NSC	Name	Index of atom H	Index of atom O
4960	4-methoxyphenol	14	7
70955	3,5-dimethoxyphenol	15	7
53558	2-kyanophenol	14	9
400524	4-kyanofenol	14	9
60108	3-kyanofenol	14	9

Table 6.3.: Information about selected phenol molecules

NSC of molecule:	4960	70955	53558	400524	60108
	H(14)	H(15)	H(14)	H(14)	H(14)
Ab-initio	**0.2020**	**0.2071**	**0.2179**	**0.2136**	**0.2115**
Yang 1994 (1a)	0.0617	0.063	0.0735	0.0703	0.0707
Bakowies 1995 (1b)	0.0621	0.0659	0.072	0.0703	0.0705
Bakowies 1995 (2b)	0.0931	0.097	0.1058	0.1037	0.1041
Bakowies 1995 (3b)	0.0756	0.0799	0.0804	0.0792	0.0794
Bakowies 1995 (4b)	-0.0272	-0.0244	-0.034	-0.0335	-0.0336
Yang 1996 (1c)	0.1844	0.1844	0.1954	0.1909	0.1914
Njo 1998 (1d)	0.0547	0.0585	0.0615	0.0607	0.0608
Njo 1998 (2d)	0.0466	0.0482	0.0542	0.053	0.0532
Njo 1998 (3d)	0.0467	0.0483	0.0543	0.053	0.0532
Njo 1998 (4d)	0.0479	0.0498	0.0549	0.0539	0.054
Njo 1998 (5d)	0.0536	0.0568	0.0636	0.0622	0.0625
Bultinck 2002 (1e)	0.1149	0.1195	0.124	0.1231	0.1233
Bultinck 2002 (1f)	0.0879	0.0966	0.0875	0.0868	0.087
Bultinck 2002 (2f)	0.095	0.1024	0.095	0.0944	0.0945
Bultinck 2002 (3f)	0.1794	0.1855	0.193	0.1917	0.192
Bultinck 2002 (4f)	0.0444	0.0488	0.0422	0.0421	0.0421
Bultinck 2004 (1g)	0.0941	0.1086	0.0932	0.0923	0.0925
Bultinck 2004 (2g)	0.0453	0.0473	0.0558	0.055	0.0551
Bultinck 2004 (3g)	0.0498	0.0528	0.0582	0.0573	0.0574
Bultinck 2004 (4g)	0.0341	0.0372	0.0367	0.0364	0.0364
Vařeková 2007 (1h)	0.1895	0.1901	0.2032	0.1985	0.1991
Vařeková 2007 (2h)	0.1841	0.1843	0.1979	0.1933	0.194
Vařeková 2007 (3h)	0.1951	0.1953	0.2082	0.2036	0.2043
Vařeková 2007 (4h)	0.1881	0.188	0.2027	0.1977	0.1984
Ouyang 2009 (1i)	0.4124	0.4131	0.4397	0.4287	0.4301
Ouyang 2009 (2i)	0.7568	0.7643	0.8605	0.8033	0.8072

Table 6.4.: Atomic charges of atom H calculated via EEM method on sample molecules from table 6.3 using parameters from publications

NSC of molecule:	4960	70955	53558	400524	60108
	O(7)	O(7)	O(9)	O(9)	O(9)
Ab-initio	**-0.3095**	**-0.3082**	**-0.2999**	**-0.3032**	**-0.3033**
Yang 1994 (1a)	-0.1511	-0.1498	-0.1377	-0.1419	-0.1414
Bakowies 1995 (1b)	-0.2207	-0.2174	-0.2119	-0.2136	-0.2133
Bakowies 1995 (2b)	-0.2555	-0.2523	-0.2449	-0.2469	-0.2466
Bakowies 1995 (3b)	-0.2636	-0.2591	-0.2585	-0.26	-0.2598
Bakowies 1995 (4b)	-0.0627	-0.0598	-0.0698	-0.0691	-0.0692
Yang 1996 (1c)	-0.3205	-0.3255	-0.318	-0.3202	-0.32
Njo 1998 (1d)	-0.1951	-0.1918	-0.1892	-0.19	-0.1899
Njo 1998 (2d)	-0.1137	-0.1124	-0.1076	-0.1087	-0.1086
Njo 1998 (3d)	-0.1138	-0.1125	-0.1078	-0.1089	-0.1087
Njo 1998 (4d)	-0.1278	-0.1261	-0.1215	-0.1226	-0.1224
Njo 1998 (5d)	-0.1843	-0.1815	-0.1757	-0.177	-0.1768
Bultinck 2002 (1e)	-0.3515	-0.3458	-0.3401	-0.3414	-0.3412
Bultinck 2002 (1f)	-0.4331	-0.4295	-0.4333	-0.4336	-0.4335
Bultinck 2002 (2f)	-0.3985	-0.3949	-0.3984	-0.3988	-0.3987
Bultinck 2002 (3f)	-0.5041	-0.4981	-0.4907	-0.4922	-0.4919
Bultinck 2002 (4f)	-0.2211	-0.2206	-0.2213	-0.2214	-0.2214
Bultinck 2004 (1g)	-0.807	-0.7882	-0.8081	-0.8093	-0.8091
Bultinck 2004 (2g)	-0.1369	-0.1344	-0.1238	-0.1251	-0.1249
Bultinck 2004 (3g)	-0.1613	-0.1587	-0.1541	-0.1549	-0.1548
Bultinck 2004 (4g)	-0.1493	-0.1466	-0.147	-0.1474	-0.1473
Vařeková 2007 (1h)	-0.3568	-0.3582	-0.3442	-0.3503	-0.3497
Vařeková 2007 (2h)	-0.3392	-0.3409	-0.3238	-0.3311	-0.3305
Vařeková 2007 (3h)	-0.3634	-0.3659	-0.3511	-0.3575	-0.3571
Vařeková 2007 (4h)	-0.3379	-0.3399	-0.3235	-0.3306	-0.3301
Ouyang 2009 (1i)	-0.7295	-0.7312	-0.7091	-0.7207	-0.72
Ouyang 2009 (2i)	-0.901	-0.9006	-0.8841	-0.8975	-0.8975

Table 6.5.: Atomic charges of atom O calculated via EEM method on sample molecules from table 6.3 using parameters from publications