotropy =	9.5436
11	H	Isotropic =	23.8162	Anisotropy =	9.8788
12	Br	Isotropic =	1959.8952	Anisotropy =	1458.3613
13	H	Isotropic =	28.7371	Anisotropy =	6.9217
14	C	Isotropic =	155.7508	Anisotropy =	36.8608
15	C	Isotropic =	155.7508	Anisotropy =	36.8608
16	H	Isotropic =	30.2582	Anisotropy =	10.2055
17	H	Isotropic =	30.3331	Anisotropy =	6.5431
18	H	Isotropic =	30.3078	Anisotropy =	8.5172
19	H	Isotropic =	30.2582	Anisotropy =	10.2055
20	H	Isotropic =	30.3078	Anisotropy =	8.5172
21	H	Isotropic =	30.3331	Anisotropy =	6.5431
22	N	Isotropic =	-99.7967	Anisotropy =	579.7513
23	C	Isotropic =	21.8353	Anisotropy =	180.8599
24	C	Isotropic =	50.6791	Anisotropy =	183.2978
25	C	Isotropic =	37.5861	Anisotropy =	211.7039
26	C	Isotropic =	50.6791	Anisotropy =	183.2978
27	C	Isotropic =	21.8353	Anisotropy =	180.8599
28	H	Isotropic =	22.5093	Anisotropy =	9.5619
29	H	Isotropic =	23.9597	Anisotropy =	5.3487
30	H	Isotropic =	23.5325	Anisotropy =	4.9016

```
31  H    Isotropic =    23.9597   Anisotropy =     5.3487
32  H    Isotropic =    22.5093   Anisotropy =     9.5619

================================================================================
X = Br    R = H
--------------------------------------------------------------------------------
Energies and NBO populations
--------------------------------------------------------------------------------

Number of atoms:  23
Full point group                 C2V     NOp   4


C      0.000000  -0.533417   0.000000
C      0.000000  -1.223190   1.214697
C      0.000000  -2.620369   1.217194
C      0.000000  -3.290044   0.000000
C      0.000000  -2.620369  -1.217194
C      0.000000  -1.223190  -1.214698
H      0.000000  -0.680227   2.153188
H      0.000000  -3.180688   2.145842
F      0.000000  -4.643773   0.000000
H      0.000000  -3.180688  -2.145842
H      0.000000  -0.680227  -2.153188
Br     0.000000   1.381934   0.000000
N      0.000000   4.506001   0.000000
C      1.145101   5.201305   0.000000
C      1.199878   6.597139   0.000000
C      0.000000   7.309837   0.000000
C     -1.199878   6.597139   0.000000
C     -1.145101   5.201305   0.000000
H      2.060514   4.613230   0.000000
H      2.158411   7.105830   0.000000
H      0.000000   8.395714   0.000000
H     -2.158411   7.105830   0.000000
H     -2.060514   4.613230   0.000000

Electronic energy:                                -3153.13011375 (  -3153.13011375)
Zero-point correction=                                0.170141
Sum of electronic and zero-point Energies=        -3152.959973
Sum of electronic and thermal Energies=           -3152.946637
Sum of electronic and thermal Enthalpies=         -3152.945693
Sum of electronic and thermal Free Energies=      -3153.007568

Lowest vibration frequency:           5.4020

Counterpoise: BSSE energy =       0.000499154561

Summary of Natural Population Analysis:

                                     Natural Population
               Natural  ----------------------------------------------
   Atom  No    Charge         Core      Valence    Rydberg      Total
--------------------------------------------------------------------------
     C    1   -0.13959      1.99867     4.11806    0.02286     6.13959
     C    2   -0.21373      1.99900     4.19601    0.01872     6.21373
     C    3   -0.25941      1.99906     4.24353    0.01683     6.25941
     C    4    0.40292      1.99849     3.57215    0.02643     5.59708
     C    5   -0.25941      1.99906     4.24353    0.01683     6.25941
     C    6   -0.21372      1.99900     4.19601    0.01872     6.21372
     H    7    0.23152      0.00000     0.76687    0.00161     0.76848
     H    8    0.23530      0.00000     0.76312    0.00157     0.76470
     F    9   -0.35452      1.99993     7.34656    0.00803     9.35452
     H   10    0.23530      0.00000     0.76312    0.00157     0.76470
     H   11    0.23152      0.00000     0.76687    0.00161     0.76848
    Br   12    0.08748     27.99929     6.89091    0.02232    34.91252
     N   13   -0.47600      1.99943     5.45407    0.02250     7.47600
     C   14    0.05178      1.99923     3.92184    0.02715     5.94822
     C   15   -0.24823      1.99917     4.23263    0.01643     6.24823
     C   16   -0.16891      1.99918     4.15230    0.01743     6.16891
     C   17   -0.24823      1.99917     4.23263    0.01643     6.24823
     C   18    0.05178      1.99923     3.92184    0.02715     5.94822
     H   19    0.19613      0.00000     0.80241    0.00146     0.80387
     H   20    0.22173      0.00000     0.77678    0.00149     0.77827
     H   21    0.21843      0.00000     0.78028    0.00129     0.78157
     H   22    0.22173      0.00000     0.77678    0.00149     0.77827
     H   23    0.19613      0.00000     0.80241    0.00146     0.80387
```

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================================================================================
  * Total *    0.00000     53.98789    71.72072    0.29139   126.00000

Contributions to pi population at N atom in pyridine:
    Val( 2p)     1.17992
    Ryd( 3p)     0.00073
    Ryd( 4p)     0.00034
    Ryd( 5p)     0.00002

    Total:       1.18101

--------------------------------------------------------------------------------
NMR properties
--------------------------------------------------------------------------------
Electronic energy (NMR):                          -3153.13011375

 1  C    Isotropic =    35.7256   Anisotropy =   128.4925
 2  C    Isotropic =    39.7298   Anisotropy =   163.1044
 3  C    Isotropic =    58.2448   Anisotropy =   153.9198
 4  C    Isotropic =     7.3155   Anisotropy =   106.5773
 5  C    Isotropic =    58.2448   Anisotropy =   153.9198
 6  C    Isotropic =    39.7298   Anisotropy =   163.1044
 7  H    Isotropic =    23.8026   Anisotropy =     9.4074
 8  H    Isotropic =    24.2712   Anisotropy =     4.6345
 9  F    Isotropic =   294.5860   Anisotropy =    99.1838
10  H    Isotropic =    24.2712   Anisotropy =     4.6345
11  H    Isotropic =    23.8026   Anisotropy =     9.4074
12  Br   Isotropic =  1951.8230   Anisotropy =  1468.1497
13  N    Isotropic =   -98.8562   Anisotropy =   576.9210
14  C    Isotropic =    21.9792   Anisotropy =   180.8271
15  C    Isotropic =    50.5665   Anisotropy =   183.5619
16  C    Isotropic =    37.4101   Anisotropy =   212.0478
17  C    Isotropic =    50.5665   Anisotropy =   183.5619
18  C    Isotropic =    21.9792   Anisotropy =   180.8271
19  H    Isotropic =    22.5229   Anisotropy =     9.4820
20  H    Isotropic =    23.9483   Anisotropy =     5.3336
21  H    Isotropic =    23.5197   Anisotropy =     4.9424
22  H    Isotropic =    23.9483   Anisotropy =     5.3336
23  H    Isotropic =    22.5229   Anisotropy =     9.4820

================================================================================
X = Br    R = Cl
--------------------------------------------------------------------------------
Energies and NBO populations
--------------------------------------------------------------------------------

Number of atoms:  23
Full point group                 C2V     NOp   4


C      0.000000  -0.494724   0.000000
C      0.000000  -1.185303   1.213717
C      0.000000  -2.582160   1.215355
C      0.000000  -3.265320   0.000000
C      0.000000  -2.582160  -1.215355
C      0.000000  -1.185303  -1.213717
H      0.000000  -0.644074   2.153359
H      0.000000  -3.128717   2.151866
Cl     0.000000  -5.027014   0.000000
H      0.000000  -3.128717  -2.151866
H      0.000000  -0.644074  -2.153359
Br     0.000000   1.419123   0.000000
N      0.000000   4.535620   0.000000
C      1.145156   5.230877   0.000000
C      1.199889   6.626687   0.000000
C      0.000000   7.339361   0.000000
C     -1.199889   6.626687   0.000000
C     -1.145156   5.230877   0.000000
H      2.060575   4.642825   0.000000
H      2.158412   7.135380   0.000000
H      0.000000   8.425232   0.000000
H     -2.158412   7.135380   0.000000
H     -2.060575   4.642825   0.000000

Electronic energy:                              -3513.45247580 (  -3513.45247580)
Zero-point correction=                              0.168823
Sum of electronic and zero-point Energies=      -3513.283653
```

Sum of electronic and thermal Energies= -3513.269931
Sum of electronic and thermal Enthalpies= -3513.268986
Sum of electronic and thermal Free Energies= -3513.331944

Lowest vibration frequency: 6.4860

Counterpoise: BSSE energy = 0.000477108347

Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.12811	1.99867	4.10651	0.02293	6.12811
C	2	-0.21531	1.99898	4.19721	0.01912	6.21531
C	3	-0.21727	1.99898	4.19972	0.01857	6.21727
C	4	-0.04592	1.99860	4.02465	0.02266	6.04592
C	5	-0.21727	1.99898	4.19972	0.01857	6.21727
C	6	-0.21531	1.99898	4.19721	0.01912	6.21531
H	7	0.23277	0.00000	0.76560	0.00163	0.76723
H	8	0.23414	0.00000	0.76419	0.00167	0.76586
Cl	9	-0.00413	9.99962	6.98454	0.01997	17.00413
H	10	0.23414	0.00000	0.76419	0.00167	0.76586
H	11	0.23277	0.00000	0.76560	0.00163	0.76723
Br	12	0.09267	27.99929	6.88569	0.02236	34.90733
N	13	-0.47657	1.99943	5.45465	0.02248	7.47657
C	14	0.05188	1.99923	3.92177	0.02712	5.94812
C	15	-0.24808	1.99917	4.23249	0.01642	6.24808
C	16	-0.16871	1.99918	4.15211	0.01742	6.16871
C	17	-0.24808	1.99917	4.23249	0.01642	6.24808
C	18	0.05188	1.99923	3.92177	0.02712	5.94812
H	19	0.19616	0.00000	0.80238	0.00146	0.80384
H	20	0.22183	0.00000	0.77668	0.00149	0.77817
H	21	0.21852	0.00000	0.78019	0.00129	0.78148
H	22	0.22183	0.00000	0.77668	0.00149	0.77817
H	23	0.19616	0.00000	0.80238	0.00146	0.80384
* Total *		0.00000	61.98749	71.70845	0.30406	134.00000

Contributions to pi population at N atom in pyridine:
Val(2p) 1.18049
Ryd(3p) 0.00073
Ryd(4p) 0.00034
Ryd(5p) 0.00002

Total: 1.18158

NMR properties

Electronic energy (NMR): -3513.45247580

1	C	Isotropic =	31.2728	Anisotropy =	136.3778
2	C	Isotropic =	40.1508	Anisotropy =	160.6059
3	C	Isotropic =	44.0364	Anisotropy =	158.6931
4	C	Isotropic =	32.3766	Anisotropy =	121.9799
5	C	Isotropic =	44.0364	Anisotropy =	158.6931
6	C	Isotropic =	40.1508	Anisotropy =	160.6059
7	H	Isotropic =	23.8349	Anisotropy =	9.4769
8	H	Isotropic =	23.9887	Anisotropy =	7.3208
9	Cl	Isotropic =	687.0565	Anisotropy =	502.4561
10	H	Isotropic =	23.9887	Anisotropy =	7.3208
11	H	Isotropic =	23.8349	Anisotropy =	9.4769
12	Br	Isotropic =	1938.5272	Anisotropy =	1453.8918
13	N	Isotropic =	-98.5006	Anisotropy =	576.1537
14	C	Isotropic =	22.0110	Anisotropy =	180.7586
15	C	Isotropic =	50.5421	Anisotropy =	183.6230
16	C	Isotropic =	37.3601	Anisotropy =	212.0979
17	C	Isotropic =	50.5421	Anisotropy =	183.6230
18	C	Isotropic =	22.0110	Anisotropy =	180.7586
19	H	Isotropic =	22.5309	Anisotropy =	9.5279
20	H	Isotropic =	23.9480	Anisotropy =	5.3443
21	H	Isotropic =	23.5196	Anisotropy =	4.9376
22	H	Isotropic =	23.9480	Anisotropy =	5.3443
23	H	Isotropic =	22.5309	Anisotropy =	9.5279

```
================================================================================
X = Br    R = OCF3
--------------------------------------------------------------------------------
Energies and NBO populations
--------------------------------------------------------------------------------

Number of atoms:  27
Full point group                 C1      NOp   1


C     -0.126249  -0.371179  -0.051567
C     -0.573703  -1.056765  -1.183617
C     -0.548480  -2.452814  -1.198687
C     -0.069803  -3.132630  -0.082885
C      0.368090  -2.459558   1.053472
C      0.341572  -1.063549   1.068058
H     -0.941469  -0.511334  -2.045333
H     -0.897839  -3.005196  -2.064031
O     -0.107043  -4.541205  -0.070219
H      0.720916  -3.017601   1.913782
H      0.679834  -0.523391   1.945043
Br    -0.161528   1.541734  -0.031455
C      0.978254  -5.197724  -0.530290
F      2.095517  -4.917457   0.168998
F      0.738165  -6.504591  -0.426288
F      1.249847  -4.920896  -1.820924
N     -0.206661   4.632312   0.003213
C     -1.351951   5.327556   0.003213
C     -1.406540   6.723365   0.002936
C     -0.206669   7.435943   0.002978
C      0.993214   6.723359   0.003227
C      0.938589   5.327564   0.003213
H     -2.267633   4.739973   0.003535
H     -2.365022   7.232123   0.002814
H     -0.206731   8.521810   0.002875
H      1.951728   7.232076   0.003236
H      1.854234   4.739878   0.002919

Electronic energy:                                -3466.16987472 (  -3466.16984624)
Zero-point correction=                                0.186972
Sum of electronic and zero-point Energies=        -3465.982903
Sum of electronic and thermal Energies=           -3465.965933
Sum of electronic and thermal Enthalpies=         -3465.964989
Sum of electronic and thermal Free Energies=      -3466.036571

Lowest vibration frequency:            8.2656

Counterpoise: BSSE energy =       0.000454462194

Summary of Natural Population Analysis:

                                     Natural Population
               Natural  -----------------------------------------------
   Atom  No    Charge         Core      Valence    Rydberg      Total
--------------------------------------------------------------------------
     C    1   -0.12393      1.99868     4.10230    0.02295     6.12393
     C    2   -0.21709      1.99899     4.19928    0.01882     6.21709
     C    3   -0.21634      1.99903     4.20032    0.01698     6.21634
     C    4    0.26082      1.99868     3.71723    0.02328     5.73918
     C    5   -0.21599      1.99903     4.19994    0.01702     6.21599
     C    6   -0.21713      1.99899     4.19931    0.01883     6.21713
     H    7    0.23351      0.00000     0.76488    0.00161     0.76649
     H    8    0.23702      0.00000     0.76128    0.00170     0.76298
     O    9   -0.56407      1.99965     6.54722    0.01719     8.56407
     H   10    0.23688      0.00000     0.76142    0.00170     0.76312
     H   11    0.23351      0.00000     0.76488    0.00161     0.76649
    Br   12    0.09776     27.99928     6.88059    0.02237    34.90224
     C   13    1.28119      1.99964     2.64817    0.07099     4.71881
     F   14   -0.35385      1.99991     7.34732    0.00662     9.35385
     F   15   -0.33622      1.99991     7.32997    0.00634     9.33622
     F   16   -0.35405      1.99991     7.34752    0.00661     9.35405
     N   17   -0.47747      1.99943     5.45551    0.02253     7.47747
     C   18    0.05219      1.99923     3.92151    0.02707     5.94781
     C   19   -0.24785      1.99917     4.23226    0.01642     6.24785
     C   20   -0.16835      1.99918     4.15176    0.01742     6.16835
     C   21   -0.24777      1.99917     4.23219    0.01642     6.24777
     C   22    0.05214      1.99923     3.92157    0.02707     5.94786
```

H	23	0.19614	0.00000	0.80241	0.00145	0.80386
H	24	0.22198	0.00000	0.77654	0.00149	0.77802
H	25	0.21869	0.00000	0.78002	0.00129	0.78131
H	26	0.22202	0.00000	0.77649	0.00149	0.77798
H	27	0.19625	0.00000	0.80229	0.00146	0.80375
* Total *		0.00000	61.98712	95.62417	0.38871	158.00000

Contributions to pi population at N atom in pyridine:

Val(2p)	1.18163
Ryd(3p)	0.00075
Ryd(4p)	0.00035
Ryd(5p)	0.00002
Total:	1.18275

NMR properties

Electronic energy (NMR): -3466.16987472

1	C	Isotropic =	29.5377	Anisotropy =	139.1897
2	C	Isotropic =	40.0842	Anisotropy =	163.0517
3	C	Isotropic =	49.2751	Anisotropy =	164.4337
4	C	Isotropic =	23.2880	Anisotropy =	112.7649
5	C	Isotropic =	49.2500	Anisotropy =	164.2909
6	C	Isotropic =	40.0754	Anisotropy =	163.0688
7	H	Isotropic =	23.6968	Anisotropy =	9.5398
8	H	Isotropic =	24.0285	Anisotropy =	6.9843
9	O	Isotropic =	167.9679	Anisotropy =	88.6697
10	H	Isotropic =	24.0339	Anisotropy =	6.8867
11	H	Isotropic =	23.6919	Anisotropy =	9.5274
12	Br	Isotropic =	1926.4558	Anisotropy =	1465.1125
13	C	Isotropic =	47.3860	Anisotropy =	10.8789
14	F	Isotropic =	240.2241	Anisotropy =	165.0153
15	F	Isotropic =	241.3086	Anisotropy =	170.1156
16	F	Isotropic =	239.9621	Anisotropy =	165.4027
17	N	Isotropic =	-98.2464	Anisotropy =	574.7700
18	C	Isotropic =	22.1848	Anisotropy =	180.9495
19	C	Isotropic =	50.4006	Anisotropy =	183.2865
20	C	Isotropic =	37.4914	Anisotropy =	212.6939
21	C	Isotropic =	50.4480	Anisotropy =	183.4432
22	C	Isotropic =	22.1509	Anisotropy =	181.1515
23	H	Isotropic =	22.5291	Anisotropy =	9.5014
24	H	Isotropic =	23.9407	Anisotropy =	5.3290
25	H	Isotropic =	23.5060	Anisotropy =	4.9418
26	H	Isotropic =	23.9341	Anisotropy =	5.3908
27	H	Isotropic =	22.5220	Anisotropy =	9.6543

X = Br R = COOCH3

Energies and NBO populations

Number of atoms: 29

Full point group CS NOp 2

C	0.000000	-0.366483	0.016488
C	0.000000	-1.071911	1.223631
C	0.000000	-2.464790	1.197212
C	0.000000	-3.154879	-0.023469
C	0.000000	-2.431918	-1.225618
C	0.000000	-1.037668	-1.209488
H	0.000000	-0.539692	2.168318
H	0.000000	-3.030613	2.122903
C	0.000000	-4.647564	0.012271
H	0.000000	-2.958947	-2.172772
H	0.000000	-0.478530	-2.138519
Br	0.000000	1.545114	0.042113
O	0.000000	-5.191545	-1.218742
C	0.000000	-6.629045	-1.271893
H	0.000000	-6.879823	-2.331934
H	-0.891477	-7.028148	-0.782490
H	0.891477	-7.028148	-0.782490
O	0.000000	-5.307733	1.030156

```
N      0.000000   4.662142   0.073352
C      1.145180   5.357398   0.073352
C      1.199895   6.753203   0.073256
C      0.000000   7.465862   0.073180
C     -1.199895   6.753203   0.073256
C     -1.145180   5.357398   0.073352
H      2.060646   4.769428   0.073362
H      2.158406   7.261900   0.073241
H      0.000000   8.551728   0.073083
H     -2.158406   7.261900   0.073241
H     -2.060646   4.769428   0.073362

Electronic energy:                                  -3281.77130994 (  -3281.77130991)
Zero-point correction=                                  0.220955
Sum of electronic and zero-point Energies=          -3281.550355
Sum of electronic and thermal Energies=             -3281.533302
Sum of electronic and thermal Enthalpies=           -3281.532358
Sum of electronic and thermal Free Energies=        -3281.603225

Lowest vibration frequency:           7.5818

Counterpoise: BSSE energy =       0.000438904398

Summary of Natural Population Analysis:

                                     Natural Population
               Natural  -----------------------------------------------
   Atom  No    Charge         Core      Valence    Rydberg      Total
------------------------------------------------------------------------
     C    1   -0.10329      1.99868     4.08139    0.02321     6.10329
     C    2   -0.23426      1.99898     4.21614    0.01914     6.23426
     C    3   -0.14665      1.99910     4.13060    0.01695     6.14665
     C    4   -0.16791      1.99893     4.15108    0.01790     6.16791
     C    5   -0.15236      1.99911     4.13698    0.01627     6.15236
     C    6   -0.23499      1.99898     4.21688    0.01913     6.23499
     H    7    0.23153      0.00000     0.76688    0.00159     0.76847
     H    8    0.23739      0.00000     0.76097    0.00164     0.76261
     C    9    0.80363      1.99930     3.15036    0.04671     5.19637
     H   10    0.23410      0.00000     0.76433    0.00157     0.76590
     H   11    0.23091      0.00000     0.76748    0.00161     0.76909
    Br   12    0.09967     27.99927     6.87871    0.02235    34.90033
     O   13   -0.55065      1.99972     6.53674    0.01419     8.55065
     C   14   -0.21746      1.99926     4.20243    0.01577     6.21746
     H   15    0.19167      0.00000     0.80726    0.00108     0.80833
     H   16    0.18987      0.00000     0.80842    0.00171     0.81013
     H   17    0.18987      0.00000     0.80842    0.00171     0.81013
     O   18   -0.61789      1.99975     6.60691    0.01122     8.61789
     N   19   -0.47695      1.99943     5.45506    0.02246     7.47695
     C   20    0.05193      1.99923     3.92173    0.02711     5.94807
     C   21   -0.24802      1.99917     4.23243    0.01642     6.24802
     C   22   -0.16863      1.99918     4.15203    0.01742     6.16863
     C   23   -0.24802      1.99917     4.23243    0.01642     6.24802
     C   24    0.05193      1.99923     3.92173    0.02711     5.94807
     H   25    0.19616      0.00000     0.80239    0.00146     0.80384
     H   26    0.22186      0.00000     0.77665    0.00149     0.77814
     H   27    0.21854      0.00000     0.78017    0.00129     0.78146
     H   28    0.22186      0.00000     0.77665    0.00149     0.77814
     H   29    0.19616      0.00000     0.80239    0.00146     0.80384
========================================================================
  * Total *    0.00000     59.98650    87.64564    0.36786   148.00000

Contributions to pi population at N atom in pyridine:
    Val( 2p)     1.18070
    Ryd( 3p)     0.00074
    Ryd( 4p)     0.00034
    Ryd( 5p)     0.00002

    Total:       1.18180

-------------------------------------------------------------------------------
NMR properties
-------------------------------------------------------------------------------
Electronic energy (NMR):                          -3281.77130994

 1  C    Isotropic =    21.8327   Anisotropy =   145.7629
 2  C    Isotropic =    41.4069   Anisotropy =   162.5556
 3  C    Isotropic =    41.5350   Anisotropy =   194.5684
```

```
 4  C    Isotropic =    45.2493   Anisotropy =   165.9925
 5  C    Isotropic =    43.0586   Anisotropy =   189.4220
 6  C    Isotropic =    41.8815   Anisotropy =   161.9002
 7  H    Isotropic =    23.6587   Anisotropy =     9.8715
 8  H    Isotropic =    23.0492   Anisotropy =     7.7344
 9  C    Isotropic =     6.3387   Anisotropy =    85.4927
10  H    Isotropic =    23.2587   Anisotropy =     8.6630
11  H    Isotropic =    23.7158   Anisotropy =     9.9977
12  Br   Isotropic =  1904.1767   Anisotropy =  1426.8812
13  O    Isotropic =   145.2928   Anisotropy =   141.8710
14  C    Isotropic =   126.7136   Anisotropy =    73.1082
15  H    Isotropic =    27.7651   Anisotropy =     7.5903
16  H    Isotropic =    27.6018   Anisotropy =     8.4582
17  H    Isotropic =    27.6018   Anisotropy =     8.4582
18  O    Isotropic =   -66.0550   Anisotropy =   603.0071
19  N    Isotropic =   -98.3306   Anisotropy =   576.0406
20  C    Isotropic =    21.9915   Anisotropy =   180.7630
21  C    Isotropic =    50.5245   Anisotropy =   183.6987
22  C    Isotropic =    37.3196   Anisotropy =   212.0982
23  C    Isotropic =    50.5245   Anisotropy =   183.6987
24  C    Isotropic =    21.9915   Anisotropy =   180.7630
25  H    Isotropic =    22.5157   Anisotropy =     9.5239
26  H    Isotropic =    23.9386   Anisotropy =     5.3378
27  H    Isotropic =    23.5127   Anisotropy =     4.9199
28  H    Isotropic =    23.9386   Anisotropy =     5.3378
29  H    Isotropic =    22.5157   Anisotropy =     9.5239

================================================================================
X = Br    R = COCH3
--------------------------------------------------------------------------------
Energies and NBO populations
--------------------------------------------------------------------------------

Number of atoms:  28
Full point group                 CS      NOp   2


C      0.000000  -0.418626   0.002964
C      0.000000  -1.057119   1.248301
C      0.000000  -2.447694   1.298754
C      0.000000  -3.213624   0.120766
C      0.000000  -2.551240  -1.117198
C      0.000000  -1.157351  -1.182328
H      0.000000  -0.472259   2.161547
H      0.000000  -2.962039   2.254143
C      0.000000  -4.711636   0.235722
H      0.000000  -3.113557  -2.045183
H      0.000000  -0.651989  -2.141693
Br     0.000000   1.490938  -0.076419
C      0.000000  -5.541767  -1.035909
O      0.000000  -5.249287   1.330544
H      0.000000  -6.598422  -0.766995
H      0.883830  -5.320901  -1.644530
H     -0.883830  -5.320901  -1.644530
N      0.000000   4.601031  -0.184643
C      1.145200   5.296265  -0.184643
C      1.199903   6.692061  -0.184939
C      0.000000   7.404709  -0.185075
C     -1.199903   6.692061  -0.184939
C     -1.145200   5.296265  -0.184643
H      2.060702   4.708352  -0.183988
H      2.158405   7.200757  -0.184668
H      0.000000   8.490572  -0.184993
H     -2.158405   7.200757  -0.184668
H     -2.060702   4.708352  -0.183988

Electronic energy:                                -3206.53574851 (  -3206.53574860)
Zero-point correction=                                0.215343
Sum of electronic and zero-point Energies=        -3206.320406
Sum of electronic and thermal Energies=           -3206.304331
Sum of electronic and thermal Enthalpies=         -3206.303387
Sum of electronic and thermal Free Energies=      -3206.371637

Lowest vibration frequency:           6.7724

Counterpoise: BSSE energy =       0.000431990517
```

Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population Core	Valence	Rydberg	Total
C	1	-0.10231	1.99868	4.08030	0.02333	6.10231
C	2	-0.23227	1.99898	4.21426	0.01903	6.23227
C	3	-0.14305	1.99909	4.12598	0.01798	6.14305
C	4	-0.16232	1.99895	4.14603	0.01733	6.16232
C	5	-0.16165	1.99911	4.14718	0.01536	6.16165
C	6	-0.23540	1.99898	4.21692	0.01950	6.23540
H	7	0.23123	0.00000	0.76718	0.00159	0.76877
H	8	0.23751	0.00000	0.76058	0.00190	0.76249
C	9	0.56546	1.99931	3.39652	0.03871	5.43454
H	10	0.22093	0.00000	0.77756	0.00150	0.77907
H	11	0.23076	0.00000	0.76760	0.00163	0.76924
Br	12	0.10167	27.99927	6.87669	0.02236	34.89833
C	13	-0.67816	1.99930	4.67054	0.00833	6.67816
O	14	-0.57824	1.99976	6.56477	0.01371	8.57824
H	15	0.23147	0.00000	0.76666	0.00187	0.76853
H	16	0.22865	0.00000	0.76994	0.00141	0.77135
H	17	0.22865	0.00000	0.76994	0.00141	0.77135
N	18	-0.47738	1.99943	5.45547	0.02248	7.47738
C	19	0.05197	1.99923	3.92170	0.02710	5.94803
C	20	-0.24790	1.99917	4.23232	0.01642	6.24790
C	21	-0.16847	1.99918	4.15187	0.01742	6.16847
C	22	-0.24790	1.99917	4.23232	0.01642	6.24790
C	23	0.05197	1.99923	3.92170	0.02710	5.94803
H	24	0.19613	0.00000	0.80241	0.00145	0.80387
H	25	0.22194	0.00000	0.77657	0.00149	0.77806
H	26	0.21864	0.00000	0.78007	0.00129	0.78136
H	27	0.22194	0.00000	0.77657	0.00149	0.77806
H	28	0.19613	0.00000	0.80241	0.00145	0.80387
* Total *		0.00000	57.98685	81.67209	0.34106	140.00000

Contributions to pi population at N atom in pyridine:

Val(2p)	1.18110
Ryd(3p)	0.00074
Ryd(4p)	0.00034
Ryd(5p)	0.00002
Total:	1.18220

NMR properties

Electronic energy (NMR): -3206.53574851

1	C	Isotropic =	21.3563	Anisotropy =	146.3676
2	C	Isotropic =	41.0054	Anisotropy =	162.3133
3	C	Isotropic =	44.6574	Anisotropy =	198.6626
4	C	Isotropic =	38.6063	Anisotropy =	179.1058
5	C	Isotropic =	42.5948	Anisotropy =	183.7303
6	C	Isotropic =	41.9697	Anisotropy =	161.2630
7	H	Isotropic =	23.6613	Anisotropy =	9.9529
8	H	Isotropic =	23.0705	Anisotropy =	6.9124
9	C	Isotropic =	-25.6912	Anisotropy =	173.4674
10	H	Isotropic =	23.3817	Anisotropy =	8.3971
11	H	Isotropic =	23.6719	Anisotropy =	10.0439
12	Br	Isotropic =	1900.9906	Anisotropy =	1420.3293
13	C	Isotropic =	153.8211	Anisotropy =	46.3282
14	O	Isotropic =	-290.6812	Anisotropy =	967.0196
15	H	Isotropic =	29.3397	Anisotropy =	6.9460
16	H	Isotropic =	28.7171	Anisotropy =	4.7002
17	H	Isotropic =	28.7171	Anisotropy =	4.7002
18	N	Isotropic =	-98.1702	Anisotropy =	575.5936
19	C	Isotropic =	22.0193	Anisotropy =	180.7786
20	C	Isotropic =	50.4957	Anisotropy =	183.7458
21	C	Isotropic =	37.2959	Anisotropy =	212.2015
22	C	Isotropic =	50.4957	Anisotropy =	183.7458
23	C	Isotropic =	22.0193	Anisotropy =	180.7786
24	H	Isotropic =	22.5165	Anisotropy =	9.4927
25	H	Isotropic =	23.9353	Anisotropy =	5.3308
26	H	Isotropic =	23.5087	Anisotropy =	4.9286
27	H	Isotropic =	23.9353	Anisotropy =	5.3308

28 H   Isotropic =   22.5165   Anisotropy =   9.4927

==
X = Br   R = CF3

Energies and NBO populations

Number of atoms: 26
Full point group   CS   NOp   2

C	0.000000	-0.436711	-0.002367
C	0.000000	-1.118666	1.215334
C	0.000000	-2.515168	1.220049
C	0.000000	-3.217185	0.013037
C	0.000000	-2.525553	-1.204607
C	0.000000	-1.132558	-1.215674
H	0.000000	-0.570559	2.150697
H	0.000000	-3.049326	2.163411
C	0.000000	-4.724055	-0.007238
H	0.000000	-3.068946	-2.144347
H	0.000000	-0.593106	-2.156043
Br	0.000000	1.474773	-0.013836
F	0.000000	-5.261841	1.228327
F	-1.083035	-5.220834	-0.652717
F	1.083035	-5.220834	-0.652717
N	0.000000	4.564201	-0.027170
C	1.145330	5.259255	-0.027170
C	1.199932	6.655015	-0.027177
C	0.000000	7.367615	-0.027088
C	-1.199932	6.655015	-0.027177
C	-1.145330	5.259255	-0.027170
H	2.060785	4.671296	-0.027116
H	2.158409	7.163731	-0.027163
H	0.000000	8.453467	-0.026882
H	-2.158409	7.163731	-0.027163
H	-2.060785	4.671296	-0.027116

Electronic energy: -3390.95045364 (-3390.95040819)
Zero-point correction=   0.182781
Sum of electronic and zero-point Energies=   -3390.767673
Sum of electronic and thermal Energies=   -3390.752474
Sum of electronic and thermal Enthalpies=   -3390.751529
Sum of electronic and thermal Free Energies=   -3390.817558

Lowest vibration frequency: -17.8666

Counterpoise: BSSE energy =   0.000446598965

Summary of Natural Population Analysis:

			Natural Population			
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.10942	1.99868	4.08734	0.02340	6.10942
C	2	-0.22541	1.99898	4.20737	0.01906	6.22541
C	3	-0.16822	1.99909	4.15248	0.01666	6.16822
C	4	-0.16011	1.99891	4.14393	0.01727	6.16011
C	5	-0.16449	1.99909	4.14838	0.01701	6.16449
C	6	-0.22419	1.99899	4.20610	0.01910	6.22419
H	7	0.23362	0.00000	0.76481	0.00157	0.76638
H	8	0.23581	0.00000	0.76258	0.00161	0.76419
C	9	1.06723	1.99912	2.87343	0.06021	4.93277
H	10	0.23184	0.00000	0.76656	0.00160	0.76816
H	11	0.23387	0.00000	0.76455	0.00158	0.76613
Br	12	0.10401	27.99928	6.87433	0.02238	34.89599
F	13	-0.35538	1.99992	7.34908	0.00638	9.35538
F	14	-0.35871	1.99992	7.35226	0.00653	9.35871
F	15	-0.35871	1.99992	7.35226	0.00653	9.35871
N	16	-0.47814	1.99943	5.45620	0.02251	7.47814
C	17	0.05216	1.99923	3.92154	0.02707	5.94784
C	18	-0.24766	1.99917	4.23208	0.01641	6.24766
C	19	-0.16815	1.99918	4.15155	0.01741	6.16815
C	20	-0.24766	1.99917	4.23208	0.01641	6.24766
C	21	0.05216	1.99923	3.92154	0.02707	5.94784

```
     H   22    0.19625      0.00000     0.80230    0.00145     0.80375
     H   23    0.22212      0.00000     0.77640    0.00149     0.77788
     H   24    0.21881      0.00000     0.77991    0.00128     0.78119
     H   25    0.22212      0.00000     0.77640    0.00149     0.77788
     H   26    0.19625      0.00000     0.80230    0.00145     0.80375
=======================================================================
  * Total *    0.00000     59.98731    89.65777    0.35492   150.00000

Contributions to pi population at N atom in pyridine:
    Val( 2p)     1.18217
    Ryd( 3p)     0.00074
    Ryd( 4p)     0.00034
    Ryd( 5p)     0.00002

    Total:       1.18327

-------------------------------------------------------------------------------
NMR properties
-------------------------------------------------------------------------------
Electronic energy (NMR):                          -3390.95045364

 1  C    Isotropic =    23.6871   Anisotropy =   146.4333
 2  C    Isotropic =    41.5398   Anisotropy =   165.1695
 3  C    Isotropic =    47.9104   Anisotropy =   186.2480
 4  C    Isotropic =    43.0928   Anisotropy =   165.9477
 5  C    Isotropic =    45.7804   Anisotropy =   188.2045
 6  C    Isotropic =    40.6052   Anisotropy =   166.5692
 7  H    Isotropic =    23.6461   Anisotropy =     9.7216
 8  H    Isotropic =    23.6154   Anisotropy =     8.4467
 9  C    Isotropic =    43.2287   Anisotropy =    10.9000
10  H    Isotropic =    23.6683   Anisotropy =     8.0035
11  H    Isotropic =    23.6020   Anisotropy =     9.7582
12  Br   Isotropic =  1904.5113   Anisotropy =  1455.1189
13  F    Isotropic =   261.2689   Anisotropy =   113.1866
14  F    Isotropic =   232.4671   Anisotropy =   148.4153
15  F    Isotropic =   232.4671   Anisotropy =   148.4153
16  N    Isotropic =   -97.7201   Anisotropy =   574.4351
17  C    Isotropic =    22.0837   Anisotropy =   180.7128
18  C    Isotropic =    50.4584   Anisotropy =   183.8129
19  C    Isotropic =    37.2429   Anisotropy =   212.3278
20  C    Isotropic =    50.4584   Anisotropy =   183.8129
21  C    Isotropic =    22.0837   Anisotropy =   180.7128
22  H    Isotropic =    22.5222   Anisotropy =     9.5678
23  H    Isotropic =    23.9324   Anisotropy =     5.3398
24  H    Isotropic =    23.5061   Anisotropy =     4.9218
25  H    Isotropic =    23.9324   Anisotropy =     5.3398
26  H    Isotropic =    22.5222   Anisotropy =     9.5678

===============================================================================
X = Br    R = CN
-------------------------------------------------------------------------------
Energies and NBO populations
-------------------------------------------------------------------------------

Number of atoms:  24
Full point group                 C2V     NOp   4


C      0.000000  -0.506352   0.000000
C      0.000000  -1.196232   1.216783
C      0.000000  -2.588631   1.217122
C      0.000000  -3.291337   0.000000
C      0.000000  -2.588631  -1.217122
C      0.000000  -1.196232  -1.216783
H      0.000000  -0.651031   2.153866
H      0.000000  -3.132122   2.155855
C      0.000000  -4.724408   0.000000
H      0.000000  -3.132122  -2.155855
H      0.000000  -0.651031  -2.153866
Br     0.000000   1.402052   0.000000
N      0.000000  -5.883218   0.000000
N      0.000000   4.475791   0.000000
C      1.145223   5.170993   0.000000
C      1.199860   6.566714   0.000000
C      0.000000   7.279468   0.000000
C     -1.199860   6.566714   0.000000
C     -1.145223   5.170993   0.000000
```

```
H      2.061115   4.583692   0.000000
H      2.158525   7.075048   0.000000
H      0.000000   8.365324   0.000000
H     -2.158525   7.075048   0.000000
H     -2.061115   4.583692   0.000000

Electronic energy:                                  -3146.13114342 (  -3146.13114342)
Zero-point correction=                                  0.177037
Sum of electronic and zero-point Energies=          -3145.954106
Sum of electronic and thermal Energies=             -3145.939838
Sum of electronic and thermal Enthalpies=           -3145.938894
Sum of electronic and thermal Free Energies=        -3146.002321

Lowest vibration frequency:           8.1378

Counterpoise: BSSE energy =       0.000455830399

Summary of Natural Population Analysis:

                                     Natural Population
               Natural  -----------------------------------------------
   Atom  No    Charge         Core      Valence    Rydberg      Total
------------------------------------------------------------------------
     C    1   -0.10571      1.99870     4.08355    0.02347     6.10571
     C    2   -0.22645      1.99898     4.20850    0.01897     6.22645
     C    3   -0.13944      1.99911     4.12487    0.01546     6.13944
     C    4   -0.19430      1.99888     4.17843    0.01699     6.19430
     C    5   -0.13944      1.99911     4.12487    0.01546     6.13944
     C    6   -0.22645      1.99898     4.20850    0.01897     6.22645
     H    7    0.23605      0.00000     0.76241    0.00154     0.76395
     H    8    0.23290      0.00000     0.76581    0.00129     0.76710
     C    9    0.30731      1.99927     3.65943    0.03400     5.69269
     H   10    0.23290      0.00000     0.76581    0.00129     0.76710
     H   11    0.23605      0.00000     0.76241    0.00154     0.76395
    Br   12    0.11419     27.99927     6.86413    0.02241    34.88581
     N   13   -0.34694      1.99959     5.32705    0.02030     7.34694
     N   14   -0.47941      1.99943     5.45743    0.02255     7.47941
     C   15    0.05234      1.99923     3.92140    0.02702     5.94766
     C   16   -0.24733      1.99917     4.23176    0.01640     6.24733
     C   17   -0.16763      1.99918     4.15105    0.01740     6.16763
     C   18   -0.24733      1.99917     4.23176    0.01640     6.24733
     C   19    0.05234      1.99923     3.92140    0.02702     5.94766
     H   20    0.19623      0.00000     0.80231    0.00145     0.80377
     H   21    0.22238      0.00000     0.77614    0.00148     0.77762
     H   22    0.21909      0.00000     0.77962    0.00128     0.78091
     H   23    0.22238      0.00000     0.77614    0.00148     0.77762
     H   24    0.19623      0.00000     0.80231    0.00145     0.80377
========================================================================
  * Total *    0.00000     55.98727    73.68712    0.32561   130.00000

Contributions to pi population at N atom in pyridine:
    Val( 2p)     1.18349
    Ryd( 3p)     0.00074
    Ryd( 4p)     0.00035
    Ryd( 5p)     0.00002

    Total:       1.18460

-------------------------------------------------------------------------------
NMR properties
-------------------------------------------------------------------------------
Electronic energy (NMR):                            -3146.13114342

 1  C    Isotropic =    21.5464   Anisotropy =   152.5853
 2  C    Isotropic =    40.5905   Anisotropy =   167.5468
 3  C    Isotropic =    39.1564   Anisotropy =   188.9566
 4  C    Isotropic =    64.0755   Anisotropy =   150.3059
 5  C    Isotropic =    39.1564   Anisotropy =   188.9566
 6  C    Isotropic =    40.5905   Anisotropy =   167.5468
 7  H    Isotropic =    23.6566   Anisotropy =     9.6805
 8  H    Isotropic =    23.6650   Anisotropy =     6.2854
 9  C    Isotropic =    55.5818   Anisotropy =   352.7752
10  H    Isotropic =    23.6650   Anisotropy =     6.2854
11  H    Isotropic =    23.6566   Anisotropy =     9.6805
12  Br   Isotropic =  1877.8646   Anisotropy =  1426.9361
13  N    Isotropic =   -43.1950   Anisotropy =   418.3365
14  N    Isotropic =   -96.9877   Anisotropy =   572.4676
```

```
15  C    Isotropic =    22.1796   Anisotropy =   180.6913
16  C    Isotropic =    50.3617   Anisotropy =   183.9565
17  C    Isotropic =    37.1421   Anisotropy =   212.5867
18  C    Isotropic =    50.3617   Anisotropy =   183.9565
19  C    Isotropic =    22.1796   Anisotropy =   180.6913
20  H    Isotropic =    22.5352   Anisotropy =     9.5175
21  H    Isotropic =    23.9261   Anisotropy =     5.3384
22  H    Isotropic =    23.4976   Anisotropy =     4.9406
23  H    Isotropic =    23.9261   Anisotropy =     5.3384
24  H    Isotropic =    22.5352   Anisotropy =     9.5175

================================================================================================
X = Br    R = NO2
------------------------------------------------------------------------------------------------
Energies and NBO populations
------------------------------------------------------------------------------------------------

Number of atoms:  25
Full point group                 C2V     NOp   4


C      0.000000  -0.453692   0.000000
C      0.000000  -1.142269   1.218524
C      0.000000  -2.534780   1.220572
C      0.000000  -3.211063   0.000000
C      0.000000  -2.534780  -1.220572
C      0.000000  -1.142269  -1.218524
H      0.000000  -0.596763   2.155148
H      0.000000  -3.093554   2.148415
N      0.000000  -4.682826   0.000000
H      0.000000  -3.093554  -2.148415
H      0.000000  -0.596763  -2.155148
Br     0.000000   1.453199   0.000000
O      0.000000  -5.257086   1.084745
O      0.000000  -5.257086  -1.084746
N      0.000000   4.508190   0.000000
C      1.145563   5.202982   0.000000
C      1.199985   6.598625   0.000000
C      0.000000   7.311126   0.000000
C     -1.199985   6.598625   0.000000
C     -1.145563   5.202982   0.000000
H      2.060990   4.615022   0.000000
H      2.158410   7.107368   0.000000
H      0.000000   8.396950   0.000000
H     -2.158410   7.107368   0.000000
H     -2.060990   4.615022   0.000000

Electronic energy:                                -3258.40070619 (  -3258.40070619)
Zero-point correction=                                0.180758
Sum of electronic and zero-point Energies=        -3258.219948
Sum of electronic and thermal Energies=           -3258.204901
Sum of electronic and thermal Enthalpies=         -3258.203956
Sum of electronic and thermal Free Energies=      -3258.269789

Lowest vibration frequency:           9.1902

Counterpoise: BSSE energy =       0.000485888843

Summary of Natural Population Analysis:

                                     Natural Population
               Natural  -----------------------------------------------
   Atom  No    Charge         Core      Valence    Rydberg      Total
------------------------------------------------------------------------
     C    1   -0.09916      1.99870     4.07691    0.02354     6.09916
     C    2   -0.22344      1.99899     4.20551    0.01895     6.22344
     C    3   -0.17166      1.99907     4.15425    0.01834     6.17166
     C    4    0.05947      1.99879     3.92098    0.02075     5.94053
     C    5   -0.17166      1.99907     4.15425    0.01834     6.17166
     C    6   -0.22344      1.99899     4.20551    0.01895     6.22344
     H    7    0.23739      0.00000     0.76111    0.00150     0.76261
     H    8    0.25222      0.00000     0.74587    0.00191     0.74778
     N    9    0.48946      1.99945     4.45611    0.05497     6.51054
     H   10    0.25222      0.00000     0.74587    0.00191     0.74778
     H   11    0.23739      0.00000     0.76111    0.00150     0.76261
    Br   12    0.12309     27.99927     6.85506    0.02258    34.87691
     O   13   -0.39117      1.99980     6.37645    0.01492     8.39117
```

```
     O   14   -0.39117      1.99980     6.37646    0.01492     8.39117
     N   15   -0.48053      1.99943     5.45853    0.02257     7.48053
     C   16    0.05256      1.99923     3.92123    0.02698     5.94744
     C   17   -0.24702      1.99917     4.23146    0.01639     6.24702
     C   18   -0.16724      1.99918     4.15067    0.01739     6.16724
     C   19   -0.24702      1.99917     4.23146    0.01639     6.24702
     C   20    0.05256      1.99923     3.92123    0.02698     5.94744
     H   21    0.19635      0.00000     0.80220    0.00145     0.80365
     H   22    0.22258      0.00000     0.77594    0.00148     0.77742
     H   23    0.21927      0.00000     0.77945    0.00128     0.78073
     H   24    0.22258      0.00000     0.77594    0.00148     0.77742
     H   25    0.19635      0.00000     0.80220    0.00145     0.80365
=======================================================================
  * Total *    0.00000     57.98733    81.64574    0.36692   140.00000

Contributions to pi population at N atom in pyridine:
    Val( 2p)     1.18471
    Ryd( 3p)     0.00074
    Ryd( 4p)     0.00035
    Ryd( 5p)     0.00002

    Total:       1.18582

-------------------------------------------------------------------------------
NMR properties
-------------------------------------------------------------------------------
Electronic energy (NMR):                          -3258.40070619

 1  C    Isotropic =    17.3987   Anisotropy =   157.5252
 2  C    Isotropic =    40.9393   Anisotropy =   163.7352
 3  C    Isotropic =    48.7081   Anisotropy =   184.6939
 4  C    Isotropic =    25.8144   Anisotropy =   115.9778
 5  C    Isotropic =    48.7081   Anisotropy =   184.6939
 6  C    Isotropic =    40.9393   Anisotropy =   163.7352
 7  H    Isotropic =    23.6108   Anisotropy =     9.8215
 8  H    Isotropic =    22.9157   Anisotropy =     5.8956
 9  N    Isotropic =  -154.2969   Anisotropy =   290.7412
10  H    Isotropic =    22.9157   Anisotropy =     5.8956
11  H    Isotropic =    23.6108   Anisotropy =     9.8215
12  Br   Isotropic =  1865.5914   Anisotropy =  1396.7917
13  O    Isotropic =  -308.0818   Anisotropy =   723.9839
14  O    Isotropic =  -308.0818   Anisotropy =   723.9839
15  N    Isotropic =   -96.6463   Anisotropy =   571.4852
16  C    Isotropic =    22.2360   Anisotropy =   180.6929
17  C    Isotropic =    50.3301   Anisotropy =   184.1171
18  C    Isotropic =    37.0635   Anisotropy =   212.7326
19  C    Isotropic =    50.3301   Anisotropy =   184.1171
20  C    Isotropic =    22.2360   Anisotropy =   180.6929
21  H    Isotropic =    22.5298   Anisotropy =     9.4931
22  H    Isotropic =    23.9168   Anisotropy =     5.3191
23  H    Isotropic =    23.4902   Anisotropy =     4.9376
24  H    Isotropic =    23.9168   Anisotropy =     5.3191
25  H    Isotropic =    22.5298   Anisotropy =     9.4931

===============================================================================
X = Cl    R = H
-------------------------------------------------------------------------------
Energies and NBO populations
-------------------------------------------------------------------------------

Number of atoms:  23
Full point group                 C2V     NOp   4


C      0.000000  -0.667475   0.000000
C      0.000000  -1.351090   1.216661
C      0.000000  -2.748591   1.208548
C      0.000000  -3.450178   0.000000
C      0.000000  -2.748591  -1.208548
C      0.000000  -1.351090  -1.216661
H      0.000000  -0.799225   2.150260
H      0.000000  -3.285858   2.152129
H      0.000000  -4.535584   0.000000
H      0.000000  -3.285858  -2.152129
H      0.000000  -0.799225  -2.150260
Cl     0.000000   1.094747   0.000000
N      0.000000   4.420709   0.000000
```

```
C      1.143941   5.117997   0.000000
C      1.199508   6.514126   0.000000
C      0.000000   7.227358   0.000000
C     -1.199508   6.514126   0.000000
C     -1.143941   5.117997   0.000000
H      2.060275   4.531207   0.000000
H      2.158273   7.022579   0.000000
H      0.000000   8.313297   0.000000
H     -2.158273   7.022579   0.000000
H     -2.060275   4.531207   0.000000

Electronic energy:                                  -940.07960339 (   -940.07960339)
Zero-point correction=                                 0.178880
Sum of electronic and zero-point Energies=          -939.900723
Sum of electronic and thermal Energies=             -939.889324
Sum of electronic and thermal Enthalpies=           -939.888380
Sum of electronic and thermal Free Energies=        -939.944792

Lowest vibration frequency:          -11.1580

Counterpoise: BSSE energy =       0.000642529394

Summary of Natural Population Analysis:

                                     Natural Population
               Natural  -----------------------------------------------
   Atom  No    Charge         Core      Valence    Rydberg      Total
------------------------------------------------------------------------
     C    1   -0.04637      1.99861     4.02429    0.02347     6.04637
     C    2   -0.23463      1.99898     4.21673    0.01892     6.23463
     C    3   -0.19425      1.99918     4.17753    0.01754     6.19425
     C    4   -0.21659      1.99918     4.19974    0.01767     6.21659
     C    5   -0.19425      1.99918     4.17753    0.01754     6.19425
     C    6   -0.23463      1.99898     4.21673    0.01892     6.23463
     H    7    0.22878      0.00000     0.76959    0.00163     0.77122
     H    8    0.21719      0.00000     0.78141    0.00140     0.78281
     H    9    0.21607      0.00000     0.78260    0.00132     0.78393
     H   10    0.21719      0.00000     0.78141    0.00140     0.78281
     H   11    0.22878      0.00000     0.76959    0.00163     0.77122
    Cl   12    0.00708      9.99963     6.97075    0.02254    16.99292
     N   13   -0.47031      1.99945     5.44858    0.02228     7.47031
     C   14    0.04915      1.99923     3.92375    0.02788     5.95085
     C   15   -0.24991      1.99917     4.23423    0.01651     6.24991
     C   16   -0.17101      1.99918     4.15432    0.01751     6.17101
     C   17   -0.24991      1.99917     4.23423    0.01651     6.24991
     C   18    0.04915      1.99923     3.92375    0.02788     5.95085
     H   19    0.19478      0.00000     0.80376    0.00147     0.80522
     H   20    0.22070      0.00000     0.77782    0.00149     0.77930
     H   21    0.21753      0.00000     0.78117    0.00130     0.78247
     H   22    0.22070      0.00000     0.77782    0.00149     0.77930
     H   23    0.19478      0.00000     0.80376    0.00147     0.80522
========================================================================
  * Total *    0.00000     33.98917    65.73108    0.27975   100.00000

Contributions to pi population at N atom in pyridine:
    Val( 2p)     1.17111
    Ryd( 3p)     0.00071
    Ryd( 4p)     0.00033
    Ryd( 5p)     0.00003

    Total:       1.17218

-------------------------------------------------------------------------------
NMR properties
-------------------------------------------------------------------------------
Electronic energy (NMR):                             -940.07960339

 1  C    Isotropic =    28.1751   Anisotropy =   130.3792
 2  C    Isotropic =    44.3823   Anisotropy =   164.0224
 3  C    Isotropic =    44.0096   Anisotropy =   188.8469
 4  C    Isotropic =    48.0597   Anisotropy =   191.3286
 5  C    Isotropic =    44.0096   Anisotropy =   188.8469
 6  C    Isotropic =    44.3823   Anisotropy =   164.0224
 7  H    Isotropic =    23.7733   Anisotropy =     8.2162
 8  H    Isotropic =    23.8717   Anisotropy =     4.9375
 9  H    Isotropic =    23.9841   Anisotropy =     4.2844
10  H    Isotropic =    23.8717   Anisotropy =     4.9375
```

```
11  H    Isotropic =    23.7733   Anisotropy =     8.2162
12  Cl   Isotropic =   663.7295   Anisotropy =   530.3794
13  N    Isotropic =  -101.8064   Anisotropy =   587.1353
14  C    Isotropic =    21.4366   Anisotropy =   181.0841
15  C    Isotropic =    50.7711   Anisotropy =   183.2567
16  C    Isotropic =    37.7710   Anisotropy =   211.3243
17  C    Isotropic =    50.7711   Anisotropy =   183.2567
18  C    Isotropic =    21.4366   Anisotropy =   181.0841
19  H    Isotropic =    22.4686   Anisotropy =     8.5699
20  H    Isotropic =    23.9689   Anisotropy =     5.3188
21  H    Isotropic =    23.5265   Anisotropy =     5.0200
22  H    Isotropic =    23.9689   Anisotropy =     5.3188
23  H    Isotropic =    22.4686   Anisotropy =     8.5699

================================================================================
X = Cl    R = OCH3
--------------------------------------------------------------------------------
Energies and NBO populations
--------------------------------------------------------------------------------

Number of atoms:  27
Full point group                 CS      NOp   2


C      0.000000  -0.498765  -0.003914
C      0.000000  -1.242496   1.171243
C      0.000000  -2.641535   1.113479
C      0.000000  -3.288952  -0.128799
C      0.000000  -2.525870  -1.307707
C      0.000000  -1.136600  -1.248302
H      0.000000  -0.741278   2.133111
H      0.000000  -3.203277   2.039939
O      0.000000  -4.640572  -0.295553
H      0.000000  -3.039198  -2.263746
H      0.000000  -0.550248  -2.160701
Cl     0.000000   1.262785   0.071544
C      0.000000  -5.461475   0.866110
H      0.000000  -6.489826   0.504112
H     -0.896165  -5.289732   1.474771
H      0.896165  -5.289732   1.474771
N      0.000000   4.602116   0.125794
C      1.143924   5.299368   0.125794
C      1.199508   6.695534   0.125990
C      0.000000   7.408777   0.126153
C     -1.199508   6.695534   0.125990
C     -1.143924   5.299368   0.125794
H      2.060229   4.712524   0.125448
H      2.158285   7.203978   0.125914
H      0.000000   8.494723   0.126279
H     -2.158285   7.203978   0.125914
H     -2.060229   4.712524   0.125448

Electronic energy:                                -1054.60194562 (  -1054.60194561)
Zero-point correction=                                0.211263
Sum of electronic and zero-point Energies=        -1054.390683
Sum of electronic and thermal Energies=           -1054.375770
Sum of electronic and thermal Enthalpies=         -1054.374826
Sum of electronic and thermal Free Energies=      -1054.440848

Lowest vibration frequency:            5.3006

Counterpoise: BSSE energy =       0.001059994696

Summary of Natural Population Analysis:

                                     Natural Population
               Natural  ----------------------------------------------
   Atom  No    Charge         Core      Valence    Rydberg      Total
-------------------------------------------------------------------------
     C    1   -0.07510      1.99859     4.05350    0.02302     6.07510
     C    2   -0.21349      1.99900     4.19561    0.01888     6.21349
     C    3   -0.28367      1.99908     4.26964    0.01495     6.28367
     C    4    0.31794      1.99881     3.66032    0.02293     5.68206
     C    5   -0.23379      1.99909     4.21773    0.01697     6.23379
     C    6   -0.21609      1.99900     4.19875    0.01833     6.21609
     H    7    0.22818      0.00000     0.77012    0.00169     0.77182
     H    8    0.22403      0.00000     0.77418    0.00179     0.77597
```

```
     O    9   -0.54407      1.99971     6.52658    0.01778     8.54407
     H   10    0.22816      0.00000     0.77008    0.00176     0.77184
     H   11    0.22937      0.00000     0.76904    0.00158     0.77063
    Cl   12    0.00042      9.99964     6.97726    0.02268    16.99958
     C   13   -0.21373      1.99928     4.19872    0.01573     6.21373
     H   14    0.19659      0.00000     0.80240    0.00101     0.80341
     H   15    0.17498      0.00000     0.82293    0.00210     0.82502
     H   16    0.17498      0.00000     0.82293    0.00210     0.82502
     N   17   -0.46961      1.99945     5.44783    0.02233     7.46961
     C   18    0.04907      1.99923     3.92378    0.02793     5.95093
     C   19   -0.25007      1.99917     4.23438    0.01652     6.25007
     C   20   -0.17125      1.99918     4.15455    0.01752     6.17125
     C   21   -0.25007      1.99917     4.23438    0.01652     6.25007
     C   22    0.04907      1.99923     3.92378    0.02793     5.95093
     H   23    0.19481      0.00000     0.80373    0.00147     0.80519
     H   24    0.22057      0.00000     0.77795    0.00149     0.77943
     H   25    0.21740      0.00000     0.78129    0.00131     0.78260
     H   26    0.22057      0.00000     0.77795    0.00149     0.77943
     H   27    0.19481      0.00000     0.80373    0.00147     0.80519
=======================================================================
  * Total *    0.00000     37.98762    77.69315    0.31923   116.00000

Contributions to pi population at N atom in pyridine:
    Val( 2p)     1.17054
    Ryd( 3p)     0.00071
    Ryd( 4p)     0.00033
    Ryd( 5p)     0.00003

    Total:       1.17161

-------------------------------------------------------------------------------
NMR properties
-------------------------------------------------------------------------------
Electronic energy (NMR):                          -1054.60194562

 1  C    Isotropic =    39.1382   Anisotropy =   113.4934
 2  C    Isotropic =    44.0029   Anisotropy =   162.3874
 3  C    Isotropic =    65.6431   Anisotropy =   161.7752
 4  C    Isotropic =    12.8669   Anisotropy =   145.2195
 5  C    Isotropic =    56.1508   Anisotropy =   151.2869
 6  C    Isotropic =    43.3237   Anisotropy =   162.0189
 7  H    Isotropic =    23.8863   Anisotropy =     8.1816
 8  H    Isotropic =    24.5286   Anisotropy =     7.5045
 9  O    Isotropic =   223.3923   Anisotropy =    84.6627
10  H    Isotropic =    24.3518   Anisotropy =     5.7834
11  H    Isotropic =    23.9381   Anisotropy =     7.7942
12  Cl   Isotropic =   685.5880   Anisotropy =   527.5842
13  C    Isotropic =   124.4901   Anisotropy =    75.5374
14  H    Isotropic =    27.4774   Anisotropy =     8.3299
15  H    Isotropic =    27.8757   Anisotropy =     8.0214
16  H    Isotropic =    27.8757   Anisotropy =     8.0214
17  N    Isotropic =  -102.0816   Anisotropy =   588.0022
18  C    Isotropic =    21.4002   Anisotropy =   181.0145
19  C    Isotropic =    50.8262   Anisotropy =   183.1693
20  C    Isotropic =    37.8113   Anisotropy =   211.1192
21  C    Isotropic =    50.8262   Anisotropy =   183.1693
22  C    Isotropic =    21.4002   Anisotropy =   181.0145
23  H    Isotropic =    22.4787   Anisotropy =     8.6452
24  H    Isotropic =    23.9801   Anisotropy =     5.3347
25  H    Isotropic =    23.5380   Anisotropy =     5.0061
26  H    Isotropic =    23.9801   Anisotropy =     5.3347
27  H    Isotropic =    22.4787   Anisotropy =     8.6452

===============================================================================
X = Cl    R = OCH2CH3
-------------------------------------------------------------------------------
Energies and NBO populations
-------------------------------------------------------------------------------

Number of atoms:  30
Full point group                 CS      NOp   2


C      0.000000  -0.389535  -0.041209
C      0.000000  -1.141658   1.128570
C      0.000000  -2.540239   1.061349
C      0.000000  -3.180381  -0.185453
```

C	0.000000	-2.407643	-1.358575
C	0.000000	-1.018747	-1.289860
H	0.000000	-0.647215	2.093970
H	0.000000	-3.107431	1.984321
O	0.000000	-4.529809	-0.362712
H	0.000000	-2.913993	-2.318363
H	0.000000	-0.426265	-2.198320
Cl	0.000000	1.371691	0.047156
C	0.000000	-5.373868	0.792891
C	0.000000	-6.815469	0.312874
H	-0.890416	-5.163370	1.400892
H	0.890416	-5.163370	1.400892
H	0.000000	-7.491210	1.174067
H	0.888633	-7.022992	-0.290358
H	-0.888633	-7.022992	-0.290358
N	0.000000	4.716345	0.141656
C	1.143915	5.413603	0.141656
C	1.199503	6.809778	0.141895
C	0.000000	7.523026	0.142098
C	-1.199503	6.809778	0.141895
C	-1.143915	5.413603	0.141656
H	2.060214	4.826752	0.141345
H	2.158282	7.318224	0.141867
H	0.000000	8.608973	0.142308
H	-2.158282	7.318224	0.141867
H	-2.060214	4.826752	0.141345

Electronic energy: -1093.91750095 (-1093.91750091)
Zero-point correction= 0.239256
Sum of electronic and zero-point Energies= -1093.678245
Sum of electronic and thermal Energies= -1093.661897
Sum of electronic and thermal Enthalpies= -1093.660953
Sum of electronic and thermal Free Energies= -1093.730744

Lowest vibration frequency: 6.5179

Counterpoise: BSSE energy = 0.000649677576

Summary of Natural Population Analysis:

			Natural Population			
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.07544	1.99859	4.05392	0.02293	6.07544
C	2	-0.21372	1.99900	4.19600	0.01872	6.21372
C	3	-0.28334	1.99908	4.26905	0.01522	6.28334
C	4	0.32094	1.99882	3.65734	0.02290	5.67906
C	5	-0.23351	1.99909	4.21781	0.01661	6.23351
C	6	-0.21661	1.99900	4.19934	0.01827	6.21661
H	7	0.22790	0.00000	0.77041	0.00170	0.77210
H	8	0.22350	0.00000	0.77466	0.00184	0.77650
O	9	-0.55774	1.99970	6.53721	0.02083	8.55774
H	10	0.22758	0.00000	0.77071	0.00171	0.77242
H	11	0.22907	0.00000	0.76934	0.00159	0.77093
Cl	12	-0.00056	9.99964	6.97825	0.02267	17.00056
C	13	-0.03606	1.99925	4.01820	0.01862	6.03606
C	14	-0.59420	1.99938	4.58625	0.00858	6.59420
H	15	0.17432	0.00000	0.82322	0.00246	0.82568
H	16	0.17432	0.00000	0.82322	0.00246	0.82568
H	17	0.21058	0.00000	0.78827	0.00115	0.78942
H	18	0.20889	0.00000	0.78943	0.00168	0.79111
H	19	0.20889	0.00000	0.78943	0.00168	0.79111
N	20	-0.46944	1.99945	5.44767	0.02233	7.46944
C	21	0.04904	1.99923	3.92379	0.02793	5.95096
C	22	-0.25010	1.99917	4.23441	0.01652	6.25010
C	23	-0.17130	1.99918	4.15460	0.01752	6.17130
C	24	-0.25010	1.99917	4.23441	0.01652	6.25010
C	25	0.04904	1.99923	3.92379	0.02793	5.95096
H	26	0.19482	0.00000	0.80372	0.00147	0.80518
H	27	0.22054	0.00000	0.77798	0.00149	0.77946
H	28	0.21737	0.00000	0.78132	0.00131	0.78263
H	29	0.22054	0.00000	0.77798	0.00149	0.77946
H	30	0.19482	0.00000	0.80372	0.00147	0.80518
* Total *		0.00000	39.98697	83.67544	0.33759	124.00000

```
Contributions to pi population at N atom in pyridine:
    Val( 2p)     1.17040
    Ryd( 3p)     0.00071
    Ryd( 4p)     0.00033
    Ryd( 5p)     0.00003

    Total:       1.17147

-------------------------------------------------------------------------------
NMR properties
-------------------------------------------------------------------------------
Electronic energy (NMR):                          -1093.91750095

 1  C    Isotropic =    39.3512   Anisotropy =   112.8807
 2  C    Isotropic =    44.0309   Anisotropy =   161.8641
 3  C    Isotropic =    65.0511   Anisotropy =   159.7368
 4  C    Isotropic =    13.2334   Anisotropy =   144.5902
 5  C    Isotropic =    56.1533   Anisotropy =   150.2302
 6  C    Isotropic =    43.3727   Anisotropy =   161.6931
 7  H    Isotropic =    23.9133   Anisotropy =     8.2133
 8  H    Isotropic =    24.5692   Anisotropy =     8.1192
 9  O    Isotropic =   193.5023   Anisotropy =    70.3399
10  H    Isotropic =    24.3401   Anisotropy =     6.2741
11  H    Isotropic =    23.9405   Anisotropy =     7.8010
12  Cl   Isotropic =   686.0261   Anisotropy =   528.0881
13  C    Isotropic =   113.4400   Anisotropy =    63.2440
14  C    Isotropic =   165.9397   Anisotropy =    25.6094
15  H    Isotropic =    27.6255   Anisotropy =     5.3967
16  H    Isotropic =    27.6255   Anisotropy =     5.3967
17  H    Isotropic =    30.2506   Anisotropy =    10.0578
18  H    Isotropic =    30.0278   Anisotropy =     8.2155
19  H    Isotropic =    30.0278   Anisotropy =     8.2155
20  N    Isotropic =  -102.1045   Anisotropy =   588.2228
21  C    Isotropic =    21.3828   Anisotropy =   180.9788
22  C    Isotropic =    50.8395   Anisotropy =   183.1583
23  C    Isotropic =    37.8117   Anisotropy =   211.0535
24  C    Isotropic =    50.8395   Anisotropy =   183.1583
25  C    Isotropic =    21.3828   Anisotropy =   180.9788
26  H    Isotropic =    22.4792   Anisotropy =     8.6712
27  H    Isotropic =    23.9817   Anisotropy =     5.3409
28  H    Isotropic =    23.5403   Anisotropy =     4.9977
29  H    Isotropic =    23.9817   Anisotropy =     5.3409
30  H    Isotropic =    22.4792   Anisotropy =     8.6712

===============================================================================
X = Cl    R = CH3
-------------------------------------------------------------------------------
Energies and NBO populations
-------------------------------------------------------------------------------

Number of atoms:  26
Full point group                 CS      NOp   2


C      0.000000  -0.565336   0.026605
C      0.000000  -1.312020   1.202577
C      0.000000  -2.708080   1.122757
C      0.000000  -3.370075  -0.111727
C      0.000000  -2.588137  -1.277652
C      0.000000  -1.194209  -1.219657
H      0.000000  -0.812988   2.165637
H      0.000000  -3.287161   2.042563
C      0.000000  -4.880235  -0.195240
H      0.000000  -3.073926  -2.250339
H      0.000000  -0.601802  -2.128288
Cl     0.000000   1.195750   0.110073
H      0.000000  -5.332139   0.800322
H     -0.882740  -5.245740  -0.732107
H      0.882740  -5.245740  -0.732107
N      0.000000   4.535869   0.173089
C      1.143928   5.233139   0.173089
C      1.199509   6.629303   0.173128
C      0.000000   7.342539   0.173175
C     -1.199509   6.629303   0.173128
C     -1.143928   5.233139   0.173089
H      2.060248   4.646319   0.173000
H      2.158287   7.137741   0.173131
```

```
H      0.000000   8.428483   0.173234
H     -2.158287   7.137741   0.173131
H     -2.060248   4.646319   0.173000

Electronic energy:                                    -979.39336250 (   -979.39336250)
Zero-point correction=                                   0.205825
Sum of electronic and zero-point Energies=           -979.187537
Sum of electronic and thermal Energies=              -979.174150
Sum of electronic and thermal Enthalpies=            -979.173206
Sum of electronic and thermal Free Energies=         -979.236786

Lowest vibration frequency:          -30.5971

Counterpoise: BSSE energy =       0.000617787437

Summary of Natural Population Analysis:

                                     Natural Population
               Natural  -----------------------------------------------
   Atom  No    Charge         Core      Valence    Rydberg      Total
------------------------------------------------------------------------
     C    1   -0.05363      1.99860     4.03195    0.02308     6.05363
     C    2   -0.22779      1.99898     4.20974    0.01906     6.22779
     C    3   -0.19681      1.99907     4.18144    0.01630     6.19681
     C    4   -0.03827      1.99907     4.02389    0.01531     6.03827
     C    5   -0.19430      1.99907     4.17882    0.01641     6.19430
     C    6   -0.22642      1.99899     4.20850    0.01893     6.22642
     H    7    0.22770      0.00000     0.77058    0.00172     0.77230
     H    8    0.21365      0.00000     0.78473    0.00162     0.78635
     C    9   -0.59674      1.99932     4.58744    0.00998     6.59674
     H   10    0.21376      0.00000     0.78467    0.00157     0.78624
     H   11    0.22764      0.00000     0.77064    0.00172     0.77236
    Cl   12    0.00235      9.99963     6.97541    0.02261    16.99765
     H   13    0.21027      0.00000     0.78845    0.00128     0.78973
     H   14    0.21660      0.00000     0.78206    0.00134     0.78340
     H   15    0.21660      0.00000     0.78206    0.00134     0.78340
     N   16   -0.46972      1.99945     5.44798    0.02228     7.46972
     C   17    0.04910      1.99923     3.92377    0.02790     5.95090
     C   18   -0.25003      1.99917     4.23435    0.01651     6.25003
     C   19   -0.17121      1.99918     4.15451    0.01751     6.17121
     C   20   -0.25003      1.99917     4.23435    0.01651     6.25003
     C   21    0.04910      1.99923     3.92377    0.02790     5.95090
     H   22    0.19479      0.00000     0.80374    0.00147     0.80521
     H   23    0.22059      0.00000     0.77793    0.00149     0.77941
     H   24    0.21742      0.00000     0.78128    0.00131     0.78258
     H   25    0.22059      0.00000     0.77793    0.00149     0.77941
     H   26    0.19479      0.00000     0.80374    0.00147     0.80521
========================================================================
  * Total *    0.00000     35.98815    71.72373    0.28811   108.00000

Contributions to pi population at N atom in pyridine:
    Val( 2p)     1.17062
    Ryd( 3p)     0.00071
    Ryd( 4p)     0.00033
    Ryd( 5p)     0.00003

    Total:       1.17169

-------------------------------------------------------------------------------
NMR properties
-------------------------------------------------------------------------------
Electronic energy (NMR):                          -979.39336250

 1  C    Isotropic =    31.9568   Anisotropy =   124.0752
 2  C    Isotropic =    44.8454   Anisotropy =   160.4289
 3  C    Isotropic =    43.3129   Anisotropy =   163.0132
 4  C    Isotropic =    35.2087   Anisotropy =   204.7690
 5  C    Isotropic =    43.2882   Anisotropy =   173.9594
 6  C    Isotropic =    44.7100   Anisotropy =   160.9874
 7  H    Isotropic =    23.9504   Anisotropy =     8.0106
 8  H    Isotropic =    24.1040   Anisotropy =     6.4765
 9  C    Isotropic =   159.7698   Anisotropy =    41.0857
10  H    Isotropic =    24.0032   Anisotropy =     7.0222
11  H    Isotropic =    23.8980   Anisotropy =     8.0818
12  Cl   Isotropic =   674.4166   Anisotropy =   527.7188
13  H    Isotropic =    29.4673   Anisotropy =     7.5835
14  H    Isotropic =    28.9648   Anisotropy =     8.4437
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15  H    Isotropic =    28.9648   Anisotropy =     8.4437
16  N    Isotropic =  -102.0120   Anisotropy =   587.7576
17  C    Isotropic =    21.4104   Anisotropy =   181.0475
18  C    Isotropic =    50.8107   Anisotropy =   183.1890
19  C    Isotropic =    37.8072   Anisotropy =   211.1837
20  C    Isotropic =    50.8107   Anisotropy =   183.1890
21  C    Isotropic =    21.4104   Anisotropy =   181.0475
22  H    Isotropic =    22.4782   Anisotropy =     8.6120
23  H    Isotropic =    23.9784   Anisotropy =     5.3299
24  H    Isotropic =    23.5357   Anisotropy =     5.0122
25  H    Isotropic =    23.9784   Anisotropy =     5.3299
26  H    Isotropic =    22.4782   Anisotropy =     8.6120

================================================================================
X = Cl    R = CHCH32
--------------------------------------------------------------------------------
Energies and NBO populations
--------------------------------------------------------------------------------

Number of atoms:  32
Full point group                 C1      NOp   1


C      0.040203  -0.392346   0.045828
C      0.039603  -1.083106  -1.163993
C      0.039476  -2.481097  -1.147822
C      0.039946  -3.202191   0.053514
C      0.040560  -2.474551   1.254334
C      0.040687  -1.079036   1.260786
H      0.039231  -0.539785  -2.102809
H      0.038996  -3.017411  -2.093589
C      0.039776  -4.726354   0.047779
H      0.040940  -2.997765   2.206796
H      0.041152  -0.529439   2.196005
Cl     0.040339   1.370742   0.042965
H      0.039301  -5.040582  -1.004130
C      1.311516  -5.300633   0.705154
C     -1.231546  -5.300341   0.706218
H      1.318452  -6.394196   0.634547
H      1.363257  -5.033847   1.767093
H      2.215001  -4.919746   0.218006
H     -2.135351  -4.919239   0.219832
H     -1.238797  -6.393902   0.635614
H     -1.282331  -5.033545   1.768200
N      0.040343   4.710220  -0.008566
C     -1.103586   5.407483  -0.008566
C     -1.159163   6.803649  -0.008479
C      0.040343   7.516891  -0.008444
C      1.239848   6.803649  -0.008477
C      1.184272   5.407483  -0.008566
H     -2.019903   4.820657  -0.008525
H     -2.117940   7.312091  -0.008404
H      0.040343   8.602836  -0.008443
H      2.198625   7.312092  -0.008401
H      2.100589   4.820657  -0.008526

Electronic energy:                                  -1058.01400536 (  -1058.01400453)
Zero-point correction=                                  0.262353
Sum of electronic and zero-point Energies=          -1057.751652
Sum of electronic and thermal Energies=             -1057.734872
Sum of electronic and thermal Enthalpies=           -1057.733928
Sum of electronic and thermal Free Energies=        -1057.805301

Lowest vibration frequency:           2.8562

Counterpoise: BSSE energy =       0.000644411013

Summary of Natural Population Analysis:

                                     Natural Population
              Natural  -----------------------------------------------
   Atom  No    Charge         Core      Valence    Rydberg      Total
-------------------------------------------------------------------------
     C    1   -0.05257      1.99860     4.03085    0.02313     6.05257
     C    2   -0.22800      1.99898     4.20998    0.01903     6.22800
     C    3   -0.19394      1.99906     4.17863    0.01625     6.19394
     C    4   -0.02450      1.99902     4.00543    0.02004     6.02450
```

```
     C    5   -0.19637      1.99906     4.18131    0.01600     6.19637
     C    6   -0.22689      1.99899     4.20879    0.01911     6.22689
     H    7    0.22782      0.00000     0.77050    0.00168     0.77218
     H    8    0.21393      0.00000     0.78434    0.00173     0.78607
     C    9   -0.24321      1.99920     4.22835    0.01566     6.24321
     H   10    0.21408      0.00000     0.78420    0.00172     0.78592
     H   11    0.22732      0.00000     0.77100    0.00168     0.77268
    Cl   12    0.00247      9.99963     6.97531    0.02258    16.99753
     H   13    0.19862      0.00000     0.79838    0.00300     0.80138
     C   14   -0.57029      1.99935     4.56146    0.00947     6.57029
     C   15   -0.57029      1.99935     4.56146    0.00947     6.57029
     H   16    0.20318      0.00000     0.79562    0.00120     0.79682
     H   17    0.19764      0.00000     0.80099    0.00137     0.80236
     H   18    0.20741      0.00000     0.79158    0.00101     0.79259
     H   19    0.20741      0.00000     0.79158    0.00101     0.79259
     H   20    0.20318      0.00000     0.79562    0.00120     0.79682
     H   21    0.19764      0.00000     0.80099    0.00137     0.80236
     N   22   -0.46969      1.99945     5.44794    0.02229     7.46969
     C   23    0.04908      1.99923     3.92377    0.02792     5.95092
     C   24   -0.25004      1.99917     4.23435    0.01652     6.25004
     C   25   -0.17121      1.99918     4.15452    0.01752     6.17121
     C   26   -0.25004      1.99917     4.23435    0.01652     6.25004
     C   27    0.04908      1.99923     3.92377    0.02792     5.95092
     H   28    0.19480      0.00000     0.80374    0.00146     0.80520
     H   29    0.22058      0.00000     0.77793    0.00149     0.77942
     H   30    0.21741      0.00000     0.78128    0.00131     0.78259
     H   31    0.22058      0.00000     0.77793    0.00149     0.77942
     H   32    0.19480      0.00000     0.80374    0.00146     0.80520
=======================================================================
  * Total *    0.00000     39.98668    83.68971    0.32361   124.00000

Contributions to pi population at N atom in pyridine:
    Val( 2p)     1.17061
    Ryd( 3p)     0.00071
    Ryd( 4p)     0.00033
    Ryd( 5p)     0.00003

    Total:       1.17168

-------------------------------------------------------------------------------
NMR properties
-------------------------------------------------------------------------------
Electronic energy (NMR):                          -1058.01400536

 1  C    Isotropic =    31.5345   Anisotropy =   123.0756
 2  C    Isotropic =    44.7029   Anisotropy =   159.7379
 3  C    Isotropic =    44.4389   Anisotropy =   157.7650
 4  C    Isotropic =    23.3905   Anisotropy =   213.5175
 5  C    Isotropic =    47.1380   Anisotropy =   187.1395
 6  C    Isotropic =    44.4256   Anisotropy =   161.6259
 7  H    Isotropic =    23.9426   Anisotropy =     7.8888
 8  H    Isotropic =    24.1068   Anisotropy =     7.1791
 9  C    Isotropic =   139.6481   Anisotropy =    24.3247
10  H    Isotropic =    23.9584   Anisotropy =     9.4514
11  H    Isotropic =    23.8595   Anisotropy =     8.2741
12  Cl   Isotropic =   673.0855   Anisotropy =   529.5101
13  H    Isotropic =    28.7223   Anisotropy =     6.9767
14  C    Isotropic =   155.7735   Anisotropy =    36.8306
15  C    Isotropic =   155.7737   Anisotropy =    36.8304
16  H    Isotropic =    30.2508   Anisotropy =    10.1418
17  H    Isotropic =    30.3292   Anisotropy =     6.5829
18  H    Isotropic =    30.3041   Anisotropy =     8.5588
19  H    Isotropic =    30.3040   Anisotropy =     8.5591
20  H    Isotropic =    30.2510   Anisotropy =    10.1417
21  H    Isotropic =    30.3292   Anisotropy =     6.5830
22  N    Isotropic =  -101.9740   Anisotropy =   587.9129
23  C    Isotropic =    21.3928   Anisotropy =   180.9730
24  C    Isotropic =    50.8189   Anisotropy =   183.1849
25  C    Isotropic =    37.7960   Anisotropy =   211.1106
26  C    Isotropic =    50.8189   Anisotropy =   183.1842
27  C    Isotropic =    21.3925   Anisotropy =   180.9724
28  H    Isotropic =    22.4747   Anisotropy =     8.7063
29  H    Isotropic =    23.9774   Anisotropy =     5.3412
30  H    Isotropic =    23.5362   Anisotropy =     4.9843
31  H    Isotropic =    23.9774   Anisotropy =     5.3412
32  H    Isotropic =    22.4747   Anisotropy =     8.7063
```

```
================================================================================
X = Cl    R = H
--------------------------------------------------------------------------------
Energies and NBO populations
--------------------------------------------------------------------------------

Number of atoms:  23
Full point group                 C2V     NOp   4


C      0.000000  -0.629188   0.000000
C      0.000000  -1.315733   1.215395
C      0.000000  -2.712382   1.217297
C      0.000000  -3.382085   0.000000
C      0.000000  -2.712382  -1.217297
C      0.000000  -1.315733  -1.215395
H      0.000000  -0.767899   2.150966
H      0.000000  -3.272603   2.145871
F      0.000000  -4.735618   0.000000
H      0.000000  -3.272603  -2.145871
H      0.000000  -0.767899  -2.150966
Cl     0.000000   1.130611   0.000000
N      0.000000   4.424939   0.000000
C      1.144030   5.122176   0.000000
C      1.199529   6.518271   0.000000
C      0.000000   7.231466   0.000000
C     -1.199529   6.518271   0.000000
C     -1.144030   5.122176   0.000000
H      2.060419   4.535473   0.000000
H      2.158275   7.026718   0.000000
H      0.000000   8.317387   0.000000
H     -2.158275   7.026718   0.000000
H     -2.060419   4.535473   0.000000

Electronic energy:                                -1039.32304625 (  -1039.32304625)
Zero-point correction=                                0.170632
Sum of electronic and zero-point Energies=        -1039.152414
Sum of electronic and thermal Energies=           -1039.140188
Sum of electronic and thermal Enthalpies=         -1039.139244
Sum of electronic and thermal Free Energies=      -1039.197216

Lowest vibration frequency:           -8.9286

Counterpoise: BSSE energy =       0.000689659556

Summary of Natural Population Analysis:

                                     Natural Population
               Natural  -----------------------------------------------
   Atom  No    Charge         Core      Valence    Rydberg      Total
--------------------------------------------------------------------------
     C    1   -0.06282      1.99861     4.04104    0.02317     6.06282
     C    2   -0.21340      1.99900     4.19625    0.01815     6.21340
     C    3   -0.25817      1.99906     4.24242    0.01670     6.25817
     C    4    0.40177      1.99849     3.57337    0.02636     5.59823
     C    5   -0.25817      1.99906     4.24242    0.01670     6.25817
     C    6   -0.21340      1.99900     4.19625    0.01815     6.21340
     H    7    0.23323      0.00000     0.76514    0.00163     0.76677
     H    8    0.23579      0.00000     0.76265    0.00156     0.76421
     F    9   -0.35410      1.99993     7.34614    0.00804     9.35410
     H   10    0.23579      0.00000     0.76265    0.00156     0.76421
     H   11    0.23323      0.00000     0.76514    0.00163     0.76677
    Cl   12    0.01419      9.99963     6.96354    0.02264    16.98581
     N   13   -0.47145      1.99945     5.44966    0.02235     7.47145
     C   14    0.04916      1.99923     3.92375    0.02787     5.95084
     C   15   -0.24961      1.99917     4.23394    0.01650     6.24961
     C   16   -0.17061      1.99918     4.15392    0.01750     6.17061
     C   17   -0.24961      1.99917     4.23394    0.01650     6.24961
     C   18    0.04916      1.99923     3.92375    0.02787     5.95084
     H   19    0.19472      0.00000     0.80381    0.00147     0.80528
     H   20    0.22092      0.00000     0.77760    0.00148     0.77908
     H   21    0.21777      0.00000     0.78092    0.00130     0.78223
     H   22    0.22092      0.00000     0.77760    0.00148     0.77908
     H   23    0.19472      0.00000     0.80381    0.00147     0.80528
==========================================================================
  * Total *    0.00000     35.98822    71.71970    0.29208   108.00000
```

```
Contributions to pi population at N atom in pyridine:
    Val( 2p)     1.17208
    Ryd( 3p)     0.00071
    Ryd( 4p)     0.00033
    Ryd( 5p)     0.00003

    Total:       1.17315

-------------------------------------------------------------------------------
NMR properties
-------------------------------------------------------------------------------
Electronic energy (NMR):                          -1039.32304625

 1  C    Isotropic =    34.3613   Anisotropy =   124.5064
 2  C    Isotropic =    42.8546   Anisotropy =   163.7865
 3  C    Isotropic =    58.1468   Anisotropy =   155.4927
 4  C    Isotropic =     7.9797   Anisotropy =   105.5043
 5  C    Isotropic =    58.1468   Anisotropy =   155.4927
 6  C    Isotropic =    42.8546   Anisotropy =   163.7865
 7  H    Isotropic =    23.8425   Anisotropy =     7.8244
 8  H    Isotropic =    24.2352   Anisotropy =     4.5838
 9  F    Isotropic =   294.5829   Anisotropy =    99.7427
10  H    Isotropic =    24.2352   Anisotropy =     4.5838
11  H    Isotropic =    23.8425   Anisotropy =     7.8244
12  Cl   Isotropic =   671.8913   Anisotropy =   528.6766
13  N    Isotropic =  -101.3641   Anisotropy =   586.1500
14  C    Isotropic =    21.4994   Anisotropy =   180.9615
15  C    Isotropic =    50.7247   Anisotropy =   183.3783
16  C    Isotropic =    37.6933   Anisotropy =   211.4531
17  C    Isotropic =    50.7247   Anisotropy =   183.3783
18  C    Isotropic =    21.4994   Anisotropy =   180.9615
19  H    Isotropic =    22.4866   Anisotropy =     8.6153
20  H    Isotropic =    23.9697   Anisotropy =     5.3257
21  H    Isotropic =    23.5267   Anisotropy =     5.0196
22  H    Isotropic =    23.9697   Anisotropy =     5.3257
23  H    Isotropic =    22.4866   Anisotropy =     8.6153

===============================================================================
X = Cl    R = Cl
-------------------------------------------------------------------------------
Energies and NBO populations
-------------------------------------------------------------------------------

Number of atoms:  23
Full point group                 C2V     NOp   4


C      0.000000  -0.615804   0.000000
C      0.000000  -1.303177   1.214455
C      0.000000  -2.699482   1.215484
C      0.000000  -3.382670   0.000000
C      0.000000  -2.699482  -1.215484
C      0.000000  -1.303177  -1.214455
H      0.000000  -0.757014   2.151147
H      0.000000  -3.246002   2.151894
Cl     0.000000  -5.144136   0.000000
H      0.000000  -3.246002  -2.151895
H      0.000000  -0.757014  -2.151147
Cl     0.000000   1.142299   0.000000
N      0.000000   4.411328   0.000000
C      1.144063   5.108544   0.000000
C      1.199540   6.504624   0.000000
C      0.000000   7.217799   0.000000
C     -1.199540   6.504624   0.000000
C     -1.144063   5.108544   0.000000
H      2.060462   4.521853   0.000000
H      2.158280   7.013067   0.000000
H      0.000000   8.303716   0.000000
H     -2.158280   7.013067   0.000000
H     -2.060462   4.521853   0.000000

Electronic energy:                              -1399.64544579 (  -1399.64544579)
Zero-point correction=                              0.169298
Sum of electronic and zero-point Energies=      -1399.476148
Sum of electronic and thermal Energies=         -1399.463521
Sum of electronic and thermal Enthalpies=       -1399.462577
Sum of electronic and thermal Free Energies=    -1399.522156
```

Lowest vibration frequency: -7.3093

Counterpoise: BSSE energy = 0.000674292501

Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.05129	1.99861	4.02936	0.02332	6.05129
C	2	-0.21495	1.99898	4.19743	0.01854	6.21495
C	3	-0.21607	1.99898	4.19867	0.01842	6.21607
C	4	-0.04731	1.99860	4.02608	0.02263	6.04731
C	5	-0.21607	1.99898	4.19867	0.01842	6.21607
C	6	-0.21496	1.99898	4.19743	0.01854	6.21496
H	7	0.23446	0.00000	0.76389	0.00165	0.76554
H	8	0.23460	0.00000	0.76375	0.00165	0.76540
Cl	9	-0.00329	9.99963	6.98371	0.01996	17.00329
H	10	0.23460	0.00000	0.76375	0.00165	0.76540
H	11	0.23446	0.00000	0.76389	0.00165	0.76554
Cl	12	0.01935	9.99963	6.95835	0.02267	16.98065
N	13	-0.47190	1.99945	5.45010	0.02235	7.47190
C	14	0.04926	1.99923	3.92368	0.02783	5.95074
C	15	-0.24949	1.99917	4.23383	0.01649	6.24949
C	16	-0.17045	1.99918	4.15377	0.01750	6.17045
C	17	-0.24949	1.99917	4.23383	0.01649	6.24949
C	18	0.04926	1.99923	3.92368	0.02783	5.95074
H	19	0.19473	0.00000	0.80380	0.00147	0.80527
H	20	0.22099	0.00000	0.77752	0.00148	0.77901
H	21	0.21785	0.00000	0.78085	0.00130	0.78215
H	22	0.22099	0.00000	0.77752	0.00148	0.77901
H	23	0.19473	0.00000	0.80380	0.00147	0.80527
* Total *		0.00000	43.98782	71.70739	0.30479	116.00000

Contributions to pi population at N atom in pyridine:

Val(2p)	1.17253
Ryd(3p)	0.00071
Ryd(4p)	0.00034
Ryd(5p)	0.00003
Total:	1.17361

NMR properties

Electronic energy (NMR): -1399.64544579

1	C	Isotropic =	30.3094	Anisotropy =	131.9130
2	C	Isotropic =	43.2424	Anisotropy =	161.2584
3	C	Isotropic =	43.8364	Anisotropy =	160.3613
4	C	Isotropic =	33.0881	Anisotropy =	120.9988
5	C	Isotropic =	43.8364	Anisotropy =	160.3613
6	C	Isotropic =	43.2424	Anisotropy =	161.2584
7	H	Isotropic =	23.8769	Anisotropy =	7.9017
8	H	Isotropic =	23.9452	Anisotropy =	7.2981
9	Cl	Isotropic =	686.8304	Anisotropy =	503.3459
10	H	Isotropic =	23.9452	Anisotropy =	7.2981
11	H	Isotropic =	23.8769	Anisotropy =	7.9017
12	Cl	Isotropic =	664.8804	Anisotropy =	519.9607
13	N	Isotropic =	-101.1319	Anisotropy =	585.5892
14	C	Isotropic =	21.5355	Anisotropy =	180.8999
15	C	Isotropic =	50.7048	Anisotropy =	183.4272
16	C	Isotropic =	37.6487	Anisotropy =	211.4858
17	C	Isotropic =	50.7048	Anisotropy =	183.4272
18	C	Isotropic =	21.5355	Anisotropy =	180.8999
19	H	Isotropic =	22.4930	Anisotropy =	8.6803
20	H	Isotropic =	23.9692	Anisotropy =	5.3345
21	H	Isotropic =	23.5266	Anisotropy =	5.0117
22	H	Isotropic =	23.9692	Anisotropy =	5.3345
23	H	Isotropic =	22.4930	Anisotropy =	8.6803

==========

X = Cl R = OCF3

Energies and NBO populations

Number of atoms: 27
Full point group C1 NOp 1

C	-0.302942	0.533297	0.010942
C	-0.210076	1.048964	-1.283116
C	0.055949	2.407340	-1.461633
C	0.226937	3.216640	-0.342598
C	0.125650	2.711680	0.950295
C	-0.139347	1.352965	1.129215
H	-0.347294	0.399608	-2.140221
H	0.125637	2.833803	-2.456176
O	0.422052	4.599488	-0.526994
H	0.247952	3.370077	1.803065
H	-0.222513	0.937222	2.126935
Cl	-0.643437	-1.176012	0.234538
C	1.692933	5.049871	-0.582570
F	2.380610	4.819441	0.553530
F	1.649155	6.366548	-0.782720
F	2.402296	4.493644	-1.583841
N	-1.124747	-4.347166	0.535040
C	-2.268971	-5.044270	0.535040
C	-2.324470	-6.440351	0.534793
C	-1.124879	-7.153342	0.534841
C	0.074734	-6.440282	0.535088
C	0.019377	-5.044290	0.535040
H	-3.185564	-4.458013	0.534955
H	-3.283281	-6.948657	0.534438
H	-1.124744	-8.239255	0.534622
H	1.033376	-6.948893	0.534949
H	0.935617	-4.457209	0.534527

Electronic energy: -1352.36289519 (-1352.36290264)
Zero-point correction= 0.187528
Sum of electronic and zero-point Energies= -1352.175367
Sum of electronic and thermal Energies= -1352.159531
Sum of electronic and thermal Enthalpies= -1352.158587
Sum of electronic and thermal Free Energies= -1352.225634

Lowest vibration frequency: -9.3817

Counterpoise: BSSE energy = 0.000736166393

Summary of Natural Population Analysis:

			Natural Population			
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.04686	1.99862	4.02492	0.02332	6.04686
C	2	-0.21670	1.99900	4.19942	0.01828	6.21670
C	3	-0.21447	1.99904	4.19853	0.01690	6.21447
C	4	0.25995	1.99868	3.71817	0.02320	5.74005
C	5	-0.21550	1.99904	4.19965	0.01681	6.21550
C	6	-0.21666	1.99900	4.19937	0.01830	6.21666
H	7	0.23533	0.00000	0.76304	0.00163	0.76467
H	8	0.23736	0.00000	0.76096	0.00168	0.76264
O	9	-0.56390	1.99965	6.54705	0.01719	8.56390
H	10	0.23767	0.00000	0.76064	0.00169	0.76233
H	11	0.23539	0.00000	0.76299	0.00163	0.76461
Cl	12	0.02384	9.99963	6.95387	0.02266	16.97616
C	13	1.28121	1.99964	2.64816	0.07098	4.71879
F	14	-0.35429	1.99991	7.34776	0.00661	9.35429
F	15	-0.33590	1.99991	7.32965	0.00634	9.33590
F	16	-0.35346	1.99991	7.34693	0.00662	9.35346
N	17	-0.47272	1.99945	5.45085	0.02242	7.47272
C	18	0.04966	1.99923	3.92336	0.02775	5.95034
C	19	-0.24939	1.99917	4.23371	0.01651	6.24939
C	20	-0.17020	1.99918	4.15352	0.01749	6.17020
C	21	-0.24923	1.99917	4.23359	0.01647	6.24923
C	22	0.04907	1.99923	3.92385	0.02785	5.95093
H	23	0.19460	0.00000	0.80399	0.00142	0.80540
H	24	0.22112	0.00000	0.77740	0.00148	0.77888
H	25	0.21797	0.00000	0.78073	0.00130	0.78203

```
     H   26    0.22115      0.00000     0.77736    0.00149     0.77885
     H   27    0.19494      0.00000     0.80352    0.00154     0.80506
=======================================================================
  * Total *    0.00000     43.98745    95.62300    0.38955   140.00000

Contributions to pi population at N atom in pyridine:
    Val( 2p)     1.17335
    Ryd( 3p)     0.00072
    Ryd( 4p)     0.00033
    Ryd( 5p)     0.00003

    Total:       1.17443

-------------------------------------------------------------------------------
NMR properties
-------------------------------------------------------------------------------
Electronic energy (NMR):                          -1352.36289519

 1  C    Isotropic =    28.9296   Anisotropy =   133.8644
 2  C    Isotropic =    43.0873   Anisotropy =   163.4936
 3  C    Isotropic =    48.9323   Anisotropy =   165.7374
 4  C    Isotropic =    23.9033   Anisotropy =   112.0735
 5  C    Isotropic =    49.0459   Anisotropy =   166.3582
 6  C    Isotropic =    43.2458   Anisotropy =   163.6983
 7  H    Isotropic =    23.7749   Anisotropy =     8.0143
 8  H    Isotropic =    24.0289   Anisotropy =     6.8015
 9  O    Isotropic =   168.2266   Anisotropy =    89.4486
10  H    Isotropic =    23.9760   Anisotropy =     6.9712
11  H    Isotropic =    23.7539   Anisotropy =     7.9261
12  Cl   Isotropic =   659.4290   Anisotropy =   522.8748
13  C    Isotropic =    47.3609   Anisotropy =    10.8939
14  F    Isotropic =   240.1274   Anisotropy =   166.1093
15  F    Isotropic =   241.1578   Anisotropy =   170.2513
16  F    Isotropic =   239.7250   Anisotropy =   165.9679
17  N    Isotropic =  -100.9009   Anisotropy =   585.2597
18  C    Isotropic =    21.5782   Anisotropy =   180.6296
19  C    Isotropic =    50.6227   Anisotropy =   183.0022
20  C    Isotropic =    37.7556   Anisotropy =   212.0828
21  C    Isotropic =    50.6197   Anisotropy =   183.3533
22  C    Isotropic =    21.6806   Anisotropy =   181.4287
23  H    Isotropic =    22.4962   Anisotropy =     8.2633
24  H    Isotropic =    23.9805   Anisotropy =     5.1806
25  H    Isotropic =    23.5022   Anisotropy =     5.0154
26  H    Isotropic =    23.9419   Anisotropy =     5.5042
27  H    Isotropic =    22.4699   Anisotropy =     9.2892

===============================================================================
X = Cl    R = COOCH3
-------------------------------------------------------------------------------
Energies and NBO populations
-------------------------------------------------------------------------------

Number of atoms:  29
Full point group                 CS      NOp   2


C      0.000000  -0.431432   0.036346
C      0.000000  -1.147700   1.235996
C      0.000000  -2.539594   1.192801
C      0.000000  -3.215216  -0.036049
C      0.000000  -2.478488  -1.229886
C      0.000000  -1.085089  -1.198046
H      0.000000  -0.621512   2.183985
H      0.000000  -3.116231   2.111647
C      0.000000  -4.708153  -0.017457
H      0.000000  -2.994629  -2.182893
H      0.000000  -0.510281  -2.117382
Cl     0.000000   1.323841   0.079878
O      0.000000  -5.238008  -1.254514
C      0.000000  -6.674923  -1.323911
H      0.000000  -6.913688  -2.386715
H     -0.891506  -7.079412  -0.839034
H      0.891506  -7.079412  -0.839034
O      0.000000  -5.379612   0.992943
N      0.000000   4.580093   0.103990
C      1.144085   5.277294   0.103990
C      1.199543   6.673362   0.103918
```

```
C      0.000000   7.386529   0.103865
C     -1.199543   6.673362   0.103918
C     -1.144085   5.277294   0.103990
H      2.060494   4.690615   0.104105
H      2.158281   7.181801   0.103986
H      0.000000   8.472444   0.103871
H     -2.158281   7.181801   0.103986
H     -2.060494   4.690615   0.104105

Electronic energy:                                  -1167.96448198 (  -1167.96445984)
Zero-point correction=                                  0.221453
Sum of electronic and zero-point Energies=          -1167.743029
Sum of electronic and thermal Energies=             -1167.726142
Sum of electronic and thermal Enthalpies=           -1167.725198
Sum of electronic and thermal Free Energies=        -1167.797118

Lowest vibration frequency:           3.5024

Counterpoise: BSSE energy =       0.000660771622

Summary of Natural Population Analysis:

                                     Natural Population
               Natural  -----------------------------------------------
   Atom  No    Charge         Core      Valence    Rydberg      Total
------------------------------------------------------------------------
     C    1   -0.02672      1.99863     4.00445    0.02364     6.02672
     C    2   -0.23370      1.99899     4.21604    0.01867     6.23370
     C    3   -0.14566      1.99911     4.12976    0.01679     6.14566
     C    4   -0.16885      1.99893     4.15210    0.01782     6.16885
     C    5   -0.15140      1.99911     4.13616    0.01613     6.15140
     C    6   -0.23440      1.99899     4.21676    0.01864     6.23440
     H    7    0.23318      0.00000     0.76521    0.00161     0.76682
     H    8    0.23788      0.00000     0.76048    0.00164     0.76212
     C    9    0.80365      1.99930     3.15032    0.04673     5.19635
     H   10    0.23459      0.00000     0.76385    0.00156     0.76541
     H   11    0.23260      0.00000     0.76578    0.00163     0.76740
    Cl   12    0.02626      9.99962     6.95145    0.02266    16.97374
     O   13   -0.55064      1.99972     6.53675    0.01417     8.55064
     C   14   -0.21745      1.99926     4.20243    0.01576     6.21745
     H   15    0.19177      0.00000     0.80715    0.00107     0.80823
     H   16    0.18996      0.00000     0.80833    0.00171     0.81004
     H   17    0.18996      0.00000     0.80833    0.00171     0.81004
     O   18   -0.61770      1.99975     6.60672    0.01123     8.61770
     N   19   -0.47223      1.99945     5.45044    0.02234     7.47223
     C   20    0.04935      1.99923     3.92362    0.02780     5.95065
     C   21   -0.24942      1.99917     4.23376    0.01649     6.24942
     C   22   -0.17036      1.99918     4.15368    0.01750     6.17036
     C   23   -0.24942      1.99917     4.23376    0.01649     6.24942
     C   24    0.04935      1.99923     3.92362    0.02780     5.95065
     H   25    0.19474      0.00000     0.80379    0.00147     0.80526
     H   26    0.22102      0.00000     0.77749    0.00149     0.77898
     H   27    0.21787      0.00000     0.78083    0.00130     0.78213
     H   28    0.22102      0.00000     0.77749    0.00149     0.77898
     H   29    0.19474      0.00000     0.80379    0.00147     0.80526
========================================================================
  * Total *    0.00000     41.98683    87.64435    0.36882   130.00000

Contributions to pi population at N atom in pyridine:
    Val( 2p)     1.17280
    Ryd( 3p)     0.00071
    Ryd( 4p)     0.00034
    Ryd( 5p)     0.00002

    Total:       1.17387

-------------------------------------------------------------------------------
NMR properties
-------------------------------------------------------------------------------
Electronic energy (NMR):                            -1167.96448198

 1  C    Isotropic =    21.9938   Anisotropy =   140.1884
 2  C    Isotropic =    44.5711   Anisotropy =   162.9121
 3  C    Isotropic =    41.0481   Anisotropy =   196.6241
 4  C    Isotropic =    45.6684   Anisotropy =   164.9862
 5  C    Isotropic =    42.6244   Anisotropy =   191.4735
 6  C    Isotropic =    45.0040   Anisotropy =   162.2187
```

```
 7  H    Isotropic =    23.7183   Anisotropy =     8.2774
 8  H    Isotropic =    22.9863   Anisotropy =     7.6766
 9  C    Isotropic =     6.5032   Anisotropy =    85.3582
10  H    Isotropic =    23.2030   Anisotropy =     8.5805
11  H    Isotropic =    23.7742   Anisotropy =     8.4070
12  Cl   Isotropic =   646.4984   Anisotropy =   506.0322
13  O    Isotropic =   145.1998   Anisotropy =   141.8686
14  C    Isotropic =   126.6954   Anisotropy =    73.0670
15  H    Isotropic =    27.7568   Anisotropy =     7.5522
16  H    Isotropic =    27.5972   Anisotropy =     8.4249
17  H    Isotropic =    27.5972   Anisotropy =     8.4249
18  O    Isotropic =   -66.1035   Anisotropy =   602.5807
19  N    Isotropic =  -100.9815   Anisotropy =   585.3997
20  C    Isotropic =    21.5267   Anisotropy =   180.9012
21  C    Isotropic =    50.6891   Anisotropy =   183.4968
22  C    Isotropic =    37.6058   Anisotropy =   211.4846
23  C    Isotropic =    50.6891   Anisotropy =   183.4968
24  C    Isotropic =    21.5267   Anisotropy =   180.9012
25  H    Isotropic =    22.4772   Anisotropy =     8.6934
26  H    Isotropic =    23.9595   Anisotropy =     5.3261
27  H    Isotropic =    23.5197   Anisotropy =     4.9915
28  H    Isotropic =    23.9595   Anisotropy =     5.3261
29  H    Isotropic =    22.4772   Anisotropy =     8.6934

================================================================================
X = Cl    R = COCH3
--------------------------------------------------------------------------------
Energies and NBO populations
--------------------------------------------------------------------------------

Number of atoms:  28
Full point group                 CS      NOp   2


C      0.000000  -0.481943  -0.013748
C      0.000000  -1.114731   1.233438
C      0.000000  -2.504654   1.286159
C      0.000000  -3.272745   0.109468
C      0.000000  -2.613057  -1.130014
C      0.000000  -1.219830  -1.198479
H      0.000000  -0.523167   2.142273
H      0.000000  -3.017289   2.242342
C      0.000000  -4.770478   0.227819
H      0.000000  -3.177307  -2.056682
H      0.000000  -0.711388  -2.156137
Cl     0.000000   1.271740  -0.088965
C      0.000000  -5.603578  -1.041774
O      0.000000  -5.305253   1.323980
H      0.000000  -6.659552  -0.770283
H      0.883869  -5.384225  -1.650889
H     -0.883869  -5.384225  -1.650889
N      0.000000   4.517036  -0.147820
C      1.144092   5.214239  -0.147820
C      1.199543   6.610294  -0.148032
C      0.000000   7.323459  -0.148192
C     -1.199543   6.610294  -0.148032
C     -1.144092   5.214239  -0.147820
H      2.060514   4.627583  -0.147352
H      2.158273   7.118748  -0.147861
H      0.000000   8.409370  -0.148232
H     -2.158273   7.118748  -0.147861
H     -2.060514   4.627583  -0.147352

Electronic energy:                                -1092.72889164 (  -1092.72889163)
Zero-point correction=                                0.215826
Sum of electronic and zero-point Energies=        -1092.513066
Sum of electronic and thermal Energies=           -1092.497154
Sum of electronic and thermal Enthalpies=         -1092.496210
Sum of electronic and thermal Free Energies=      -1092.565212

Lowest vibration frequency:            3.6457

Counterpoise: BSSE energy =       0.000660964606

Summary of Natural Population Analysis:

                                     Natural Population
```

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.02563	1.99863	4.00327	0.02374	6.02563
C	2	-0.23163	1.99899	4.21411	0.01853	6.23163
C	3	-0.14206	1.99910	4.12514	0.01782	6.14206
C	4	-0.16328	1.99895	4.14705	0.01728	6.16328
C	5	-0.16066	1.99911	4.14635	0.01520	6.16066
C	6	-0.23486	1.99899	4.21683	0.01904	6.23486
H	7	0.23292	0.00000	0.76547	0.00161	0.76708
H	8	0.23801	0.00000	0.76009	0.00190	0.76199
C	9	0.56552	1.99931	3.39647	0.03870	5.43448
H	10	0.22143	0.00000	0.77708	0.00149	0.77857
H	11	0.23240	0.00000	0.76594	0.00165	0.76760
Cl	12	0.02812	9.99962	6.94960	0.02266	16.97188
C	13	-0.67819	1.99930	4.67057	0.00833	6.67819
O	14	-0.57799	1.99976	6.56452	0.01371	8.57799
H	15	0.23168	0.00000	0.76645	0.00187	0.76832
H	16	0.22870	0.00000	0.76989	0.00141	0.77130
H	17	0.22870	0.00000	0.76989	0.00141	0.77130
N	18	-0.47249	1.99945	5.45069	0.02236	7.47249
C	19	0.04935	1.99923	3.92363	0.02779	5.95065
C	20	-0.24933	1.99917	4.23367	0.01649	6.24933
C	21	-0.17024	1.99918	4.15357	0.01749	6.17024
C	22	-0.24933	1.99917	4.23367	0.01649	6.24933
C	23	0.04935	1.99923	3.92363	0.02779	5.95065
H	24	0.19470	0.00000	0.80383	0.00147	0.80530
H	25	0.22109	0.00000	0.77743	0.00149	0.77891
H	26	0.21795	0.00000	0.78075	0.00130	0.78205
H	27	0.22109	0.00000	0.77743	0.00149	0.77891
H	28	0.19470	0.00000	0.80383	0.00147	0.80530
* Total *		0.00000	39.98718	81.67084	0.34198	122.00000

Contributions to pi population at N atom in pyridine:

Val(2p)	1.17305
Ryd(3p)	0.00071
Ryd(4p)	0.00034
Ryd(5p)	0.00002
Total:	1.17412

NMR properties

Electronic energy (NMR): -1092.72889164

1	C	Isotropic =	21.6608	Anisotropy =	140.6032
2	C	Isotropic =	44.1279	Anisotropy =	162.7140
3	C	Isotropic =	44.1431	Anisotropy =	200.8762
4	C	Isotropic =	38.9715	Anisotropy =	178.0566
5	C	Isotropic =	42.1423	Anisotropy =	185.7860
6	C	Isotropic =	45.1391	Anisotropy =	161.5029
7	H	Isotropic =	23.7139	Anisotropy =	8.3628
8	H	Isotropic =	23.0059	Anisotropy =	6.8433
9	C	Isotropic =	-25.4626	Anisotropy =	173.2921
10	H	Isotropic =	23.3223	Anisotropy =	8.2842
11	H	Isotropic =	23.7382	Anisotropy =	8.4444
12	Cl	Isotropic =	644.6731	Anisotropy =	503.6200
13	C	Isotropic =	153.8157	Anisotropy =	46.2593
14	O	Isotropic =	-290.5811	Anisotropy =	966.6546
15	H	Isotropic =	29.3320	Anisotropy =	6.8790
16	H	Isotropic =	28.7107	Anisotropy =	4.7318
17	H	Isotropic =	28.7107	Anisotropy =	4.7318
18	N	Isotropic =	-100.9063	Anisotropy =	585.1174
19	C	Isotropic =	21.5566	Anisotropy =	180.9173
20	C	Isotropic =	50.6662	Anisotropy =	183.5312
21	C	Isotropic =	37.5895	Anisotropy =	211.5769
22	C	Isotropic =	50.6662	Anisotropy =	183.5312
23	C	Isotropic =	21.5566	Anisotropy =	180.9173
24	H	Isotropic =	22.4775	Anisotropy =	8.6674
25	H	Isotropic =	23.9566	Anisotropy =	5.3194
26	H	Isotropic =	23.5159	Anisotropy =	4.9999
27	H	Isotropic =	23.9566	Anisotropy =	5.3194
28	H	Isotropic =	22.4775	Anisotropy =	8.6674

==========

X = Cl R = CF3

Energies and NBO populations

Number of atoms: 26
Full point group CS NOp 2

C	0.000000	-0.504189	0.003614
C	0.000000	-1.154517	1.237438
C	0.000000	-2.549947	1.273832
C	0.000000	-3.279655	0.083272
C	0.000000	-2.616575	-1.150230
C	0.000000	-1.224819	-1.194102
H	0.000000	-0.580006	2.156737
H	0.000000	-3.062089	2.229191
C	0.000000	-4.786605	0.098022
H	0.000000	-3.181471	-2.077053
H	0.000000	-0.702280	-2.143921
Cl	0.000000	1.250039	-0.048432
F	0.000000	-5.295159	1.345801
F	-1.083009	-5.298069	-0.535705
F	1.083009	-5.298069	-0.535705
N	0.000000	4.469259	-0.152330
C	1.144140	5.166423	-0.152330
C	1.199552	6.562450	-0.152678
C	0.000000	7.275607	-0.152827
C	-1.199552	6.562450	-0.152678
C	-1.144140	5.166423	-0.152330
H	2.060600	4.579799	-0.151799
H	2.158292	7.070861	-0.152587
H	0.000000	8.361511	-0.152727
H	-2.158292	7.070861	-0.152587
H	-2.060600	4.579799	-0.151799

Electronic energy: -1277.14351629 (-1277.14349265)
Zero-point correction= 0.183262
Sum of electronic and zero-point Energies= -1276.960254
Sum of electronic and thermal Energies= -1276.945197
Sum of electronic and thermal Enthalpies= -1276.944253
Sum of electronic and thermal Free Energies= -1277.011746

Lowest vibration frequency: -20.6925

Counterpoise: BSSE energy = 0.000702091274

Summary of Natural Population Analysis:

			Natural Population			
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.03251	1.99863	4.01008	0.02380	6.03251
C	2	-0.22492	1.99899	4.20732	0.01861	6.22492
C	3	-0.16720	1.99909	4.15158	0.01653	6.16720
C	4	-0.16100	1.99891	4.14488	0.01721	6.16100
C	5	-0.16341	1.99910	4.14743	0.01688	6.16341
C	6	-0.22357	1.99899	4.20594	0.01864	6.22357
H	7	0.23538	0.00000	0.76303	0.00159	0.76462
H	8	0.23635	0.00000	0.76205	0.00160	0.76365
C	9	1.06724	1.99913	2.87339	0.06024	4.93276
H	10	0.23241	0.00000	0.76599	0.00159	0.76759
H	11	0.23566	0.00000	0.76274	0.00160	0.76434
Cl	12	0.03049	9.99962	6.94726	0.02262	16.96951
F	13	-0.35519	1.99992	7.34890	0.00638	9.35519
F	14	-0.35851	1.99992	7.35206	0.00653	9.35851
F	15	-0.35851	1.99992	7.35206	0.00653	9.35851
N	16	-0.47310	1.99945	5.45126	0.02240	7.47310
C	17	0.04940	1.99923	3.92359	0.02778	5.95060
C	18	-0.24917	1.99917	4.23352	0.01649	6.24917
C	19	-0.17001	1.99918	4.15335	0.01749	6.17001
C	20	-0.24917	1.99917	4.23352	0.01649	6.24917
C	21	0.04940	1.99923	3.92359	0.02778	5.95060
H	22	0.19471	0.00000	0.80382	0.00147	0.80529
H	23	0.22121	0.00000	0.77730	0.00148	0.77879
H	24	0.21809	0.00000	0.78062	0.00130	0.78191

```
     H   25    0.22121      0.00000     0.77730    0.00148     0.77879
     H   26    0.19471      0.00000     0.80382    0.00147     0.80529
=======================================================================
  * Total *    0.00000     41.98764    89.65637    0.35599   132.00000

Contributions to pi population at N atom in pyridine:
    Val( 2p)     1.17366
    Ryd( 3p)     0.00071
    Ryd( 4p)     0.00035
    Ryd( 5p)     0.00002

    Total:       1.17474

-------------------------------------------------------------------------------
NMR properties
-------------------------------------------------------------------------------
Electronic energy (NMR):                          -1277.14351629

 1  C    Isotropic =    23.6832   Anisotropy =   140.6107
 2  C    Isotropic =    44.6953   Anisotropy =   165.3909
 3  C    Isotropic =    47.4982   Anisotropy =   188.0796
 4  C    Isotropic =    43.5520   Anisotropy =   165.0126
 5  C    Isotropic =    45.3527   Anisotropy =   190.0943
 6  C    Isotropic =    43.6433   Anisotropy =   166.8862
 7  H    Isotropic =    23.7090   Anisotropy =     8.1524
 8  H    Isotropic =    23.5607   Anisotropy =     8.3974
 9  C    Isotropic =    43.3245   Anisotropy =    11.1560
10  H    Isotropic =    23.6108   Anisotropy =     7.9677
11  H    Isotropic =    23.6522   Anisotropy =     8.1844
12  Cl   Isotropic =   648.1771   Anisotropy =   517.0619
13  F    Isotropic =   261.1212   Anisotropy =   113.2111
14  F    Isotropic =   232.4395   Anisotropy =   148.1981
15  F    Isotropic =   232.4395   Anisotropy =   148.1981
16  N    Isotropic =  -100.6470   Anisotropy =   584.5135
17  C    Isotropic =    21.5954   Anisotropy =   180.8371
18  C    Isotropic =    50.6402   Anisotropy =   183.5792
19  C    Isotropic =    37.5455   Anisotropy =   211.6399
20  C    Isotropic =    50.6402   Anisotropy =   183.5792
21  C    Isotropic =    21.5954   Anisotropy =   180.8371
22  H    Isotropic =    22.4819   Anisotropy =     8.7353
23  H    Isotropic =    23.9543   Anisotropy =     5.3290
24  H    Isotropic =    23.5141   Anisotropy =     4.9943
25  H    Isotropic =    23.9543   Anisotropy =     5.3290
26  H    Isotropic =    22.4819   Anisotropy =     8.7353

===============================================================================
X = Cl    R = CN
-------------------------------------------------------------------------------
Energies and NBO populations
-------------------------------------------------------------------------------

Number of atoms:  24
Full point group                 C2V     NOp   4


C      0.000000  -0.580025   0.000000
C      0.000000  -1.265573   1.217808
C      0.000000  -2.657539   1.217479
C      0.000000  -3.359784   0.000000
C      0.000000  -2.657539  -1.217479
C      0.000000  -1.265573  -1.217808
H      0.000000  -0.715693   2.152006
H      0.000000  -3.201334   2.155875
C      0.000000  -4.792848   0.000000
H      0.000000  -3.201334  -2.155875
H      0.000000  -0.715693  -2.152006
Cl     0.000000   1.172339   0.000000
N      0.000000  -5.951610   0.000000
N      0.000000   4.375484   0.000000
C      1.144216   5.072633   0.000000
C      1.199568   6.468615   0.000000
C      0.000000   7.181731   0.000000
C     -1.199568   6.468615   0.000000
C     -1.144216   5.072633   0.000000
H      2.060688   4.486066   0.000000
H      2.158260   6.977084   0.000000
H      0.000000   8.267619   0.000000
```

```
H     -2.158260   6.977084   0.000000
H     -2.060688   4.486066   0.000000

Electronic energy:                                  -1032.32414890 (  -1032.32414890)
Zero-point correction=                                  0.177563
Sum of electronic and zero-point Energies=          -1032.146586
Sum of electronic and thermal Energies=             -1032.133446
Sum of electronic and thermal Enthalpies=           -1032.132502
Sum of electronic and thermal Free Energies=        -1032.192173

Lowest vibration frequency:           -4.5567

Counterpoise: BSSE energy =       0.000699445229

Summary of Natural Population Analysis:

                                     Natural Population
               Natural  ----------------------------------------------
   Atom  No    Charge         Core      Valence    Rydberg      Total
------------------------------------------------------------------------
     C    1   -0.02765      1.99864     4.00509    0.02392     6.02765
     C    2   -0.22591      1.99899     4.20838    0.01854     6.22591
     C    3   -0.13822      1.99911     4.12379    0.01531     6.13822
     C    4   -0.19491      1.99888     4.17917    0.01686     6.19491
     C    5   -0.13822      1.99911     4.12379    0.01531     6.13822
     C    6   -0.22591      1.99899     4.20838    0.01854     6.22591
     H    7    0.23802      0.00000     0.76042    0.00156     0.76198
     H    8    0.23354      0.00000     0.76519    0.00127     0.76646
     C    9    0.30686      1.99927     3.65991    0.03397     5.69314
     H   10    0.23354      0.00000     0.76519    0.00127     0.76646
     H   11    0.23802      0.00000     0.76042    0.00156     0.76198
    Cl   12    0.03905      9.99962     6.93870    0.02263    16.96095
     N   13   -0.34594      1.99959     5.32604    0.02031     7.34594
     N   14   -0.47432      1.99945     5.45245    0.02242     7.47432
     C   15    0.04946      1.99923     3.92356    0.02775     5.95054
     C   16   -0.24889      1.99917     4.23324    0.01648     6.24889
     C   17   -0.16960      1.99918     4.15294    0.01748     6.16960
     C   18   -0.24889      1.99917     4.23324    0.01648     6.24889
     C   19    0.04946      1.99923     3.92356    0.02775     5.95054
     H   20    0.19466      0.00000     0.80386    0.00147     0.80534
     H   21    0.22143      0.00000     0.77709    0.00148     0.77857
     H   22    0.21832      0.00000     0.78039    0.00130     0.78168
     H   23    0.22143      0.00000     0.77709    0.00148     0.77857
     H   24    0.19466      0.00000     0.80386    0.00147     0.80534
========================================================================
  * Total *    0.00000     37.98761    73.68576    0.32663   112.00000

Contributions to pi population at N atom in pyridine:
    Val( 2p)     1.17464
    Ryd( 3p)     0.00071
    Ryd( 4p)     0.00035
    Ryd( 5p)     0.00002

    Total:       1.17572

-------------------------------------------------------------------------------
NMR properties
-------------------------------------------------------------------------------
Electronic energy (NMR):                            -1032.32414890

 1  C    Isotropic =    22.1177   Anisotropy =   145.4172
 2  C    Isotropic =    43.6752   Anisotropy =   167.7108
 3  C    Isotropic =    38.5504   Anisotropy =   190.9058
 4  C    Isotropic =    64.4477   Anisotropy =   149.6068
 5  C    Isotropic =    38.5504   Anisotropy =   190.9058
 6  C    Isotropic =    43.6752   Anisotropy =   167.7108
 7  H    Isotropic =    23.7129   Anisotropy =     8.1021
 8  H    Isotropic =    23.5999   Anisotropy =     6.2722
 9  C    Isotropic =    55.7019   Anisotropy =   352.4979
10  H    Isotropic =    23.5999   Anisotropy =     6.2722
11  H    Isotropic =    23.7129   Anisotropy =     8.1021
12  Cl   Isotropic =   635.4230   Anisotropy =   501.9735
13  N    Isotropic =   -43.1212   Anisotropy =   418.8143
14  N    Isotropic =  -100.1296   Anisotropy =   583.1468
15  C    Isotropic =    21.6740   Anisotropy =   180.8288
16  C    Isotropic =    50.5690   Anisotropy =   183.7129
17  C    Isotropic =    37.4713   Anisotropy =   211.8935
```

```
18  C    Isotropic =    50.5690   Anisotropy =   183.7129
19  C    Isotropic =    21.6740   Anisotropy =   180.8288
20  H    Isotropic =    22.4933   Anisotropy =     8.6844
21  H    Isotropic =    23.9497   Anisotropy =     5.3256
22  H    Isotropic =    23.5071   Anisotropy =     5.0138
23  H    Isotropic =    23.9497   Anisotropy =     5.3256
24  H    Isotropic =    22.4933   Anisotropy =     8.6844

================================================================================
X = Cl    R = NO2
--------------------------------------------------------------------------------
Energies and NBO populations
--------------------------------------------------------------------------------

Number of atoms:  25
Full point group                 C2V     NOp   4


C      0.000000  -0.523839   0.000000
C      0.000000  -1.208898   1.219473
C      0.000000  -2.600805   1.220719
C      0.000000  -3.276925   0.000000
C      0.000000  -2.600805  -1.220719
C      0.000000  -1.208898  -1.219473
H      0.000000  -0.658447   2.153103
H      0.000000  -3.159663   2.148415
N      0.000000  -4.748707   0.000000
H      0.000000  -3.159663  -2.148415
H      0.000000  -0.658447  -2.153103
Cl     0.000000   1.225940   0.000000
O      0.000000  -5.322659   1.084754
O      0.000000  -5.322659  -1.084754
N      0.000000   4.410788   0.000000
C      1.144287   5.107911   0.000000
C      1.199588   6.503863   0.000000
C      0.000000   7.216948   0.000000
C     -1.199588   6.503863   0.000000
C     -1.144287   5.107911   0.000000
H      2.060809   4.521437   0.000000
H      2.158259   7.012336   0.000000
H      0.000000   8.302823   0.000000
H     -2.158259   7.012336   0.000000
H     -2.060809   4.521437   0.000000

Electronic energy:                                -1144.59363475 (  -1144.59363475)
Zero-point correction=                               0.181246
Sum of electronic and zero-point Energies=        -1144.412389
Sum of electronic and thermal Energies=           -1144.398448
Sum of electronic and thermal Enthalpies=         -1144.397504
Sum of electronic and thermal Free Energies=      -1144.459770

Lowest vibration frequency:           -2.6025

Counterpoise: BSSE energy =       0.000703144081

Summary of Natural Population Analysis:

                                     Natural Population
               Natural  -----------------------------------------------
   Atom  No    Charge         Core      Valence    Rydberg      Total
--------------------------------------------------------------------------
     C    1   -0.02105      1.99865     3.99835    0.02405     6.02105
     C    2   -0.22263      1.99899     4.20515    0.01849     6.22263
     C    3   -0.17049      1.99908     4.15320    0.01821     6.17049
     C    4    0.05864      1.99879     3.92190    0.02067     5.94136
     C    5   -0.17049      1.99908     4.15320    0.01821     6.17049
     C    6   -0.22263      1.99899     4.20515    0.01849     6.22263
     H    7    0.23935      0.00000     0.75912    0.00152     0.76065
     H    8    0.25285      0.00000     0.74525    0.00190     0.74715
     N    9    0.48964      1.99945     4.45591    0.05500     6.51036
     H   10    0.25285      0.00000     0.74525    0.00190     0.74715
     H   11    0.23935      0.00000     0.75912    0.00152     0.76065
    Cl   12    0.04747      9.99962     6.93015    0.02277    16.95253
     O   13   -0.39053      1.99980     6.37582    0.01491     8.39053
     O   14   -0.39053      1.99980     6.37582    0.01491     8.39053
     N   15   -0.47525      1.99945     5.45336    0.02244     7.47525
     C   16    0.04956      1.99923     3.92349    0.02772     5.95044
```

```
     C   17   -0.24867      1.99917     4.23304    0.01647     6.24867
     C   18   -0.16931      1.99918     4.15265    0.01748     6.16931
     C   19   -0.24867      1.99917     4.23304    0.01647     6.24867
     C   20    0.04956      1.99923     3.92349    0.02772     5.95044
     H   21    0.19466      0.00000     0.80387    0.00147     0.80534
     H   22    0.22159      0.00000     0.77693    0.00148     0.77841
     H   23    0.21847      0.00000     0.78023    0.00129     0.78153
     H   24    0.22159      0.00000     0.77693    0.00148     0.77841
     H   25    0.19466      0.00000     0.80387    0.00147     0.80534
=======================================================================
  * Total *    0.00000     39.98767    81.64428    0.36805   122.00000

Contributions to pi population at N atom in pyridine:
    Val( 2p)     1.17542
    Ryd( 3p)     0.00071
    Ryd( 4p)     0.00035
    Ryd( 5p)     0.00002

    Total:       1.17650

-------------------------------------------------------------------------------
NMR properties
-------------------------------------------------------------------------------
Electronic energy (NMR):                          -1144.59363475

 1  C    Isotropic =    18.5101   Anisotropy =   149.2264
 2  C    Isotropic =    44.0109   Anisotropy =   164.0343
 3  C    Isotropic =    48.0320   Anisotropy =   186.9534
 4  C    Isotropic =    26.3551   Anisotropy =   114.8458
 5  C    Isotropic =    48.0320   Anisotropy =   186.9534
 6  C    Isotropic =    44.0109   Anisotropy =   164.0343
 7  H    Isotropic =    23.6762   Anisotropy =     8.2354
 8  H    Isotropic =    22.8504   Anisotropy =     5.7965
 9  N    Isotropic =  -153.8258   Anisotropy =   290.0595
10  H    Isotropic =    22.8504   Anisotropy =     5.7965
11  H    Isotropic =    23.6762   Anisotropy =     8.2354
12  Cl   Isotropic =   630.0636   Anisotropy =   485.7990
13  O    Isotropic =  -308.1745   Anisotropy =   723.9803
14  O    Isotropic =  -308.1745   Anisotropy =   723.9803
15  N    Isotropic =   -99.7796   Anisotropy =   582.4600
16  C    Isotropic =    21.7005   Anisotropy =   180.8271
17  C    Isotropic =    50.5275   Anisotropy =   183.8457
18  C    Isotropic =    37.4027   Anisotropy =   212.0086
19  C    Isotropic =    50.5275   Anisotropy =   183.8457
20  C    Isotropic =    21.7005   Anisotropy =   180.8271
21  H    Isotropic =    22.4887   Anisotropy =     8.6534
22  H    Isotropic =    23.9414   Anisotropy =     5.3096
23  H    Isotropic =    23.5003   Anisotropy =     5.0097
24  H    Isotropic =    23.9414   Anisotropy =     5.3096
25  H    Isotropic =    22.4887   Anisotropy =     8.6534
```