Table 3.

	Zavodnik *et al* [1]			theory		
	x	y	z	x	y	z
O1A	0.1932(3)	0.6505(2)	0.3265(2)	0.18670	0.65377	0.32690
H1A	0.2998(59)	0.6239(36)	0.3444(24)	0.31552	0.60182	0.35082
C2A	0.2217(4)	0.8023(2)	0.3261(2)	0.21346	0.80367	0.32580
C3A	0.0468(4)	0.8900(3)	0.2954(2)	0.04578	0.89037	0.29580
H3A	-0.0950(52)	0.8444(41)	0.2809(31)	-0.10213	0.83907	0.27380
C4A	0.0694(4)	1.0450(3)	0.2937(2)	0.06951	1.04169	0.29354
H4A	-0.0488(61)	1.1008(42)	0.2633(34)	-0.06125	1.10896	0.26895
C5A	0.2624(5)	1.1125(3)	0.3233(2)	0.25853	1.10725	0.32148
H5A	0.2875(70)	1.2289(38)	0.3241(28)	0.27469	1.22592	0.32010
C6A	0.4367(4)	1.0241(3)	0.3540(2)	0.42536	1.02006	0.35159
H6A	0.5961(56)	1.0658(42)	0.3727(41)	0.57370	1.06991	0.37448
C7A	0.4182(4)	0.8698(3)	0.3556(2)	0.40334	0.86867	0.35372
H7A	0.5407(53)	0.8116(38)	0.3754(32)	0.53342	0.80026	0.37793
O1B	0.8467(3)	0.5161(2)	0.2500(-)	0.84992	0.51060	0.25462
H1B	0.9665(50)	0.5570(34)	0.2581(26)	0.98580	0.56096	0.27329
C2B	0.8848(4)	0.4102(3)	0.1834(2)	0.87875	0.40847	0.18729
C3B	1.0825(5)	0.4048(3)	0.1366(2)	1.06937	0.40001	0.13962
H3B	1.2010(63)	0.4695(46)	0.1472(35)	1.19704	0.47819	0.15327
C4B	1.1130(6)	0.2959(4)	0.0698(2)	1.09389	0.29327	0.07367
H4B	1.2568(75)	0.3008(61)	0.0403(40)	1.24305	0.28845	0.03628
C5B	0.9429(7)	0.1936(4)	0.0504(2)	0.92954	0.19581	0.05445
H5B	0.9776(90)	0.1242(53)	-0.0019(34)	0.94906	0.11242	0.00272
C6B	0.7460(6)	0.2018(3)	0.0967(2)	0.73782	0.20791	0.10083
H6B	0.6226(81)	0.1477(47)	0.0860(40)	0.60700	0.13334	0.08545
C7B	0.7131(5)	0.3101(3)	0.1636(2)	0.71162	0.31327	0.16728
H7B	0.5606(51)	0.3176(45)	0.1985(34)	0.56186	0.32208	0.20387
O1C	0.5509(3)	0.4999(2)	0.3849(2)	0.54607	0.50202	0.38233
H1C	0.6757(44)	0.5123(32)	0.3514(23)	0.66261	0.50296	0.33563
C2C	0.5886(4)	0.3961(3)	0.4526(2)	0.58728	0.40138	0.44931
C3C	0.7887(4)	0.3190(3)	0.4567(2)	0.78176	0.32846	0.45491
H3C	0.9132(62)	0.3376(44)	0.4183(34)	0.90712	0.35149	0.40622
C4C	0.8198(6)	0.2127(3)	0.5249(3)	0.81399	0.22537	0.52237
H4C	0.9579(72)	0.1767(50)	0.5280(38)	0.96628	0.16868	0.52613
C5C	0.6561(7)	0.1848(4)	0.5885(2)	0.65416	0.19372	0.58432
H5C	0.6625(90)	0.1095(56)	0.6383(35)	0.68026	0.11223	0.63672
C6C	0.4595(7)	0.2640(4)	0.5845(2)	0.46257	0.26974	0.57936
H6C	0.3263(90)	0.2578(63)	0.6227(38)	0.33788	0.24926	0.62884
C7C	0.4254(5)	0.3706(3)	0.5170(2)	0.42843	0.37296	0.51233
H7C	0.3031(63)	0.4194(49)	0.5128(31)	0.27861	0.43269	0.50865

Table 3: Fractional coordinates for the ambient-pressure monoclinic, $P112_1$, phenol structure obtained from the *ab initio* calculations (second set of coordinates) and, for comparison, the coordinates obtained from the experimental study of Zavodnik *et al* [1]. The standard deviations obtained from the experimental work are shown in parenthesis.

Table 4.

	experiment			theory		
	x	y	z	x	y	z
O1A	0.7050(10)	0.4386(19)	0.3000(15)	0.71126	0.44422	0.30056
H1A	0.6716	0.3230	0.3235	0.69033	0.29217	0.33282
C2A	0.6911(8)	0.4219(16)	0.1876(15)	0.69424	0.42362	0.18807
C3A	0.6275(9)	0.2301(18)	0.1293(17)	0.63125	0.23658	0.13281
H3A	0.5935	0.1113	0.1675	0.59312	0.10191	0.17866
C4A	0.6146(10)	0.216(2)	0.0139(17)	0.61763	0.22242	0.01955
H4A	0.5721	0.0877	-0.0251	0.56780	0.07574	-0.02288
C5A	0.6654(11)	0.394(3)	-0.0432(15)	0.66588	0.39451	-0.03877
H5A	0.6568	0.3842	-0.1204	0.65587	0.38251	-0.12753
C6A	0.7290(11)	0.585(3)	0.0150(15)	0.72717	0.58276	0.01721
H6A	0.7629	0.7043	-0.0232	0.76559	0.71904	-0.02749
C7A	0.7418(9)	0.5996(18)	0.1304(15)	0.74174	0.59851	0.13037
H7A	0.7844	0.7279	0.1694	0.79100	0.74506	0.17397
O1B	0.6823(10)	0.937(2)	0.3864(14)	0.67878	0.94285	0.38739
H1B	0.7209	0.8193	0.3720	0.70328	0.78813	0.36015
C2B	0.6694(11)	0.923(2)	0.4937(14)	0.66498	0.91994	0.49480
C3B	0.7169(10)	0.726(2)	0.5603(15)	0.71200	0.73004	0.56043
H3B	0.7597	0.6059	0.5317	0.76167	0.59304	0.52719
C4B	0.7005(9)	0.709(3)	0.6697(15)	0.69602	0.71761	0.66844
H4B	0.7322	0.5776	0.7143	0.73503	0.57017	0.71920
C5B	0.6366(10)	0.889(3)	0.7124(14)	0.63330	0.89194	0.71140
H5B	0.6256	0.8773	0.7856	0.62076	0.88149	0.79602
C6B	0.5891(9)	1.085(3)	0.6458(14)	0.58742	1.08187	0.64526
H6B	0.5463	1.2053	0.6744	0.53838	1.22112	0.67753
C7B	0.6055(10)	1.102(2)	0.5364(14)	0.60298	1.09665	0.53728
H7B	0.5737	1.2337	0.4918	0.56633	1.24510	0.48556
O1C	1.0164(12)	0.860(2)	0.4541(16)	1.00983	0.86120	0.45488
H1C	0.9818	0.9714	0.4791	0.99169	1.01681	0.48602
C2C	1.0088(13)	0.893(2)	0.3444(13)	1.01206	0.88574	0.34465
C3C	0.9567(10)	1.0874(15)	0.2791(17)	0.96011	1.07771	0.28353
H3C	0.9167	1.2084	0.3103	0.91506	1.21464	0.32183
C4C	0.9644(10)	1.101(2)	0.1671(16)	0.96582	1.09261	0.17292
H4C	0.9295	1.2314	0.1235	0.92559	1.24459	0.12613
C5C	1.0241(12)	0.920(4)	0.1205(13)	1.02267	0.91911	0.12300
H5C	1.0293	0.9295	0.0456	1.02819	0.93448	0.03668
C6C	1.0762(10)	0.726(3)	0.1858(17)	1.07385	0.72806	0.18498
H6C	1.1162	0.6046	0.1546	1.12009	0.59183	0.14765
C7C	1.0686(11)	0.7119(15)	0.2977(16)	1.06928	0.71142	0.29554
H7C	1.1034	0.5817	0.3414	1.11154	0.56416	0.34440

Table 4: Fractional coordinates for the high-pressure monoclinic, $P2_1$, phenol structure obtained from the *ab initio* calculations (second set of coordinates) and, for comparison, the coordinates obtained from the Bruker APEX CCD single-crystal x-ray diffraction results. The standard deviations obtained from the single-crystal refinements are shown in parenthesis.