Table 5.1: Computed values of dipole moment and polarizability of the compounds responsible for off-flavor and cork-taint in wine. Gaussian results obtained with B_3LYP on a 6-31+G(d,p) basis. In square brackets: QuantumEspresso results with BLYP level of theory on a plane-wave basis with cutoff 40 Ry.

Molecule name (Formula)	**Molecular mass** (a.m.u.)	**CAS Number**	**Dipole Moment** μ_D (Debye)	**Polarizability** α (Å^3)
2,4,6-Trichloroanisole ($C_7H_5Cl_3O$)	211.47	87-40-1	1.57[1,2] [1.41]	18.36 [21.47]
2,4,6-Tribromoanisole ($C_7H_5Br_3O$)	344.83	607-99-8	1.54 [1.44]	22.11 [25.67]
Pentachlorophenol (C_6Cl_5OH)	266.34	87-86-5	1.78 [1.90]	20.33 [25.45]
Pentabromophenol (C_6Br_5OH)	488.59	608-71-9	1.55 [2.06]	26.14 [30.11]
2,4,6-Trichlorophenol ($C_6H_2Cl_3OH$)	197-45	88-06-2	1.47[3] [1.49]	16.53 [19.67]
2,4,6-Tribromophenol ($C_6H_2Br_3OH$)	330.80	118-79-6	1.40[4] [1.46]	20.29 [23.26]
2,3,4-Trichloroanisole ($C_7H_5Cl_3O$)	211.47	54134-80-7	4.42 [4.34]	18.38 [21.21]
2,3,6-Trichloroanisole ($C_7H_5Cl_3O$)	211.47	50375-10-5	1.91 [1.57]	18.21 [21.04]
2,3,4,5-Tetrachloroanisole ($C_7H_4Cl_4O$)	245.91	938-86-3	3.75 [4.09]	20.42 [23.73]
2,3,4,6-Tetrachloroanisole ($C_7H_4Cl_4O$)	245.91	938-22-7	2.00 [1.83]	20.27 [23.58]
2,3,5,6-Tetrachloroanisole ($C_7H_4Cl_4O$)	245.91	6936-40-9	1.61 [1.57]	20.28 [23.53]
2,4-Dichloroanisole ($C_7H_6Cl_2O$)	177.03	553-82-2	3.40[5] [3.45]	16.55 [19.12]

[1] 1.42: G. Klages, J. Naturforschg 1965
[2] 1.57: M. Bowyer, Uni. of newcastle, 2002
[3] 1.42: G. Klages, J. Naturforschg 1965
[4] 1.45: G. Klages, J. Naturforschg 1965
[5] 2.77: G. Klages, J. Naturforschg 1965

Table 5.1: continued

Molecule name (Formula)	**Molecular mass** (a.m.u.)	**CAS Number**	**Dipole Moment** μ_D (Debye)	**Polarizability** α (Å^3)
2,6-Dichloroanisole ($C_7H_6Cl_2O$)	177.03	1984-65-2	2.04 [2.17]	16.21 [18.53]
Cis-1,5-octadien-3-one ($C_8H_{12}O$)	124.18	65767-22-8	3.02 [2.60]	15.20 [16.96]
Cis-1,5-octadien-3-ol ($C_8H_{14}O$)	126.20	50306-18-8	2.00 [1.66]	15.64 [17.31]
1-Octene-3-ol ($C_8H_{16}O$)	128.22	3391-86-4	1.44 [1.57]	15.39 [17.12]
1-Octene-3-one ($C_8H_{14}O$)	126.20	4312-99-6	3.16 [3.07]	14.70 [16.43]
Octanal ($C_8H_{16}O$)	128.21	124-13-0	3.33 [2.70]	14.85 [16.57]
2-Sec-butyl-3-methoxypyrazine ($C_9H_{14}N_2O$)	166.22	24168-70-5	1.33 [1.30]	18.43 [20.47]
3-Iso-butyl-2-methoxypyrazine ($C_9H_{14}N_2O$)	166.22	24683-00-9	1.41 [1.43]	18.38 [20.20]
2-Iso-propyl-3-methoxypyrazine ($C_8H_{12}N_2O$)	152.19	25773-40-4	1.38 [1.36]	16.74 [18.45]
2-Methoxy-3,5-dimethylpyrazine ($C_7H_{10}N_2O$)	138.17	92508-08-2	1.13 [1.18]	15.10 [16.88]
2-Methylisoborneol ($C_{11}H_{20}O$)	168.21	2371-42-8	1.53 [1.47]	18.71 [20.31]
Geosmin ($C_{12}H_{22}O$)	182.31	19700-21-1	1.43 [1.37]	20.28 [22.02]
Guaiacol ($C_7H_8O_2$)	124.14	90-05-1	2.87 [3.00]	13.26 [14.84]

Table 5.1: continued

Molecule name (Formula)	**Molecular mass** (a.m.u.)	**CAS Number**	**Dipole Moment** μ_D (Debye)	**Polarizability** α (Å^3)
4-Ethylguaiacol ($C_9H_{12}O_2$)	152.19	2785-89-9	1.19 [2.60]	17.19 [19.08]
4-Ethylphenol ($C_8H_{10}O$)	122.16	123-07-9	1.45 [1.62]	14.46 [15.82]
Eucalyptol ($C_8H_{10}O$)	154.25	470-82-6	1.55 [6] [1.51]	17.01[7] [18.56]
4-Ethylcatechol ($C_8H_{10}O_2$)	138.17	1124-39-6	2.38 [2.22]	15.14 [16.79]
4-Methylguaiacol ($C_8H_{10}O_2$)	138.17	93-51-6	1.21 [1.29]	15.32 [17.16]
Rotundone ($C_{15}H_{22}O$)	218.34	18374-76-0	3.97 [4.06]	26.10 [28.34]
Geraniol ($C_{10}H_{18}O$)	154.25	106-24-1	2.45 [1.55]	19.43 [21.69]
Hotrienol ($C_{10}H_{16}O$)	152.24	53834-70-1	1.74 [1.80]	19.83 [21.71]
Linalool ($C_{10}H_{18}O$)	154.25	78-70-6	1.93[8] [1.85]	18.93[9] [20.81]
Nerol ($C_{10}H_{18}O$)	154.25	106-25-2	2.64 [2.62]	18.61 [20.66]
$\alpha-$Terpineol ($C_{10}H_{18}O$)	154.25	98-55-5	1.66 [1.74]	17.98 [19.90]
Indole (C_8H_7N)	117.15	120-72-9	2.16 [2.44]	14.72 [16.00]
1-Methylindole (C_9H_9N)	131.18	603-76-9	2.48 [2.78]	16.73 [18.24]

[6] 1.57: G. Amadei,Rapid Commun. Mass Spectrom. 2011
[7] 18.1: G. Amadei,Rapid Commun. Mass Spectrom. 2011
[8] 1.58: G. Amadei,Rapid Commun. Mass Spectrom. 2011
[9] 19.6: G. Amadei,Rapid Commun. Mass Spectrom. 2011

Table 5.1: continued

Molecule name (Formula)	**Molecular mass** (a.m.u.)	**CAS Number**	**Dipole Moment** μ_D (Debye)	**Polarizability** α ($\dot{A}^3$)
2-Aminoacetophenone (C_8H_9NO)	135.16	551-93-9	1.96 [1.86]	16.08 [17.71]
2-Chloro-6-methylphenol (C_7H_7ClO)	142.58	87-64-9	0.88 [0.82]	14.37 [16.26]
3-Octanone ($C_8H_{16}O$)	128.21	106-68-3	2.74 [2.68]	14.60 [16.41]
Fenchone ($C_{10}H_{16}O$)	152.23	1195-79-5	3.10 [3.06]	16.60 [18.06]
Fenchol ($C_{10}H_{18}O$)	154.25	1632-73-1	1.46 [1.29]	17.05 [18.56]
Trans-2-octen-1-ol ($C_8H_{16}O$)	128.21	18409-17-1	1.74 [1.88]	15.59 [17.75]
Pentachloroanisole ($C_7H_3Cl_5O$)	280.35	1825-21-4	2.12 [2.18]	22.22 [26.10]

Table 5.2: Dipole moment and polarizability of Sulfur compounds responsible for off-flavor and cork-taint in wine. Gaussian results are presented with B_3LYP/Aug-cc-PVTZ level of theory.

Molecule name (Formula)	**Molecular mass** (a.m.u.)	**CAS Number**	**Dipole Moment** μ_D (Debye)	**Polarizability** α ($\dot{A}^3$)
Hydrogen Sulfide (H_2S)	34.08	7783-06-4	0.99[10]	3.71
Methanethiol (CH_4S)	48.11	74-93-1	1.56[11]	5.55[12]
Ethanethiol (C_2H_6S)	62.14	75-08-1	1.68[13][14]	7.43
Dimethyl Sulfide (C_2H_6S)	62.14	75-18-3	1.60[15][16]	7.46
Diethyl Sulfide ($C_4H_{10}S$)	90.19	352-93-2	1.64[17]	11.34
Dimethyl Disulfide ($C_2H_6S_2$)	94.2	624-92-0	2.03[18]	10.79[19]
Diethyl Disulfide ($C_4H_{10}S_2$)	122.3	110-81-6	2.15	14.67
Methyl Thioacetate (C_3H_6OS)	90.15	1534-08-3	1.36	9.64
3-Mercaptohexan-1-ol ($C_6H_{14}OS$)	134.24	51755-83-0	1.68	15.43

[10] 0.97: Carl L. Yaws, Thermophysical Properties of Chemicals and Hydrocarbons.
[11] 1.52: Carl L. Yaws, Thermophysical Properties of Chemicals and Hydrocarbons.
[12] 5.55: NIST data base.
[13] 1.68: NIST data base.
[14] 1.58: Carl L. Yaws, Thermophysical Properties of Chemicals and Hydrocarbons.
[15] 1.60: NIST data base.
[16] 1.50: Carl L. Yaws, Thermophysical Properties of Chemicals and Hydrocarbons.
[17] 1.54: Carl L. Yaws, Thermophysical Properties of Chemicals and Hydrocarbons.
[18] 1.99: Carl L. Yaws, Thermophysical Properties of Chemicals and Hydrocarbons.
[19] 10.79: NIST data base.

Table 5.2: continued

Molecule name (Formula)	**Molecular mass** (a.m.u.)	**CAS Number**	**Dipole Moment** μ_D (Debye)	**Polarizability** α (Å^3)
4-Mercapto-4-methylpentan-2-one ($C_6H_{12}OS$)	132.23	19872-72-7	2.27	14.86
4-Mercapto-4-methylpentan-2-ol ($C_6H_{14}OS$)	134.24	255391-65-2	2.53	15.34
Benzothiazole (C_7H_5NS)	135.19	95-16-9	1.34	15.91
2-Furanmethanethiol (C_5H_6OS)	114.17	98-02-2	1.94	12.81
2-Mercaptoethanol (C_2H_6OS)	78.14	60-24-2	2.50	8.14
Benzenemethanethiol (C_7H_8S)	124.21	100-53-8	1.48[20]	15.74
2-Mercaptoethyl acetate ($C_4H_8O_2S$)	120.17	5862-40-8	1.83	11.91
3-mercaptopropyl acetate ($C_5H_{10}O_2S$)	134.2	26473-61-0	1.61	13.97
Cis-3,6-dimethyl-1,2,4,5-tetrathiane ($C_4H_8S_4$)	184.4	75100-46-8	0	19.83
Prenyl-mercaptan ($C_5H_{10}S$)	102.2	5287-45-6	1.78	13.35
Trans-3,6-dimethyl-1,2,4,5-tetrathiane ($C_4H_8S_4$)	184.8	75100-47-9	0	19.11

[20] 1.44 (in benzene): Carl L. Yaws, Thermophysical Properties of Chemicals and Hydrocarbons.

Table 5.2: continued

Molecule name (Formula)	**Molecular mass** (a.m.u.)	**CAS Number**	**Dipole Moment** μ_D (Debye)	**Polarizability** α ($\dot{A}^3$)
2-Methyl-3-furanthiol (C_5H_6OS)	114.17	28588-74-1	0.90	12.47
2-Methylthiolane-3-ol ($C_5H_{10}OS$)	118.2	149834-43-5	2.12	12.71
3-Mercapto-3-methylbutan-1-ol ($C_5H_{12}OS$)	120.22	34300-94-2	1.84	13.52
Ethyl-3-mercaptopropionate ($C_5H_{10}O_2S$)	134.2	5466-06-08	2.76	13.91
5-2-hydroxyethyl-4-methylthiazole (C_6H_9NOS)	143.21	137-00-8	2.79	15.29
2-Methyltetrahydro thiophen-3-one (C_5H_8OS)	116.18	13679-85-1	1.72	12.14
3-Methylsulfanyl propan-1-ol ($C_4H_{10}OS$)	106.19	0505-10-02	3.06	12.03
3-Mercaptohexylacatate ($C_8H_{16}O_2S$)	176.28	136954-20-6	1.47	19.32
Ethylthioacetate (C_4H_8OS)	104.17	625-60-5	1.41	11.57