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# *Developing and Understanding Iridium-Catalysed Arene Borylation*

PETER HARRISSON

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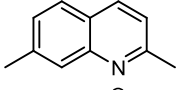
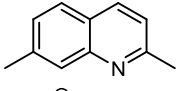
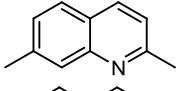
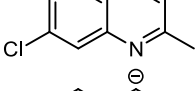
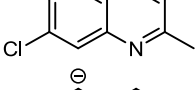
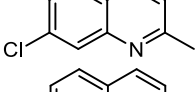
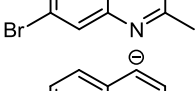
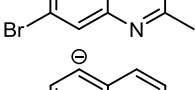
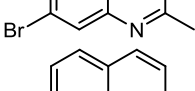
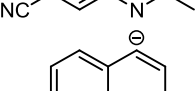
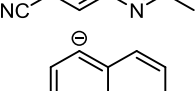
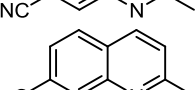
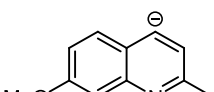
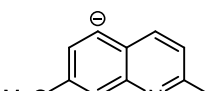

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# APPENDIX III - DFT CALCULATION DATA TABLES

### 1.1 2,7-disubstituted Quinolines

The following methods were utilised for the optimisation and frequency calculation:

Optimisation (gas phase)	Frequency (gas phase)	Optimisation + Frequency (solution phase)
B3LYP/6-31G(g)	B3LYP/6-311++G(2df,2p)	B3LYP/6-311++G(2df,2p) scrf=(iefpcm,solvent=dms) (tsnum=60, tsare=0.4, radii=bondi, alpha=1.20)

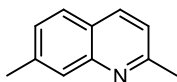
Compound	$E_{PCM}$	E	$G_{(gas)}$	$\Delta_{solv}G$ (kcal/mol)
	-480.724889	-480.721971076	-480.566817	-1.83
	-480.178022	-480.090341051	-479.950153	-54.98
	-480.173373	-480.084309413	-479.944374	-55.84
	-901.023019	-901.018068824	-900.900400	-3.10
	-900.479028	-900.396356065	-900.293523	-51.84
	-900.478655	-900.395415435	-900.292781	-52.19
	-3014.937349	-3014.931912370	-3014.815936	-3.41
	-3014.393640	-3014.311177440	-3014.210002	-51.70
	-3014.393659	-3014.311755680	-3014.210830	-51.35
	-533.667003	-533.662103031	-533.536371	-3.07
	-533.130622	-533.050370520	-532.939265	-50.32
	-533.129284	-533.046739213	-532.935717	-51.76
	-555.960492	-555.954574425	-555.796041	-3.71
	-555.414390	-555.323151119	-555.179716	-57.21
	-555.411910	-555.320901799	-555.177478	-57.06

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	-778.560983	-778.557598966	-778.429267	-2.12
	-778.018293	-777.940624889	-777.827186	-48.70
	-778.015854	-777.935691812	-777.822317	-50.26
	-850.129534	-850.129604211	-849.908034	0.04
	-849.580754	-849.513920632	-849.306915	-41.90
	-849.575036	-849.507196843	-849.300347	-42.54

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## 1.2 Optimised Geometry Cartesian coordinates

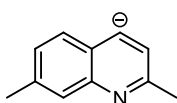


## Gas phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-2.397784	-0.435179	-0.000024
2	C	-1.183648	-1.092324	-0.000037
3	C	0.045169	-0.381969	-0.000022
4	C	0.019406	1.046227	0.000007
5	C	-1.234854	1.709343	-0.000005
6	C	-2.406113	0.988675	-0.000035
7	H	-1.131249	-2.177461	-0.000073
8	C	1.268809	1.716501	0.000025
9	H	-1.256835	2.797032	-0.000017
10	H	-3.360862	1.510006	-0.000073
11	C	2.427981	0.981973	0.00002
12	C	2.356296	-0.442441	-0.000005
13	H	1.294168	2.804235	0.00004
14	H	3.398917	1.469999	0.000032
15	N	1.209283	-1.098148	-0.000034
16	C	3.625092	-1.259803	0.00001
17	H	4.239249	-1.038419	-0.882194
18	H	4.238947	-1.038796	0.882525
19	H	3.378571	-2.323476	-0.000234
20	C	-3.704823	-1.190974	0.000054
21	H	-4.308558	-0.942556	0.882316
22	H	-4.30957	-0.94105	-0.881077
23	H	-3.540938	-2.272638	-0.000936

## Solution phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	2.394268	-0.432316	0.00008
2	C	1.186643	-1.092634	-0.000173
3	C	-0.040314	-0.387415	-0.000368
4	C	-0.018856	1.03488	-0.000171
5	C	1.229854	1.701131	-0.000017
6	C	2.399719	0.987442	0.000109
7	H	1.148116	-2.177218	-0.000166
8	C	-1.263506	1.705038	-0.00006
9	H	1.246327	2.786899	0.000147
10	H	3.350098	1.51214	0.000354
11	C	-2.419727	0.975821	0.000025
12	C	-2.354107	-0.443504	-0.000168
13	H	-1.287511	2.791042	0.000165
14	H	-3.38702	1.466246	0.000337
15	N	-3.240533	-1.095992	-0.000449
16	C	-3.626605	-1.24485	0.000362
17	H	-4.232852	-1.010144	0.877866
18	H	-4.233394	-1.010263	-0.876801
19	H	-3.40595	-2.309348	0.000365
20	C	3.699894	-1.181447	0.000335
21	H	4.298343	-0.926391	-0.876972
22	H	4.298612	-0.92535	0.87715
23	H	3.541387	-2.258536	0.000976

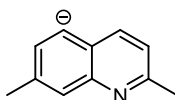


## Gas phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	2.381164	-0.420851	0.00008
2	C	1.164233	-1.066197	-0.003842
3	C	-0.060621	-0.352325	-0.005012
4	C	-0.054967	1.076194	-0.002992
5	C	1.216318	1.70942	0.001666
6	C	2.390885	0.99668	0.002981
7	H	1.120401	-2.149619	-0.004309
8	C	-1.279127	1.833729	-0.002667
9	H	1.239144	2.792948	0.006084
10	H	3.340443	1.520013	0.007429
11	C	-2.40721	1.023568	-0.000091
12	C	-2.362726	-0.39627	0.000008
13	H	-3.403838	1.462935	0.002972
14	N	-1.225513	-1.071808	-0.005369
15	C	-3.644383	-1.190945	0.005769
16	H	-3.436626	-2.259334	0.002787
17	H	-4.244562	-0.95507	0.887575
18	H	-4.256535	-0.950909	-0.866533
19	C	3.680545	-1.183957	0.002653
20	H	4.280485	-0.936902	0.881577
21	H	3.510268	-2.259757	0.001736
22	H	4.284743	-0.935925	-0.873044
1	C	2.381164	-0.420851	0.00008

## Solution phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	2.383772	-0.414626	0.000003
2	C	1.16681	-1.0698	-0.000231
3	C	-0.068095	-0.362279	-0.000058
4	C	-0.070523	1.073781	0.000067
5	C	1.202607	1.710441	0.000364
6	C	2.39002	1.0068	0.000374
7	H	1.120441	-2.158989	-0.000483
8	C	-1.283385	1.872925	-0.000213
9	H	1.191598	2.799738	0.000542
10	H	3.345079	1.534394	0.000616
11	C	-2.402228	1.027436	-0.000551
12	C	-2.353255	-0.391627	-0.000243
13	H	-3.414074	1.461176	-0.001208
14	N	-1.224219	-1.096169	-0.000169
15	C	-3.636194	-1.204486	0.000518
16	H	-4.249933	-0.986139	0.88638
17	H	-4.258548	-0.974381	-0.876218
18	H	-3.40214	-2.273787	-0.007293
19	C	3.689311	-1.179126	-0.000137
20	H	4.303653	-0.942215	0.881246
21	H	3.516603	-2.261642	-0.000535
22	H	4.303818	-0.941602	-0.881241
1	C	2.383772	-0.414626	0.000003

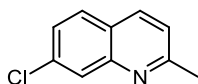


## Gas phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	2.394306	-0.388777	-0.000029
2	C	1.19661	-1.084628	-0.000027
3	C	-0.025212	-0.369989	-0.00002
4	C	0.03243	1.073008	0
5	C	1.249878	1.861372	-0.000042
6	C	2.383408	1.037647	-0.000071
7	H	1.161213	-2.173323	-0.000017
8	C	-1.229933	1.719065	0.000053
9	H	3.381504	1.504873	-0.000136
10	C	-2.408566	1.00052	0.000059
11	C	-2.341558	-0.417385	0.000004
12	H	-3.379035	1.496739	0.000105
13	N	-1.199723	-1.086508	-0.00004
14	C	-3.615528	-1.238594	-0.000018
15	H	-4.236985	-1.027483	0.882452
16	H	-4.237086	-1.027282	-0.882367
17	H	-3.361611	-2.302304	-0.000148
18	C	3.711451	-1.138676	0.000083
19	H	4.320014	-0.884881	0.880481
20	H	3.563995	-2.226343	-0.0003
21	H	4.320474	-0.884297	-0.879822
22	H	-1.218127	2.808481	0.000076
1	C	2.394306	-0.388777	-0.000029

## Solution phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	2.399932	-0.387604	-0.000253
2	C	1.202641	-1.066981	-0.000346
3	C	-0.019234	-0.356411	-0.000548
4	C	0.016961	1.077031	-0.000178
5	C	1.244993	1.827662	0.000321
6	C	2.387887	1.036936	-0.000602
7	H	1.170713	-2.152153	-0.000195
8	C	-1.247793	1.713801	0.000339
9	H	3.369813	1.513775	0.000272
10	C	-2.40977	0.985246	0.000325
11	C	-2.339439	-0.429566	-0.000155
12	H	-3.378023	1.474383	0.000731
13	N	-1.188021	-1.073976	-0.000577
14	C	-3.607843	-1.242295	0.000298
15	H	-4.217707	-1.016574	0.877982
16	H	-4.218495	-1.016289	-0.876763
17	H	-3.37776	-2.305289	0.000031
18	C	3.713353	-1.12933	0.000591
19	H	4.312251	-0.87051	0.87723
20	H	3.566491	-2.209268	0.000712
21	H	4.313229	-0.870803	-0.875456
22	H	-1.274489	2.79962	0.000743
1	C	2.399932	-0.387604	-0.000253

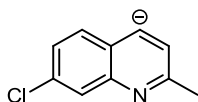


## Gas phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-2.042498	-0.117144	-0.000017
2	C	-0.918296	-0.909241	-0.000018
3	C	0.364533	-0.301649	-0.000002
4	C	0.46227	1.12414	0.000013
5	C	-0.72513	1.898868	0.000013
6	C	-1.962544	1.295885	-0.000002
7	H	-0.978432	-1.991258	-0.000029
8	C	1.766744	1.681654	0.000026
9	H	-0.649989	2.983674	0.000025
10	H	-2.873604	1.883986	-0.000002
11	C	2.855341	0.847346	0.000024
12	C	2.659077	-0.566334	0.00001
13	H	1.8882	2.762567	0.000035
14	H	3.865525	1.247296	0.000033
15	N	1.459251	-1.118431	-0.000003
16	C	3.850924	-1.490989	0.000032
17	H	4.481153	-1.322361	-0.882262
18	H	4.480895	-1.322636	0.882566
19	H	3.513556	-2.529281	-0.000168
20	Cl	-3.635564	-0.862246	-0.000039

## Solution phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	2.035805	-0.113726	0.000104
2	C	0.921305	-0.909395	0.00012
3	C	-0.358869	-0.307142	0.000037
4	C	-0.458532	1.112165	-0.000012
5	C	0.722502	1.889591	-0.000013
6	C	1.957721	1.292847	0.000023
7	H	0.994973	-1.990354	0.000137
8	C	-1.758183	1.671338	-0.000079
9	H	0.642868	2.972352	-0.000076
10	H	2.864551	1.885601	-0.000025
11	C	-2.8443	0.843353	-0.00006
12	C	-2.655008	-0.566211	-0.00006
13	H	-1.876771	2.750963	-0.000098
14	H	-3.851027	1.246814	-0.000045
15	N	-1.457761	-1.116352	-0.00003
16	C	-3.85193	-1.474867	-0.000027
17	H	-4.475837	-1.291944	0.877311
18	H	-4.47594	-1.291759	-0.877254
19	H	-3.540172	-2.516165	-0.000158
20	Cl	3.626978	-0.857574	0.000013

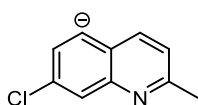


## Gas phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	2.013419	-0.094219	-0.000013
2	C	0.893898	-0.89167	-0.000264
3	C	-0.394803	-0.285764	-0.000127
4	C	-0.52025	1.146613	0.000075
5	C	0.686536	1.897394	0.000364
6	C	1.940235	1.314225	0.000343
7	H	0.961823	-1.975371	-0.000513
8	C	-1.798525	1.836107	-0.000107
9	H	0.576532	2.980523	0.000557
10	H	2.850381	1.906688	0.000556
11	C	-2.838685	0.896303	-0.000396
12	C	-2.666405	-0.513156	-0.000188
13	H	-3.883751	1.23998	-0.000921
14	N	-1.480252	-1.117249	-0.0002
15	C	-3.873573	-1.433406	0.000476
16	H	-4.502872	-1.266624	0.886147
17	H	-4.511965	-1.256203	-0.876542
18	H	-3.549256	-2.478565	-0.006933
19	Cl	3.633517	-0.85672	-0.000114

## Solution phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	2.015546	-0.101013	0.000352
2	C	0.893597	-0.886662	-0.000243
3	C	-0.384658	-0.275239	0.000672
4	C	-0.499144	1.150033	-0.001489
5	C	0.706121	1.897124	0.000644
6	C	1.94656	1.302553	0.001901
7	H	0.962635	-1.965795	-0.002837
8	C	-1.784631	1.800664	-0.004236
9	H	0.632016	2.97758	0.003298
10	H	2.851988	1.892462	0.004144
11	C	-2.835975	0.895031	0.000719
12	C	-2.669618	-0.516849	0.001911
13	H	-3.867187	1.245003	0.002827
14	N	-1.479822	-1.094006	0.001935
15	C	-3.879698	-1.415125	-0.000726
16	H	-3.586423	-2.46297	-0.009942
17	H	-4.49981	-1.232551	0.879651
18	H	-4.504929	-1.21915	-0.874538
19	Cl	3.607169	-0.863508	-0.000775

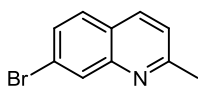


## Gas phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	2.014766	-0.047253	-0.000021
2	C	0.924184	-0.889311	-0.000026
3	C	-0.358422	-0.287071	0.000002
4	C	-0.428577	1.15335	0.000022
5	C	0.711207	2.041923	0.000029
6	C	1.935975	1.360346	0.00001
7	H	1.013751	-1.969363	-0.000047
8	C	-1.743423	1.686887	0.000037
9	H	2.88599	1.904481	0.000017
10	C	-2.850384	0.864331	0.000034
11	C	-2.656918	-0.543091	0.000016
12	H	-3.861377	1.270096	0.000044
13	N	-1.46092	-1.107912	0
14	C	-3.853335	-1.472548	0.000023
15	H	-4.489458	-1.314397	0.882541
16	H	-4.489525	-1.314325	-0.882434
17	H	-3.508495	-2.510014	-0.00003
18	H	-1.831737	2.772208	0.000051
19	Cl	3.666873	-0.840511	-0.000052

## Solution phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-2.025589	-0.067372	0.000233
2	C	-0.927955	-0.885994	-0.001915
3	C	0.349022	-0.278655	-0.001947
4	C	0.429955	1.150954	-0.000762
5	C	-0.723157	2.006752	0.00195
6	C	-1.944018	1.340523	0.002675
7	H	-1.011801	-1.963079	-0.003402
8	C	1.744295	1.682903	-0.001728
9	H	-2.882962	1.886903	0.004847
10	C	2.838273	0.858936	-0.001544
11	C	2.651533	-0.546951	-0.000771
12	H	3.84246	1.262331	-0.001036
13	N	1.450443	-1.093715	-0.002068
14	C	3.848961	-1.457941	0.003401
15	H	4.513178	-1.228366	-0.832435
16	H	4.431076	-1.327156	0.918073
17	H	3.540897	-2.498277	-0.069457
18	H	1.862053	2.760228	-0.002268
19	Cl	-3.640936	-0.826795	0.000153

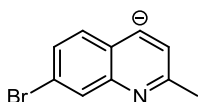


## Gas phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-1.393624	0.166834	-0.00001
2	C	-0.343762	-0.720253	-0.00001
3	C	0.98787	-0.22746	0.000006
4	C	1.209447	1.184477	0.00002
5	C	0.094125	2.060029	0.000019
6	C	-1.191106	1.56686	0.000004
7	H	-0.496837	-1.793056	-0.000021
8	C	2.55747	1.626108	0.000032
9	H	0.263243	3.134248	0.00003
10	H	-2.046561	2.233127	0.000005
11	C	3.569052	0.699988	0.00003
12	C	3.250586	-0.691271	0.000017
13	H	2.772672	2.69231	0.00004
14	H	4.610193	1.010693	0.000038
15	N	2.007127	-1.136619	0.000004
16	C	4.357559	-1.715948	0.000037
17	H	5.000198	-1.602872	-0.882221
18	H	4.999925	-1.603117	0.882528
19	H	3.931282	-2.721002	-0.000158
20	Br	-3.190563	-0.488291	-0.000032

## Solution phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-1.386726	0.172356	-0.000595
2	C	-0.347296	-0.718769	-0.001515
3	C	0.98173	-0.231524	-0.001267
4	C	1.205605	1.173206	-0.000499
5	C	0.09795	2.051244	0.000122
6	C	-1.186124	1.566309	0.000148
7	H	-0.509621	-1.786874	-0.002105
8	C	2.549838	1.615719	0.000023
9	H	0.272096	3.120238	0.000659
10	H	-2.030645	2.240124	0.000693
11	C	3.558053	0.695301	0.000381
12	C	3.246753	-0.693247	-0.000179
13	H	2.76142	2.678183	0.00047
14	H	4.594102	1.006684	0.001335
15	N	2.004926	-1.134861	-0.001306
16	C	4.360733	-1.700707	0.001294
17	H	5.000473	-1.567306	-0.873843
18	H	4.994033	-1.571241	0.8817
19	H	3.962542	-2.712376	-0.002354
20	Br	-3.187485	-0.486935	0.000432

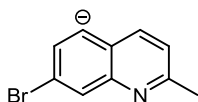


## Gas phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	1.35596	0.186444	0.000028
2	C	0.311724	-0.706209	-0.000276
3	C	-1.024613	-0.213329	-0.000146
4	C	-1.272768	1.203155	0.000149
5	C	-0.135459	2.055538	0.000474
6	C	1.164147	1.583006	0.000433
7	H	0.472086	-1.779892	-0.000578
8	C	-2.605374	1.780104	-0.000082
9	H	-0.337866	3.12537	0.00071
10	H	2.019215	2.251934	0.000679
11	C	-3.560303	0.754187	-0.000417
12	C	-3.267564	-0.635467	-0.000308
13	H	-4.630941	1.007126	-0.000715
14	N	-2.034049	-1.135397	-0.000273
15	C	-4.39094	-1.655913	0.000554
16	H	-5.032294	-1.543433	0.886106
17	H	-5.041986	-1.534396	-0.876605
18	H	-3.978174	-2.669405	-0.00649
19	Br	3.180556	-0.486246	-0.000104

## Solution phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	1.364545	0.184711	0.000016
2	C	0.314868	-0.6968	-0.00337
3	C	-1.01236	-0.19921	-0.00322
4	C	-1.25292	1.211006	-0.00126
5	C	-0.11795	2.05981	0.004929
6	C	1.171332	1.576317	0.005131
7	H	0.472536	-1.76683	-0.00604
8	C	-2.59111	1.743195	-0.00549
9	H	-0.28272	3.130724	0.010954
10	H	2.017491	2.24933	0.009914
11	C	-3.55912	0.751489	-0.00525
12	C	-3.26775	-0.64364	-0.00199
13	H	-4.6179	1.008931	-0.00584
14	N	-2.03223	-1.11058	-0.00253
15	C	-4.39598	-1.6428	0.007278
16	H	-4.99141	-1.54535	0.918674
17	H	-5.07376	-1.47274	-0.83274
18	H	-4.01583	-2.66116	-0.05106
19	Br	3.165596	-0.49238	-0.0002

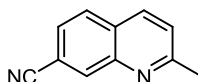


## Gas phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	1.341259	0.237282	-0.000008
2	C	0.332445	-0.699222	-0.000012
3	C	-0.999538	-0.213216	0.000012
4	C	-1.192335	1.215484	0.000003
5	C	-0.130948	2.193918	0.000036
6	C	1.151821	1.632156	0.000002
7	H	0.518163	-1.766542	-0.000031
8	C	-2.547499	1.636201	0.000043
9	H	2.048849	2.258488	0.000025
10	C	-3.579364	0.72162	0.000039
11	C	-3.266767	-0.664497	0.000021
12	H	-4.621201	1.039739	0.000005
13	N	-2.026978	-1.125228	0.000008
14	C	-4.37991	-1.69189	0.000003
15	H	-5.027122	-1.588087	0.882521
16	H	-5.027199	-1.588018	-0.882397
17	H	-3.948566	-2.696413	-0.000026
18	H	-2.72929	2.709754	0.000057
19	Br	3.21715	-0.477124	-0.000043

## Solution phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-1.361154	0.212448	0.000921
2	C	-0.339875	-0.698549	-0.000494
3	C	0.985091	-0.202276	-0.001144
4	C	1.186825	1.215515	-0.000137
5	C	0.11009	2.164521	0.00301
6	C	-1.165579	1.607735	0.003072
7	H	-0.511324	-1.764893	-0.001488
8	C	2.541869	1.633292	-0.002387
9	H	-2.051159	2.236356	0.003418
10	C	3.560676	0.718308	-0.002494
11	C	3.255216	-0.667121	-0.002143
12	H	4.595728	1.03466	-0.002436
13	N	2.011794	-1.108906	-0.001525
14	C	4.371311	-1.675517	0.003551
15	H	5.025311	-1.533998	-0.859374
16	H	4.991041	-1.56068	0.895462
17	H	3.975963	-2.688021	-0.018757
18	H	2.751983	2.696274	-0.003069
19	Br	-3.192198	-0.471643	-0.000389

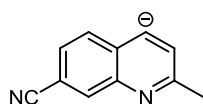


## Gas phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-2.179846	-0.145382	-0.000006
2	C	-1.035448	-0.927577	-0.000008
3	C	0.243929	-0.320342	-0.000003
4	C	0.336039	1.105738	0.000003
5	C	-0.852056	1.881563	0.000004
6	C	-2.085878	1.276891	0.000001
7	H	-1.090278	-2.010521	-0.000013
8	C	1.639899	1.666658	0.000006
9	H	-0.774793	2.965948	0.000009
10	H	-2.995853	1.867482	0.000003
11	C	2.729008	0.833878	0.000003
12	C	2.538285	-0.582016	-0.000001
13	H	1.759396	2.747574	0.000008
14	H	3.738155	1.236419	0.000003
15	N	1.34007	-1.135645	-0.000006
16	C	3.733116	-1.501723	0.000016
17	H	4.362342	-1.330032	-0.88229
18	H	4.362086	-1.330311	0.882562
19	H	3.400067	-2.541294	-0.000185
20	C	-3.474387	-0.763925	-0.00001
21	N	-4.528226	-1.256905	-0.000012

## Solution phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-2.172387	-0.14235	-0.00009
2	C	-1.037139	-0.929758	-0.000159
3	C	0.237168	-0.326187	-0.000116
4	C	0.329546	1.093417	-0.000013
5	C	-0.851686	1.871803	0.000005
6	C	-2.083303	1.274269	-0.000026
7	H	-1.105769	-2.011937	-0.000213
8	C	1.628526	1.657342	0.000061
9	H	-0.769771	2.954255	0.000065
10	H	-2.990556	1.867412	0.000007
11	C	2.71477	0.831804	0.000031
12	C	2.531847	-0.581147	-0.000043
13	H	1.744051	2.737221	0.000125
14	H	3.720546	1.238176	0.000083
15	N	1.337977	-1.133908	-0.000133
16	C	3.732996	-1.482806	0.000115
17	H	4.356585	-1.294442	-0.876291
18	H	4.354659	-1.296503	0.878343
19	H	3.426765	-2.525655	-0.001389
20	C	-3.460014	-0.760979	-0.000006
21	N	-4.503472	-1.251945	0.000234

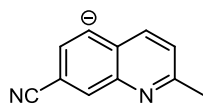


## Gas phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-2.164319	-0.131305	-0.000003
2	C	-1.010645	-0.909508	-0.000008
3	C	0.269448	-0.305064	-0.000004
4	C	0.389465	1.129273	0
5	C	-0.821352	1.878901	0.000005
6	C	-2.067037	1.29121	0.000004
7	H	-1.069373	-1.994928	-0.000012
8	C	1.664728	1.822786	-0.000005
9	H	-0.711041	2.961633	0.000009
10	H	-2.976694	1.886156	0.000008
11	C	2.705724	0.885579	-0.000009
12	C	2.540969	-0.528043	-0.000002
13	H	3.74958	1.232097	-0.00002
14	N	1.358961	-1.134466	-0.000003
15	C	3.75349	-1.439554	0.000024
16	H	4.385604	-1.261897	-0.881179
17	H	4.385334	-1.262199	0.881483
18	H	3.436781	-2.486838	-0.000191
19	C	-3.452637	-0.7556	-0.000006
20	N	-4.50856	-1.252117	-0.000007

## Solution phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-2.156161	-0.13187	-0.000384
2	C	-1.009764	-0.907026	-0.0002
3	C	0.260868	-0.295391	-0.000166
4	C	0.368471	1.131015	0.001152
5	C	-0.838058	1.879084	-0.001628
6	C	-2.073534	1.283863	-0.002088
7	H	-1.072668	-1.986942	0.000217
8	C	1.651916	1.786726	0.003741
9	H	-0.761021	2.958894	-0.004293
10	H	-2.979089	1.87408	-0.003987
11	C	2.703421	0.883661	0.001074
12	C	2.544308	-0.532151	-0.001069
13	H	3.73344	1.236881	0.000634
14	N	1.358726	-1.112434	-0.00157
15	C	3.759525	-1.421662	-0.000385
16	H	4.383786	-1.223304	-0.874304
17	H	4.377149	-1.230108	0.879788
18	H	3.473903	-2.471533	-0.005182
19	C	-3.435059	-0.762487	0.000821
20	N	-4.474597	-1.264785	0.001844

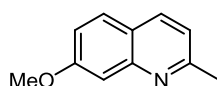


## Gas phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-2.17215	-0.116407	-0.000007
2	C	-1.039041	-0.926147	-0.00001
3	C	0.228828	-0.308288	-0.000004
4	C	0.286658	1.133313	0.000006
5	C	-0.854099	2.022035	0.000009
6	C	-2.061734	1.312514	0.000002
7	H	-1.102841	-2.010032	-0.000017
8	C	1.601283	1.676291	0.000012
9	H	-3.014974	1.852529	0.000003
10	C	2.711543	0.862803	0.000006
11	C	2.53004	-0.549279	-0.000003
12	H	3.719645	1.275617	0.000009
13	N	1.340407	-1.121322	-0.000009
14	C	3.734897	-1.466594	0.000014
15	H	4.369015	-1.300919	-0.882357
16	H	4.368778	-1.301189	0.882609
17	H	3.400797	-2.50743	-0.000018
18	C	-3.469244	-0.731974	-0.000011
19	N	-4.540569	-1.195874	-0.000014
20	H	1.678819	2.7622	0.000017

## Solution phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-2.170435	-0.116125	-0.001472
2	C	-1.042083	-0.915691	-0.004786
3	C	0.223372	-0.299191	-0.005007
4	C	0.29392	1.131136	-0.002238
5	C	-0.860272	1.985737	-0.00082
6	C	-2.071509	1.308254	-0.000106
7	H	-1.111908	-1.994479	-0.00544
8	C	1.607874	1.671273	0.0015
9	H	-3.012517	1.851603	0.001476
10	C	2.703125	0.853303	0.002508
11	C	2.526209	-0.557289	-0.000656
12	H	3.70532	1.261611	0.00673
13	N	1.330789	-1.109426	-0.004962
14	C	3.730693	-1.457341	0.003925
15	H	4.358714	-1.265996	-0.868678
16	H	4.346685	-1.272371	0.886443
17	H	3.430209	-2.50228	-0.00169
18	C	-3.460346	-0.726717	0.002411
19	N	-4.519192	-1.189312	0.005599
20	H	1.719023	2.748984	0.005148

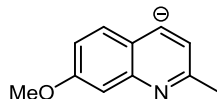


## Gas phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-1.986667	-0.339962	-0.000016
2	C	-0.794635	-1.045392	-0.000015
3	C	0.442685	-0.367051	-0.000013
4	C	0.456489	1.065182	-0.000008
5	C	-0.776267	1.758048	-0.000009
6	C	-1.977216	1.080211	-0.000014
7	H	-0.80256	-2.129662	-0.000017
8	C	1.722889	1.703662	-0.000004
9	H	-2.906385	1.638279	-0.00002
10	C	2.862737	0.941311	-0.000005
11	C	2.752641	-0.482629	-0.000005
12	N	1.592616	-1.111432	-0.000012
13	C	4.001707	-1.329923	0.000009
14	H	4.620579	-1.122152	-0.882231
15	H	4.620376	-1.122403	0.882453
16	H	3.730452	-2.387524	-0.000163
17	O	-3.129191	-1.087029	-0.000028
18	C	-4.381977	-0.421909	0.000079
19	H	-4.512386	0.200711	-0.894992
20	H	-5.136603	-1.210627	0.00013
21	H	-4.512242	0.200692	0.895182
22	H	3.846119	1.403342	-0.000005
23	H	1.774703	2.790556	-0.000004
24	H	-0.771151	2.845756	-0.000009

## Solution phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	1.981493	-0.339405	-0.000726
2	C	0.795549	-1.046497	-0.000555
3	C	-0.439023	-0.372368	-0.000157
4	C	-0.454909	1.053386	-0.000104
5	C	0.773168	1.747511	-0.000295
6	C	1.971762	1.075846	-0.000532
7	H	0.810986	-2.130444	-0.00059
8	C	-1.715767	1.692874	0.00023
9	H	2.894102	1.63893	-0.000536
10	C	-2.853993	0.936842	0.000465
11	C	-2.751587	-0.481925	0.000426
12	N	-1.593064	-1.108606	0.000111
13	C	-4.004401	-1.313628	0.000521
14	H	-4.616161	-1.092736	0.877814
15	H	-4.616213	-1.092918	-0.876787
16	H	-3.758454	-2.372547	0.000628
17	O	3.124169	-1.079535	-0.000785
18	C	4.385437	-0.41451	0.000826
19	H	4.507567	0.201617	0.893538
20	H	5.134364	-1.201259	0.000604
21	H	4.508942	0.20334	-0.890506
22	H	-3.833186	1.402494	0.00067
23	H	-1.764901	2.778064	0.000264
24	H	0.76468	2.833217	-0.000191

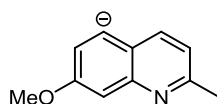


## Gas phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-1.962847	-0.325414	-0.000047
2	C	-0.773852	-1.029399	-0.000045
3	C	0.472027	-0.350465	-0.000023
4	C	0.509775	1.088813	-0.000003
5	C	-0.741903	1.753939	-0.000003
6	C	-1.958331	1.090079	-0.000025
7	H	-0.785232	-2.116486	-0.000059
8	C	1.741274	1.860364	0.000012
9	H	-2.88684	1.653527	-0.000033
10	C	2.840389	0.990371	0.000008
11	C	2.756568	-0.427198	0.000005
12	N	1.613299	-1.108423	-0.000015
13	C	4.020984	-1.268669	0.000041
14	H	4.643574	-1.057048	-0.881125
15	H	4.643268	-1.057425	0.881517
16	H	3.763459	-2.332488	-0.000216
17	O	-3.127193	-1.088791	-0.000086
18	C	-4.355583	-0.406252	0.000112
19	H	-4.483267	0.227681	-0.891275
20	H	-5.135292	-1.175142	0.000164
21	H	-4.483033	0.227576	0.891607
22	H	3.862095	1.399724	0.000007
23	H	-0.705278	2.842366	0.000011

## Solution phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	1.961336	-0.330358	-0.005472
2	C	0.768454	-1.024495	-0.010462
3	C	-0.464848	-0.33954	-0.010628
4	C	-0.493584	1.092486	-0.006191
5	C	0.757551	1.753928	-0.002086
6	C	1.959963	1.081556	-0.001711
7	H	0.777091	-2.107247	-0.012046
8	C	-1.734925	1.819996	0.001981
9	H	2.886275	1.635695	0.003031
10	C	-2.845159	0.986761	0.004258
11	C	-2.766222	-0.432347	0.00274
12	N	-1.615487	-1.083917	-0.006553
13	C	-4.029552	-1.255475	0.009192
14	H	-4.629185	-1.040468	0.896506
15	H	-4.651269	-1.019703	-0.857466
16	H	-3.799478	-2.319163	-0.006241
17	O	3.104989	-1.080773	-0.000897
18	C	4.36771	-0.413339	0.013273
19	H	4.481155	0.198744	0.909338
20	H	5.118089	-1.198609	0.015215
21	H	4.496004	0.208571	-0.873969
22	H	-3.851242	1.403482	0.007837
23	H	0.756718	2.837261	0.001474

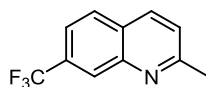


## Gas phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-1.973891	-0.298066	-0.00006
2	C	-0.801882	-1.039314	-0.000028
3	C	0.431113	-0.354959	-0.000016
4	C	0.410219	1.091052	-0.000034
5	C	-0.787707	1.90408	-0.000081
6	C	-1.954286	1.121773	-0.000075
7	H	-0.82505	-2.124971	-0.000002
8	C	1.684399	1.708305	-0.000025
9	H	-2.924738	1.630142	-0.000077
10	C	2.847904	0.963604	0
11	C	2.746435	-0.451878	0.000039
12	N	1.591367	-1.097589	0.000023
13	C	4.001678	-1.301871	0.000067
14	H	4.627408	-1.103607	-0.882236
15	H	4.627158	-1.1039	0.882615
16	H	3.724131	-2.359593	-0.000136
17	O	-3.140136	-1.066134	-0.000047
18	C	-4.373433	-0.389968	0.000138
19	H	-4.504602	0.243914	-0.889571
20	H	-5.148294	-1.165607	0.000256
21	H	-4.504325	0.243919	0.889884
22	H	3.829159	1.437512	-0.000009
23	H	1.697385	2.797828	-0.000054

## Solution phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	1.978247	-0.301477	-0.000621
2	C	0.80322	-1.025532	-0.001303
3	C	-0.426571	-0.343281	-0.001035
4	C	-0.423139	1.093447	-0.000706
5	C	0.785299	1.867945	-0.000574
6	C	1.958693	1.116923	-0.000082
7	H	0.822534	-2.109326	-0.001609
8	C	-1.699722	1.703183	-0.000113
9	H	2.915366	1.628674	0.000354
10	C	-2.847254	0.951045	0.000465
11	C	-2.745379	-0.462099	0.000295
12	N	-1.582544	-1.084994	-0.000546
13	C	-3.996736	-1.300833	0.00146
14	H	-4.610012	-1.087244	0.879781
15	H	-4.612468	-1.086184	-0.874866
16	H	-3.745355	-2.358941	0.000529
17	O	3.131979	-1.049115	-0.000684
18	C	4.389095	-0.384095	0.001701
19	H	4.513939	0.234515	0.892742
20	H	5.141529	-1.168898	0.001649
21	H	4.516226	0.236615	-0.887562
22	H	-3.825688	1.419088	0.001189
23	H	-1.748622	2.788228	0.00016

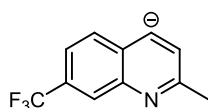


## Gas phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-1.457874	0.11661	-0.000139
2	C	-0.381157	-0.740997	-0.000134
3	C	0.941671	-0.226798	-0.000089
4	C	1.135248	1.18809	-0.000043
5	C	0.003494	2.044758	-0.000061
6	C	-1.268145	1.523413	-0.00011
7	H	-0.511153	-1.816763	-0.000169
8	C	2.475364	1.655388	0.000012
9	H	0.155703	3.121323	-0.000048
10	H	-2.133166	2.179247	-0.000161
11	C	3.503352	0.74787	0.000022
12	C	3.212305	-0.649801	-0.000027
13	H	2.670749	2.725307	0.000046
14	H	4.538521	1.078162	0.000066
15	N	1.977191	-1.117049	-0.000086
16	C	4.338558	-1.652992	0.000001
17	H	4.978857	-1.527722	-0.882263
18	H	4.978544	-1.528006	0.882535
19	H	3.931451	-2.665937	-0.000224
20	C	-2.867958	-0.407664	0.000054
21	F	-2.921864	-1.754801	-0.001206
22	F	-3.55291	0.024489	1.085593
23	F	-3.554002	0.026587	-1.083954

## Solution phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-1.450132	0.120099	-0.001356
2	C	-0.381814	-0.741171	-0.0021
3	C	0.937163	-0.231105	-0.001615
4	C	1.132917	1.176625	-0.000593
5	C	0.008532	2.035407	-0.000127
6	C	-1.261202	1.521956	-0.000394
7	H	-0.518643	-1.812701	-0.002668
8	C	2.469306	1.644828	0.000307
9	H	0.163498	3.10679	0.000789
10	H	-2.116776	2.183851	0.000076
11	C	3.493094	0.742687	0.000492
12	C	3.209041	-0.652578	-0.000292
13	H	2.663351	2.71029	0.001115
14	H	4.523425	1.072667	0.001505
15	N	1.976071	-1.116014	-0.001579
16	C	4.342322	-1.637656	0.001418
17	H	4.980487	-1.490168	-0.872536
18	H	4.97134	-1.496313	0.883054
19	H	3.964135	-2.656937	-0.003767
20	C	-2.856982	-0.401821	0.000182
21	F	-2.926124	-1.744988	-0.008671
22	F	-3.550415	0.01675	1.087419
23	F	-3.558658	0.031682	-1.075641

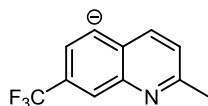


## Gas phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	1.434972	0.129655	-0.000022
2	C	0.348519	-0.723812	-0.000292
3	C	-0.975731	-0.210614	-0.000125
4	C	-1.1971	1.20926	0.000151
5	C	-0.040783	2.040551	0.000466
6	C	1.242091	1.536551	0.000399
7	H	0.478468	-1.801895	-0.000586
8	C	-2.51873	1.811448	-0.000019
9	H	-0.224434	3.113437	0.000711
10	H	2.106065	2.197317	0.00063
11	C	-3.491564	0.802969	-0.000318
12	C	-3.226308	-0.593642	-0.000186
13	H	-4.557413	1.075711	-0.000713
14	N	-2.003079	-1.114749	-0.000217
15	C	-4.369731	-1.591419	0.000528
16	H	-5.008928	-1.466173	0.8859
17	H	-5.018038	-1.457182	-0.876785
18	H	-3.976971	-2.612787	-0.006301
19	C	2.831184	-0.396255	-0.000123
20	F	3.548772	0.023079	1.0831
21	F	2.902508	-1.750686	-0.000632
22	F	3.548928	0.023903	-1.082922

## Solution phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	1.429432	0.1309	-0.006276
2	C	0.349537	-0.718754	-0.008922
3	C	-0.966718	-0.199529	-0.005208
4	C	-1.177196	1.212825	-0.002314
5	C	-0.026328	2.044123	0.004137
6	C	1.246919	1.532391	0.002372
7	H	0.48063	-1.791872	-0.013149
8	C	-2.504053	1.772508	-0.00483
9	H	-0.178819	3.116473	0.012979
10	H	2.104213	2.192249	0.007541
11	C	-3.490291	0.799039	-0.002366
12	C	-3.229374	-0.599581	-0.000506
13	H	-4.541488	1.082058	-0.001765
14	N	-2.003091	-1.091771	-0.004014
15	C	-4.375921	-1.576741	0.008089
16	H	-5.002381	-1.427638	0.890662
17	H	-5.017049	-1.430634	-0.863512
18	H	-4.013222	-2.602585	0.009532
19	C	2.827253	-0.402565	-0.000874
20	F	3.509974	-0.044707	1.119772
21	F	2.891629	-1.746097	-0.071354
22	F	3.563975	0.072653	-1.038862

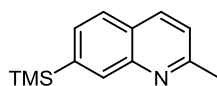


## Gas phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-1.439379	0.146768	-0.000011
2	C	-0.375478	-0.738752	-0.000009
3	C	0.93659	-0.212573	-0.000005
4	C	1.096878	1.220943	-0.000001
5	C	0.020305	2.188694	-0.000003
6	C	-1.231891	1.556175	-0.000009
7	H	-0.511973	-1.81482	-0.000012
8	C	2.446084	1.668644	0.000005
9	H	-2.142989	2.16681	-0.000015
10	C	3.497145	0.778622	0.000006
11	C	3.215629	-0.61563	0.000001
12	H	4.532054	1.119458	0.000011
13	N	1.98716	-1.101577	-0.000005
14	C	4.351304	-1.617945	0.000001
15	H	4.996311	-1.500039	-0.882431
16	H	4.996311	-1.50004	0.882433
17	H	3.94209	-2.631752	0
18	C	-2.84153	-0.376018	0.000001
19	H	2.600171	2.746576	0.000009
20	F	-2.928137	-1.735665	-0.000086
21	F	-3.556786	0.041719	1.084067
22	F	-3.556859	0.041864	-1.08396

## Solution phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-1.439256	0.145044	-0.004609
2	C	-0.377455	-0.726371	-0.003285
3	C	0.932737	-0.200859	-0.001566
4	C	1.106196	1.21982	-0.000758
5	C	0.012403	2.152564	0.001332
6	C	-1.241053	1.551761	-0.001965
7	H	-0.51301	-1.798402	-0.004164
8	C	2.455006	1.66245	0.000675
9	H	-2.137854	2.167079	-0.000162
10	C	3.489764	0.767856	0.000451
11	C	3.211631	-0.624395	-0.000671
12	H	4.518425	1.103913	0.001283
13	N	1.978005	-1.088148	-0.002162
14	C	4.347832	-1.610156	0.001789
15	H	4.990043	-1.462222	-0.868867
16	H	4.974435	-1.475224	0.88606
17	H	3.97243	-2.630574	-0.008409
18	C	-2.8416	-0.378542	-0.000428
19	H	2.645831	2.728441	0.001511
20	F	-3.56293	0.063319	-1.065808
21	F	-2.923618	-1.726072	-0.024436
22	F	-3.539404	0.021532	1.097142

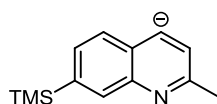


## Gas phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-1.106891	-0.264099	0.000032
2	C	-0.042315	0.624198	-0.000028
3	C	1.307896	0.183514	-0.000029
4	C	1.576852	-1.218629	0.000035
5	C	0.487357	-2.126791	0.000098
6	C	-0.807737	-1.661728	0.000096
7	H	-0.196542	1.699682	-0.000008
8	C	2.938655	-1.61624	0.000032
9	H	0.691876	-3.195642	0.000147
10	H	-1.622176	-2.383781	0.000145
11	C	3.919911	-0.657636	-0.000032
12	C	3.556123	0.722361	-0.000096
13	N	2.298705	1.125787	-0.000093
14	C	4.629511	1.78321	-0.000178
15	H	5.276016	1.693109	0.882108
16	H	5.275853	1.693129	-0.882586
17	H	4.169458	2.773418	-0.000129
18	Si	-2.908026	0.328136	0.000036
19	C	-3.779947	-0.338236	-1.545369
20	H	-3.747679	-1.433525	-1.588046
21	H	-4.835287	-0.038891	-1.562173
22	H	-3.310821	0.041053	-2.460732
23	C	-3.779847	-0.337933	1.545627
24	H	-3.310667	0.041538	2.460887
25	H	-4.835188	-0.038596	1.562438
26	H	-3.747565	-1.433214	1.588516
27	C	-2.964731	2.218698	-0.000156
28	H	-2.475365	2.641144	-0.88551
29	H	-4.003745	2.570129	-0.000152
30	H	-2.475297	2.641332	0.88507
31	H	4.970868	-0.934327	-0.000035
32	H	3.188672	-2.675117	0.000081

## Solution phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-1.103154	-0.254098	-0.000321
2	C	-0.043425	0.631843	-0.000383
3	C	1.302623	0.191829	-0.000216
4	C	1.570222	-1.204369	-0.000095
5	C	0.484077	-2.110478	-0.000144
6	C	-0.806948	-1.647576	-0.000247
7	H	-0.203126	1.703445	-0.000508
8	C	2.926213	-1.607488	0.000093
9	H	0.689293	-3.177056	-0.000108
10	H	-1.616487	-2.371045	-0.00027
11	C	3.908415	-0.6581	0.000199
12	C	3.555724	0.719578	0.000049
13	N	2.301972	1.124178	-0.000194
14	C	4.639636	1.761546	0.000106
15	H	5.280975	1.654162	0.877492
16	H	5.281198	1.654049	-0.877108
17	H	4.208428	2.759459	-0.000019
18	Si	-2.908442	0.327443	0.000062
19	C	-3.765485	-0.347308	-1.537155
20	H	-3.772897	-1.433262	-1.572418
21	H	-4.817871	-0.055783	-1.550688
22	H	-3.300001	0.034214	-2.447636
23	C	-3.763478	-0.343687	1.539988
24	H	-3.296783	0.039909	2.448977
25	H	-4.815838	-0.052093	1.554221
26	H	-3.720848	-1.433658	1.577681
27	C	-2.981878	2.207184	-0.002171
28	H	-2.501096	2.630566	-0.885712
29	H	-4.022185	2.538942	-0.001965
30	H	-2.500077	2.632745	0.879769
31	H	4.955426	-0.941456	0.000375
32	H	3.171004	-2.665751	0.000193



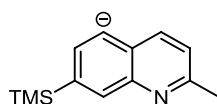
## Gas phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-1.078628	-0.277401	-0.000047
2	C	-0.006735	0.609762	-0.000026
3	C	1.3445	0.168286	-0.000016
4	C	1.639398	-1.23708	-0.00002
5	C	0.524045	-2.121696	-0.000055
6	C	-0.781448	-1.675618	-0.000068
7	H	-0.163295	1.688061	-0.000009
8	C	2.990351	-1.771699	0.000023
9	H	0.758988	-3.185527	-0.000063
10	H	-1.596664	-2.401374	-0.000096
11	C	3.910771	-0.71525	0.000046
12	C	3.573989	0.666282	0.000019
13	N	2.326187	1.124318	-0.000006
14	C	4.665712	1.72126	-0.000024
15	H	5.316221	1.625178	0.881024
16	H	5.315629	1.625709	-0.881573
17	H	4.22106	2.721353	0.000399
18	Si	-2.852295	0.313455	-0.000003
19	C	-3.782986	-0.326577	-1.534289
20	H	-3.742752	-1.4212	-1.59216
21	H	-4.840618	-0.030642	-1.525484
22	H	-3.330775	0.063962	-2.45397
23	C	-3.782592	-0.326103	1.534723
24	H	-3.330372	0.065077	2.454127
25	H	-4.840347	-0.030611	1.525963
26	H	-3.741884	-1.420681	1.593128
27	C	-2.955455	2.210904	-0.000304
28	H	-2.465825	2.637442	-0.883627
29	H	-3.999976	2.549125	-0.000351
30	H	-2.465831	2.637689	0.882904
31	H	4.989739	-0.932577	0.000103

## Solution phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-1.080258	-0.268658	-0.000165
2	C	-0.009094	0.605387	-0.000564
3	C	1.33601	0.157321	-0.000486
4	C	1.619878	-1.242659	-0.000397
5	C	0.504991	-2.121488	-0.000153
6	C	-0.789983	-1.661689	0.000018
7	H	-0.16297	1.679089	-0.000588
8	C	2.972893	-1.736116	0.000019
9	H	0.707475	-3.188631	0.000258
10	H	-1.602352	-2.382768	0.000405
11	C	3.909992	-0.713295	0.000426
12	C	3.576938	0.66893	0.000192
13	N	2.32886	1.100672	-0.000185
14	C	4.673562	1.704503	0.000216
15	H	5.315624	1.594192	0.877102
16	H	5.315974	1.593869	-0.876383
17	H	4.254287	2.708688	-0.000067
18	Si	-2.872963	0.327587	0.0001
19	C	-3.752048	-0.332552	-1.534081
20	H	-3.720331	-1.422969	-1.572362
21	H	-4.801649	-0.030354	-1.540821
22	H	-3.288351	0.045614	-2.447052
23	C	-3.750771	-0.329797	1.536181
24	H	-3.286329	0.050025	2.448086
25	H	-4.800385	-0.02765	1.543249
26	H	-3.718945	-1.420144	1.576375
27	C	-2.941153	2.210119	-0.001626
28	H	-2.457554	2.631745	-0.884509
29	H	-3.979969	2.54708	-0.001618
30	H	-2.456998	2.633417	0.880155
31	H	4.976192	-0.942162	0.000192

Negative frequency at -16.39 associated with Si(CH<sub>3</sub>)<sub>3</sub> rotational mode



## Gas phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-1.076639	-0.273046	0.000039
2	C	-0.02574	0.641229	0.00004
3	C	1.310635	0.176572	0.000033
4	C	1.536168	-1.24839	0.000068
5	C	0.501126	-2.260538	0.00007
6	C	-0.774884	-1.675749	0.000054
7	H	-0.183706	1.718383	0.000037
8	C	2.903404	-1.635599	0.000079
9	H	-1.649001	-2.346742	0.000085
10	C	3.915009	-0.700067	0.000034
11	C	3.571445	0.680051	0.000029
12	N	2.322333	1.110895	0.000019
13	C	4.661506	1.73239	-0.000134
14	H	5.312053	1.644338	0.882004
15	H	5.311448	1.644693	-0.88276
16	H	4.206853	2.726816	0.000208
17	Si	-2.860922	0.296435	-0.000067
18	C	-3.784219	-0.353454	-1.53542
19	H	-3.711207	-1.445776	-1.595594
20	H	-4.849366	-0.084662	-1.52332
21	H	-3.343848	0.052583	-2.454416
22	C	-3.784296	-0.352793	1.535528
23	H	-3.344003	0.053759	2.454335
24	H	-4.849424	-0.083939	1.523167
25	H	-3.711371	-1.445079	1.596351
26	C	-3.010268	2.196017	-0.000214
27	H	-2.529647	2.633493	-0.883604
28	H	-4.061617	2.513737	0.000043
29	H	-2.529231	2.633453	0.882973
30	H	4.964158	-0.995107	-0.000009
31	H	3.105007	-2.706042	0.000056

## Solution phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-1.085828	-0.270199	0.000484
2	C	-0.03149	0.62327	-0.000309
3	C	1.305079	0.163248	-0.000397
4	C	1.546647	-1.249229	-0.000522
5	C	0.490677	-2.223683	-0.000171
6	C	-0.785887	-1.668809	0.001065
7	H	-0.188477	1.696107	-0.000789
8	C	2.912221	-1.630306	-0.000442
9	H	-1.643323	-2.343628	0.001851
10	C	3.90899	-0.690702	-0.000041
11	C	3.566242	0.685814	0.00005
12	N	2.313261	1.09455	-0.000218
13	C	4.655406	1.726129	0.000693
14	H	5.297357	1.620524	0.87814
15	H	5.29785	1.621143	-0.876473
16	H	4.226477	2.725565	0.000914
17	Si	-2.884592	0.306094	0.00012
18	C	-3.763206	-0.362914	-1.532193
19	H	-3.718669	-1.452762	-1.569678
20	H	-4.81596	-0.071697	-1.538137
21	H	-3.304646	0.019243	-2.446226
22	C	-3.761446	-0.353482	1.537518
23	H	-3.301908	0.034237	2.448709
24	H	-4.814227	-0.062342	1.542844
25	H	-3.716774	-1.443084	1.581538
26	C	-2.987172	2.189513	-0.005901
27	H	-2.509603	2.616717	-0.889529
28	H	-4.030912	2.511081	-0.006593
29	H	-2.508957	2.622622	0.874491
30	H	4.954034	-0.982263	0.000253
31	H	3.147779	-2.690533	-0.00047

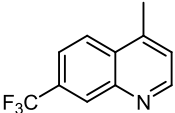
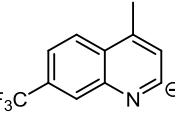
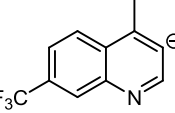
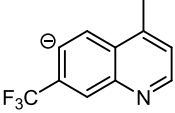
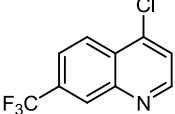
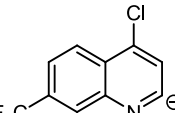
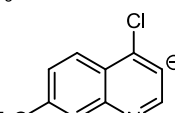
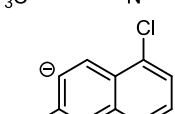
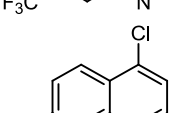
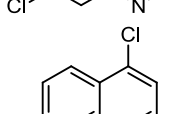
Negative frequency at -60.22 associated with Si(CH<sub>3</sub>)<sub>3</sub> rotational mode

### 1.3 4,7-disubstituted Quinolines

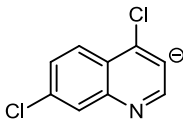
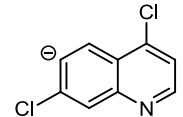
The following methods were utilised for the optimisation and frequency calculation:

Optimisation (gas phase)	Frequency (gas phase)	Optimisation + Frequency (solution phase)
B3LYP/6-31G(g)	B3LYP/6-311++G(2df,2p)	B3LYP/6-311++G(2df,2p) scrf=(iefpcm,solvent=dms) (tsnum=60, tsare=0.4, radii=bondi, alpha=1.20)

Frequency (gas phase)

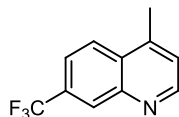
Compound	$E_{\text{PCM}}$	E	$G_{(\text{gas})}$	$\Delta_{\text{solv}}G$ (kcal/mol)
	-778.558118	-778.554351419	-778.425354	-2.36
	-778.007776	-777.919605635	-777.806429	-55.28
	-778.011277	-777.933161332	-777.819361	-48.98
	-778.015850	-777.932765289	-777.818715	-52.09
	-1198.852551	-1198.848461820	-1198.757314	-2.56
	-1198.309249	-1198.228356360	-1198.153231	-50.72
	-1198.322467	-1198.247618080	-1198.171522	-46.93
	-1198.308343	-1198.233858150	-1198.157617	-46.70
	-1321.315271	-1321.309588410	-1321.228975	-3.56
	-1320.770563	-1320.685317650	-1320.620113	-53.45

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	-1320.783390	-1320.703636640-1320.638036	-50.01
	-1320.778536	-1320.695912170-1320.630764	-51.81

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## 1.4 Optimised Geometry Cartesian coordinates

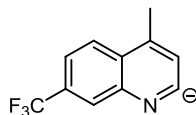


## Gas phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	1.35934	-0.097346	-0.000099
2	C	0.544737	1.010732	-0.000121
3	C	-0.867577	0.865442	0.000004
4	C	-1.438347	-0.446998	0.000049
5	C	-0.563493	-1.567848	0.000209
6	C	0.800904	-1.401051	0.000136
7	H	0.94965	2.015903	-0.000155
8	C	-2.864833	-0.56001	-0.000068
9	H	-0.978069	-2.570821	0.000448
10	C	-3.590038	0.612678	-0.000079
11	C	-2.925106	1.862969	0.000101
12	N	-1.616884	2.007144	0.000107
13	H	-3.513178	2.780414	0.000177
14	C	2.857659	0.035235	-0.000025
15	F	3.403642	-0.565102	-1.084481
16	F	3.403497	-0.563397	1.085366
17	F	3.265943	1.319461	-0.000958
18	H	-4.676497	0.588109	-0.00032
19	H	1.459071	-2.264481	0.000251
20	C	-3.547275	-1.903856	-0.000129
21	H	-3.27064	-2.494427	-0.882154
22	H	-3.271032	-2.494239	0.882155
23	H	-4.634684	-1.788791	-0.000362

## Solution phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-1.349355	-0.098143	0.000355
2	C	-0.542183	1.009315	0.000801
3	C	0.865505	0.864478	0.000695
4	C	1.434701	-0.442132	0.000239
5	C	0.564296	-1.560933	0.000173
6	C	-0.795367	-1.398826	0.000203
7	H	-0.951086	2.009189	0.001022
8	C	2.857469	-0.560304	-0.00021
9	H	0.976257	-2.559843	-0.000152
10	C	3.582829	0.60677	-0.000952
11	C	2.926942	1.8548	-0.000569
12	N	1.620913	1.999817	0.000764
13	H	3.518586	2.764559	-0.000801
14	C	-2.84392	0.035387	-0.000164
15	F	-3.40445	-0.558113	1.081776
16	F	-3.403693	-0.560115	-1.081421
17	F	-3.263621	1.313183	-0.001475
18	H	4.664473	0.58271	-0.001618
19	H	-1.444246	-2.264362	0.00017
20	C	3.534612	-1.8994	0.000238
21	H	3.253153	-2.48394	0.87851
22	H	3.252827	-2.484889	-0.877246
23	H	4.616333	-1.782813	-0.000003

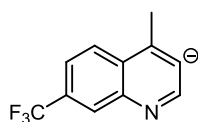


## Gas phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	1.327914	-0.102097	-0.000069
2	C	0.508779	1.010385	-0.000073
3	C	-0.909427	0.895543	-0.000028
4	C	-1.472611	-0.425769	0.000004
5	C	-0.605553	-1.548857	0.000024
6	C	0.765818	-1.404484	-0.000024
7	H	0.914202	2.017226	-0.000106
8	C	-2.90092	-0.504777	-0.000057
9	H	-1.031394	-2.550514	0.000028
10	C	-3.583884	0.691156	-0.000332
11	C	-3.007713	2.039958	-0.00005
12	N	-1.63808	2.052675	0.000118
13	C	2.814656	0.025241	0.000036
14	F	3.390225	-0.576264	-1.082953
15	F	3.389995	-0.575044	1.083823
16	F	3.249778	1.307148	-0.000063
17	H	-4.679765	0.627495	-0.000632
18	H	1.416146	-2.275591	-0.000042
19	C	-3.607636	-1.842051	0.000115
20	H	-3.352362	-2.449261	-0.881042
21	H	-3.352678	-2.448856	0.881645
22	H	-4.69411	-1.697265	-0.000108

## Solution phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	1.318084	-0.09739	-0.00015
2	C	0.516358	1.017698	-0.00029
3	C	-0.89511	0.895792	-0.00022
4	C	-1.46647	-0.40866	-0.00017
5	C	-0.60897	-1.53649	-0.00032
6	C	0.75483	-1.3935	0.000051
7	H	0.93848	2.012873	-0.00024
8	C	-2.89095	-0.49801	0.000279
9	H	-1.03297	-2.53094	-0.00017
10	C	-3.58741	0.685812	0.001108
11	C	-2.99031	1.998123	0.000635
12	N	-1.64106	2.046191	-0.00056
13	C	2.810252	0.022478	0.000082
14	F	3.373043	-0.58247	-1.07898
15	F	3.372128	-0.574	1.084361
16	F	3.249006	1.294998	-0.0048
17	H	-4.67219	0.627521	0.000177
18	H	1.394252	-2.2658	0.000908
19	C	-3.58935	-1.83095	-0.00078
20	H	-3.32446	-2.42177	-0.88053
21	H	-3.31937	-2.42594	0.874576
22	H	-4.66967	-1.69553	0.002492

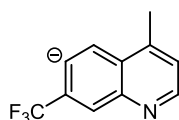


## Gas phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	1.32677	-0.106256	-0.034521
2	C	0.50631	1.006895	-0.025006
3	C	-0.9034	0.878777	-0.013032
4	C	-1.497331	-0.429796	-0.00583
5	C	-0.615372	-1.550402	-0.015173
6	C	0.754182	-1.404375	-0.028813
7	H	0.91634	2.011758	-0.030064
8	C	-2.92748	-0.508834	0.007689
9	H	-1.037965	-2.551933	-0.015223
10	C	-3.752902	0.626331	0.014818
11	C	-2.972525	1.838156	0.005631
12	N	-1.651592	2.020262	-0.008084
13	H	-3.516953	2.794119	0.010179
14	C	2.810628	0.026873	0.002612
15	F	3.43156	-0.811394	-0.877365
16	F	3.34164	-0.28574	1.2224
17	F	3.246324	1.278289	-0.284615
18	H	1.403425	-2.276542	-0.043176
19	C	-3.578934	-1.883796	0.015001
20	H	-3.318154	-2.486719	-0.870412
21	H	-3.298251	-2.486784	0.894182
22	H	-4.662691	-1.737567	0.027061

## Solution phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	1.312368	-0.101886	-0.026531
2	C	0.507757	1.010403	-0.016187
3	C	-0.900039	0.876647	-0.007485
4	C	-1.489415	-0.421913	-0.00482
5	C	-0.617395	-1.544405	-0.015581
6	C	0.745434	-1.397047	-0.025256
7	H	0.925908	2.006965	-0.016593
8	C	-2.919009	-0.515379	0.009092
9	H	-1.03198	-2.542291	-0.018152
10	C	-3.717111	0.627426	0.005485
11	C	-2.972926	1.845997	-0.00033
12	N	-1.655735	2.009433	-0.003392
13	H	-3.51794	2.790293	0.002627
14	C	2.80201	0.028047	-0.000365
15	F	3.407484	-0.784326	-0.902366
16	F	3.32743	-0.315702	1.207796
17	F	3.23541	1.278086	-0.256343
18	H	1.386146	-2.268402	-0.03465
19	C	-3.546676	-1.891697	0.015103
20	H	-3.293615	-2.460203	-0.884671
21	H	-3.212468	-2.490546	0.867146
22	H	-4.628811	-1.801519	0.067503

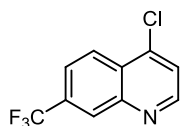


## Gas phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	1.338264	-0.171135	-0.000253
2	C	0.559891	0.973519	-0.000699
3	C	-0.851562	0.856421	-0.000596
4	C	-1.4161	-0.467382	-0.000449
5	C	-0.531355	-1.584834	-0.001274
6	C	0.868813	-1.53358	-0.001147
7	H	0.977607	1.97753	-0.00089
8	C	-2.845399	-0.559964	0.000224
9	H	-1.016087	-2.569166	-0.002169
10	C	-3.578926	0.61054	0.000382
11	C	-2.915351	1.859997	0.000128
12	N	-1.604598	2.000269	-0.000349
13	H	-3.505096	2.780212	0.000332
14	C	2.837794	-0.00412	0.000388
15	F	3.432173	-0.566708	-1.085085
16	F	3.431559	-0.568079	1.085385
17	F	3.250515	1.304648	0.001298
18	C	-3.538869	-1.900672	0.001023
19	H	-3.260522	-2.496616	-0.877435
20	H	-3.258219	-2.496536	0.878853
21	H	-4.628572	-1.779595	0.002482
22	H	-4.668358	0.580803	0.000524

## Solution phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-1.340582	-0.169372	-0.006182
2	C	-0.559751	0.965891	-0.00496
3	C	0.847167	0.847772	-0.001924
4	C	1.418114	-0.458436	-0.000314
5	C	0.542044	-1.580602	0.001358
6	C	-0.847003	-1.510523	-0.000471
7	H	-0.981563	1.962333	-0.006209
8	C	2.844125	-0.55977	0.000386
9	H	1.019493	-2.556219	0.004413
10	C	3.566721	0.610528	0.002536
11	C	2.906369	1.856171	0.002287
12	N	1.598337	1.990703	-0.000966
13	H	3.492874	2.769128	0.003927
14	C	-2.836337	-0.000446	-0.001553
15	F	-3.418051	-0.510691	1.117819
16	F	-3.442706	-0.627634	-1.042979
17	F	-3.247947	1.291462	-0.066213
18	C	3.537184	-1.892706	-0.002324
19	H	3.258261	-2.486745	0.87009
20	H	3.265632	-2.478164	-0.882967
21	H	4.618052	-1.765069	0.002727
22	H	4.648931	0.590522	0.004113

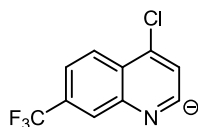


## Gas phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	1.612839	-0.100551	-0.000037
2	C	0.904722	1.077267	-0.000026
3	C	-0.515398	1.063964	-0.000011
4	C	-1.197044	-0.198213	-0.000006
5	C	-0.434371	-1.395913	-0.000012
6	C	0.938374	-1.34888	-0.000028
7	H	1.399888	2.040882	-0.000035
8	C	-2.618174	-0.139254	0.000003
9	H	-0.948032	-2.350733	-0.000008
10	C	-3.261779	1.074406	0.00001
11	C	-2.474138	2.251463	0.000001
12	N	-1.158007	2.266308	-0.000004
13	H	-2.972596	3.21975	0.000027
14	Cl	-3.56588	-1.61419	0.000007
15	C	3.118268	-0.104745	0.000007
16	F	3.604593	-0.751315	-1.084803
17	F	3.604547	-0.750527	1.085299
18	F	3.639219	1.13772	-0.000435
19	H	-4.344221	1.134888	0.00002
20	H	1.515953	-2.267883	-0.000046

## Solution phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-1.600884	-0.100008	-0.001848
2	C	-0.899003	1.075591	-0.00081
3	C	0.515991	1.060907	-0.000363
4	C	1.194355	-0.195426	-0.000569
5	C	0.434945	-1.389395	-0.001466
6	C	-0.9326	-1.345939	-0.0021
7	H	-1.395726	2.034629	-0.000735
8	C	2.611388	-0.13994	-0.000027
9	H	0.941409	-2.34334	-0.002173
10	C	3.256999	1.064687	-0.000042
11	C	2.479236	2.241876	-0.0003
12	N	1.166189	2.256565	-0.000052
13	H	2.983498	3.20195	-0.000177
14	Cl	3.547002	-1.611722	0.001042
15	C	-3.102923	-0.10133	0.000017
16	F	-3.60276	-0.721902	1.095111
17	F	-3.605531	-0.764841	-1.067986
18	F	-3.63292	1.133535	-0.023379
19	H	4.335453	1.128849	0.000764
20	H	-1.501119	-2.266035	-0.003692

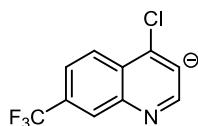


## Gas phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	1.58889	-0.10201	-0.000057
2	C	0.890739	1.087588	-0.000031
3	C	-0.532401	1.117906	-0.000013
4	C	-1.225116	-0.147988	-0.000013
5	C	-0.47963	-1.352367	-0.000038
6	C	0.897467	-1.340431	-0.00006
7	H	1.397733	2.046333	-0.000031
8	C	-2.638899	-0.036292	0.000004
9	H	-1.016245	-2.296118	-0.000048
10	C	-3.252499	1.17608	0.000018
11	C	-2.504072	2.445991	0.000022
12	N	-1.153013	2.330129	0.000005
13	Cl	-3.634777	-1.601115	0.000005
14	C	3.083154	-0.126271	0.000006
15	F	3.589648	-0.782414	-1.083003
16	F	3.589591	-0.781441	1.083633
17	F	3.642968	1.105514	-0.000519
18	H	-4.341818	1.221553	0.000027
19	H	1.456967	-2.271886	-0.0001

## Solution phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	1.576173	-0.100375	-0.001169
2	C	0.882434	1.083027	-0.00042
3	C	-0.533815	1.0935	-0.001095
4	C	-1.217911	-0.159232	-0.002245
5	C	-0.473162	-1.361396	-0.003626
6	C	0.896816	-1.339457	-0.003146
7	H	1.393146	2.035065	0.001283
8	C	-2.631315	-0.06664	-0.000271
9	H	-0.992912	-2.308344	-0.00496
10	C	-3.25314	1.144102	0.001109
11	C	-2.516632	2.389393	-0.001352
12	N	-1.172909	2.302558	-0.00078
13	Cl	-3.596431	-1.558487	0.001891
14	C	3.074459	-0.114236	0.000777
15	F	3.580211	-0.764818	-1.078176
16	F	3.577319	-0.75906	1.084623
17	F	3.621202	1.115368	-0.001723
18	H	-4.335912	1.180608	0.007393
19	H	1.453338	-2.266484	-0.004279

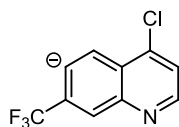


## Gas phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	1.578489	-0.105975	-0.020516
2	C	0.88239	1.086021	-0.014507
3	C	-0.53418	1.105503	-0.007169
4	C	-1.251806	-0.144568	-0.003619
5	C	-0.49983	-1.350946	-0.009141
6	C	0.876285	-1.338545	-0.017359
7	H	1.395694	2.0414	-0.017704
8	C	-2.663034	0.003511	0.003028
9	H	-1.039375	-2.29154	-0.009487
10	H	1.433293	-2.271908	-0.027544
11	C	-3.372576	1.150284	0.007383
12	C	-2.491984	2.285774	0.003839
13	N	-1.161652	2.316039	-0.003944
14	H	-2.936079	3.289375	0.006609
15	Cl	-3.610229	-1.655958	0.005399
16	C	3.071007	-0.131236	0.001469
17	F	3.587353	-0.952274	-0.956145
18	F	3.568563	-0.600155	1.18174
19	F	3.631125	1.08718	-0.189651

## Solution phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	1.566716	-0.098427	-0.00431
2	C	0.874634	1.085651	-0.005678
3	C	-0.539296	1.088211	-0.003697
4	C	-1.241609	-0.156484	-0.001448
5	C	-0.489095	-1.35712	-0.000909
6	C	0.880535	-1.334092	-0.00173
7	H	1.38521	2.037498	-0.006817
8	C	-2.656435	-0.03883	0.000882
9	H	-1.006069	-2.304729	0.00062
10	H	1.43544	-2.262438	-0.001205
11	C	-3.366039	1.116929	0.004319
12	C	-2.509428	2.26268	0.00319
13	N	-1.186058	2.285786	-0.002497
14	H	-2.96277	3.252268	0.005741
15	Cl	-3.575391	-1.623769	-0.000135
16	C	3.063789	-0.117766	0.000189
17	F	3.569468	-0.798804	-1.059852
18	F	3.563406	-0.735665	1.101583
19	F	3.614861	1.109631	-0.033221

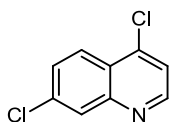


## Gas phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-1.591963	-0.174794	-0.001116
2	C	-0.922628	1.035318	-0.001396
3	C	0.493204	1.052153	-0.001003
4	C	1.173385	-0.224632	-0.000814
5	C	0.398159	-1.419843	-0.002268
6	C	-1.000022	-1.488332	-0.002467
7	H	-1.430298	1.996214	-0.001686
8	C	2.588676	-0.131679	0.00028
9	H	0.977409	-2.347792	-0.003565
10	C	3.241831	1.079048	0.000698
11	C	2.452594	2.252761	0.000225
12	N	1.134257	2.258189	-0.000588
13	H	2.94883	3.22522	0.000516
14	Cl	3.588048	-1.605939	0.001046
15	C	-3.101715	-0.143734	0.000477
16	F	-3.637576	-0.758529	1.086273
17	F	-3.640307	-0.757223	-1.084423
18	F	-3.62741	1.12313	0.001929
19	H	4.325949	1.136	0.00135

## Solution phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	1.588645	-0.169506	-0.002964
2	C	0.915724	1.031213	-0.005334
3	C	-0.496065	1.042789	-0.002699
4	C	-1.176143	-0.215411	-0.001312
5	C	-0.409833	-1.412505	0.001215
6	C	0.978853	-1.46246	0.001622
7	H	1.422786	1.989042	-0.006913
8	C	-2.591279	-0.137591	0.001493
9	H	-0.979004	-2.337828	0.000787
10	C	-3.23647	1.068702	0.004602
11	C	-2.453619	2.242387	0.001842
12	N	-1.14001	2.244933	-0.002129
13	H	-2.952923	3.208442	0.005466
14	Cl	-3.555461	-1.60445	-0.001707
15	C	3.095141	-0.135161	0.000181
16	F	3.635898	-0.773573	-1.069959
17	F	3.630008	-0.737054	1.094468
18	F	3.618576	1.116581	-0.019491
19	H	-4.317994	1.133143	0.00754

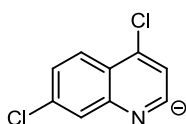


## Gas phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-0.877845	-2.0164	0
2	C	0.473888	-1.771581	0
3	C	0.948532	-0.433458	0
4	C	0	0.644493	0
5	C	-1.385545	0.341864	0
6	C	-1.822121	-0.962475	0
7	H	1.203999	-2.572345	0
8	C	0.546858	1.956723	0
9	H	-2.881848	-1.193043	0
10	C	1.907912	2.142785	0
11	C	2.738997	0.996083	0
12	N	2.299211	-0.244487	0
13	Cl	-0.511022	3.355957	0
14	Cl	-1.468615	-3.669505	0
15	H	3.820023	1.128916	0
16	H	2.338803	3.137483	0
17	H	-2.105672	1.152501	0

## Solution phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-0.867608	-2.008879	0
2	C	0.478028	-1.766114	0
3	C	0.947368	-0.431143	0
4	C	0	0.639662	0
5	C	-1.380783	0.334659	0
6	C	-1.813841	-0.965045	0
7	H	1.201526	-2.568492	0
8	C	0.53913	1.949681	0
9	H	-2.869956	-1.1933	0
10	C	1.892131	2.145972	0
11	C	2.729399	1.011562	0
12	N	2.293876	-0.228039	0
13	Cl	-0.523281	3.335278	0
14	Cl	-1.450313	-3.660759	0
15	H	3.804358	1.155071	0
16	H	2.319975	3.137517	0
17	H	-2.104887	1.136534	0

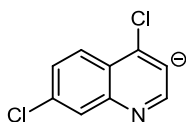


## Gas phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-0.71575	-2.04594	0
2	C	0.61823	-1.72289	0
3	C	1.030559	-0.35713	0
4	C	0	0.654109	0
5	C	-1.35873	0.264805	0
6	C	-1.72934	-1.06591	0
7	H	1.398163	-2.47657	0
8	C	0.492398	1.985218	0
9	H	-2.77402	-1.35943	0
10	C	1.824114	2.248382	0
11	C	2.840899	1.180793	0
12	N	2.365647	-0.08897	0
13	Cl	-0.74551	3.36843	0
14	Cl	-1.20982	-3.76313	0
15	H	2.165289	3.283635	0
16	H	-2.12264	1.036432	0

## Solution phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-0.743174	-2.030835	0
2	C	0.590093	-1.722347	0
3	C	1.004381	-0.367064	0
4	C	0	0.649133	0
5	C	-1.36347	0.280448	0
6	C	-1.740784	-1.03977	0
7	H	1.347445	-2.493411	0
8	C	0.493901	1.976324	0
9	H	-2.784476	-1.317707	0
10	C	1.831434	2.227498	0
11	C	2.812788	1.164798	0
12	N	2.346715	-0.098783	0
13	Cl	-0.659872	3.328915	0
14	Cl	-1.243199	-3.718918	0
15	H	2.174513	3.254902	0
16	H	-2.123295	1.048655	0

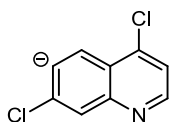


## Gas phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-0.679362	-2.046824	0
2	C	0.650454	-1.701968	0
3	C	1.027041	-0.331902	0
4	C	0	0.679823	0
5	C	-1.355298	0.260617	0
6	C	-1.701677	-1.075512	0
7	H	1.438173	-2.447327	0
8	C	0.504126	2.007424	0
9	H	-2.128506	1.021072	0
10	H	-2.742512	-1.384308	0
11	C	1.79098	2.402879	0
12	C	2.664359	1.263673	0
13	N	2.356001	-0.032446	0
14	Cl	-1.144462	-3.767686	0
15	H	3.748319	1.436708	0
16	Cl	-0.867963	3.347198	0

## Solution phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-0.679362	-2.046824	0
2	C	0.650454	-1.701968	0
3	C	1.027041	-0.331902	0
4	C	0	0.679823	0
5	C	-1.355298	0.260617	0
6	C	-1.701677	-1.075512	0
7	H	1.438173	-2.447327	0
8	C	0.504126	2.007424	0
9	H	-2.128506	1.021072	0
10	H	-2.742512	-1.384308	0
11	C	1.79098	2.402879	0
12	C	2.664359	1.263673	0
13	N	2.356001	-0.032446	0
14	Cl	-1.144462	-3.767686	0
15	H	3.748319	1.436708	0
16	Cl	-0.867963	3.347198	0



## Gas phase

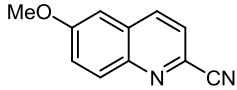
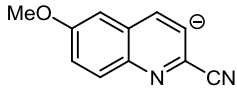
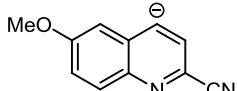
Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-1.085712	-1.859806	0
2	C	0.288983	-1.794019	0
3	C	0.883741	-0.507066	0
4	C	0	0.640659	0
5	C	-1.40887	0.422835	0
6	C	-2.02185	-0.83334	0
7	H	0.941185	-2.66229	0
8	C	0.662858	1.891093	0
9	H	-2.025388	1.325698	0
10	C	2.035729	1.991732	0
11	C	2.780566	0.790283	0
12	N	2.246546	-0.4154	0
13	Cl	-1.717913	-3.642738	0
14	H	3.870966	0.843867	0
15	Cl	-0.273679	3.406824	0
16	H	2.531814	2.956837	0

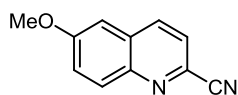
## Solution phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-1.035679	-1.901041	0
2	C	0.331095	-1.787127	0
3	C	0.892132	-0.490132	0
4	C	0	0.629253	0
5	C	-1.401475	0.3908	0
6	C	-1.984266	-0.872854	0
7	H	0.995611	-2.640057	0
8	C	0.620972	1.901686	0
9	H	-2.035264	1.271207	0
10	C	1.983708	2.026853	0
11	C	2.758391	0.849471	0
12	N	2.250184	-0.363423	0
13	Cl	-1.644684	-3.622846	0
14	H	3.839383	0.932428	0
15	Cl	-0.35566	3.35848	0
16	H	2.465554	2.99315	0

## 1.5 6-methoxyquinoline-2-carbonitrile

Optimisation (gas phase)	Frequency (gas phase)	Optimisation + Frequency (solution phase)
B3LYP/6-31G(g)	B3LYP/6-311++G(2df,2p)	B3LYP/6-311++G(2df,2p) scrf=(iefpcm,solvent=dms) (tsnum=60, tsare=0.4, radii=bondi, alpha=1.20)

Compound	$E_{\text{PCM}}$	E	$G_{(\text{gas})}$	$\Delta_{\text{solv}}G$ (kcal/mol)
	-608.900824	-608.889413540	-608.760202	-7.15
	-608.366231	-608.276715283	-608.162407	-56.13
	-608.363298	-608.279357538	-608.165597	-52.63

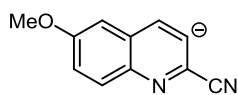


## Gas phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-1.950157	-1.204933	-0.000071
2	C	-0.618646	-1.551749	-0.000035
3	C	0.394844	-0.559378	-0.000004
4	C	0.003258	0.821826	-0.000028
5	C	-1.366006	1.157703	-0.000088
6	C	-2.33326	0.165532	-0.000065
7	H	-2.704402	-1.983329	-0.000156
8	H	-0.308215	-2.591616	-0.000044
9	C	1.044611	1.788762	-0.000009
10	H	-1.679426	2.197413	-0.000112
11	C	2.353032	1.377001	0.000027
12	C	2.625389	-0.02178	0.000015
13	H	0.794353	2.846501	-0.000005
14	H	3.175125	2.084754	0.000063
15	N	1.693072	-0.960706	0.000029
16	C	4.000476	-0.463104	0.000057
17	O	-3.626363	0.586236	0.000049
18	C	-4.668512	-0.381191	0.00009
19	H	-4.632483	-1.013737	0.896015
20	H	-5.598857	0.188835	-0.000054
21	H	-4.632264	-1.014027	-0.895626
22	N	5.119342	-0.778841	-0.000002

## Solution phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	1.942343	-1.197871	-0.000985
2	C	0.618251	-1.547678	-0.000293
3	C	-0.39427	-0.559588	-0.000043
4	C	-0.008121	0.819346	-0.000195
5	C	1.355612	1.158156	-0.000682
6	C	2.321048	0.17105	-0.001161
7	H	2.693398	-1.973317	-0.002137
8	H	0.324029	-2.588565	0.000004
9	C	-1.042546	1.785841	0.000349
10	H	1.655305	2.197904	-0.000429
11	C	-2.348803	1.381205	0.000722
12	C	-2.618233	-0.008951	0.00058
13	H	-0.793072	2.839094	0.000726
14	H	-3.163401	2.091353	0.001262
15	N	-1.691091	-0.949175	0.00027
16	C	-3.984194	-0.461692	0.000827
17	O	3.609515	0.582884	-0.002068
18	C	4.661357	-0.390089	0.001227
19	H	4.618691	-1.01528	-0.89139
20	H	5.585313	0.180248	0.002026
21	H	4.615474	-1.012492	0.895603
22	N	-5.084127	-0.805166	0.000987

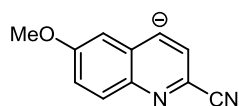


## Gas phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	1.918185	-1.204835	-0.000285
2	C	0.578099	-1.537515	-0.00036
3	C	-0.434159	-0.544999	-0.000237
4	C	-0.047644	0.838005	-0.000115
5	C	1.335604	1.154545	0.000014
6	C	2.296567	0.163916	-0.000198
7	H	2.66801	-1.989269	-0.000325
8	H	0.261106	-2.577504	-0.000408
9	C	-1.092559	1.804831	-0.000116
10	H	1.651569	2.195965	0.000247
11	C	-2.456658	1.501921	-0.000082
12	C	-2.630976	0.071216	-0.000011
13	N	-1.738107	-0.928368	-0.000177
14	C	-4.011306	-0.407315	0.000223
15	O	3.617323	0.586735	-0.000038
16	C	4.626725	-0.395088	0.0006
17	H	4.583782	-1.038067	-0.891547
18	H	5.57811	0.145274	0.000461
19	H	4.583455	-1.037286	0.893319
20	N	-5.11819	-0.773783	0.000504
21	H	-0.761804	2.853973	-0.000323

## Solution phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	1.918185	-1.204835	-0.000285
2	C	0.578099	-1.537515	-0.00036
3	C	-0.434159	-0.544999	-0.000237
4	C	-0.047644	0.838005	-0.000115
5	C	1.335604	1.154545	0.000014
6	C	2.296567	0.163916	-0.000198
7	H	2.66801	-1.989269	-0.000325
8	H	0.261106	-2.577504	-0.000408
9	C	-1.092559	1.804831	-0.000116
10	H	1.651569	2.195965	0.000247
11	C	-2.456658	1.501921	-0.000082
12	C	-2.630976	0.071216	-0.000011
13	N	-1.738107	-0.928368	-0.000177
14	C	-4.011306	-0.407315	0.000223
15	O	3.617323	0.586735	-0.000038
16	C	4.626725	-0.395088	0.0006
17	H	4.583782	-1.038067	-0.891547
18	H	5.57811	0.145274	0.000461
19	H	4.583455	-1.037286	0.893319
20	N	-5.11819	-0.773783	0.000504
21	H	-0.761804	2.853973	-0.000323



## Gas phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-1.93709	-1.179803	0.000078
2	C	-0.606557	-1.52579	0.000017
3	C	0.408191	-0.541412	-0.000003
4	C	0.046169	0.847875	0.000028
5	C	-1.334149	1.160893	0.000089
6	C	-2.302557	0.18526	0.000115
7	H	-2.68811	-1.95668	0.000098
8	H	-0.305821	-2.566324	-0.000012
9	C	1.027817	1.902218	0.000005
10	H	-1.613538	2.206218	0.000119
11	C	2.323582	1.397144	-0.000058
12	C	2.608944	0.006723	-0.000092
13	H	3.183985	2.063304	-0.000101
14	N	1.70227	-0.957705	-0.000069
15	C	3.988155	-0.424402	-0.000178
16	O	-3.619217	0.612008	0.000191
17	C	-4.639645	-0.356371	0.000091
18	H	-4.601453	-0.994521	0.889526
19	H	-5.580331	0.191454	0.000103
20	H	-4.601395	-0.99439	-0.889435
21	N	5.106765	-0.710742	-0.000272

## Solution phase

Number	Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-1.935701	-1.179346	0.000349
2	C	-0.607562	-1.523804	-0.001822
3	C	0.405624	-0.535772	-0.00177
4	C	0.042519	0.853283	-0.000662
5	C	-1.336296	1.1668	0.001451
6	C	-2.30691	0.187318	0.001953
7	H	-2.686092	-1.955351	0.000885
8	H	-0.314964	-2.566113	-0.003065
9	C	1.03494	1.895351	-0.001847
10	H	-1.631249	2.208512	0.002722
11	C	2.334146	1.404594	-0.002482
12	C	2.615066	0.014053	-0.001608
13	H	3.192435	2.070915	-0.002953
14	N	1.702621	-0.944647	-0.00184
15	C	3.986548	-0.42522	0.001118
16	O	-3.605769	0.607186	0.003828
17	C	-4.652338	-0.366766	-0.001124
18	H	-4.614697	-0.990523	0.893123
19	H	-5.580116	0.197387	-0.010508
20	H	-4.601432	-0.995324	-0.891296
21	N	5.097673	-0.736775	0.004573