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

Table 5.3: Computed values of proton affinity and ionization energy of the targeted compounds using Gaussian B_3LYP/6-31+G(d,p) level of theory.

Molecule name (Formula)	**Proton Affinity** (Kcal/mol)	**Ionization Energy** (eV)
2,4,6-Trichloroanisole ($C_7H_5Cl_3O$)	183.51	8.28
2,4,6-Tribromoanisole ($C_7H_5Br_3O$)	186.17	8.19
Pentachlorophenol (C_6Cl_5OH)	167.15	8.56
Pentabromophenol (C_6Br_5OH)	174.17	8.60
2,4,6-Trichlorophenol ($C_6H_2Cl_3OH$)	174.35	8.79
2,4,6-Tribromophenol ($C_6H_2Br_3OH$)	178.56	8.62
2,3,4-Trichloroanisole ($C_7H_5Cl_3O$)	181.32	8.15
2,3,6-Trichloroanisole ($C_7H_5Cl_3O$)	183.87	8.37
2,3,4,5-Tetrachloroanisole ($C_7H_4Cl_4O$)	178.40	8.23
2,3,4,6-Tetrachloroanisole ($C_7H_4Cl_4O$)	181.96	8.35
2,3,5,6-Tetrachloroanisole ($C_7H_4Cl_4O$)	181.49	8.67
2,4-Dichloroanisole ($C_7H_6Cl_2O$)	182.77	8.04
2,6-Dichloroanisole ($C_7H_6Cl_2O$)	186.69	8.30
Cis-1,5-octadien-3-one ($C_8H_{12}O$)	211.13	8.39
Cis-1,5-octadien-3-ol ($C_8H_{14}O$)	200.87	8.28

Table 5.3: continued

Molecule name (Formula)	**Proton Affinity** (Kcal/mol)	**Ionization Energy** (eV)
1-Octene-3-ol ($C_8H_{16}O$)	197.68	8.92
1-Octene-3-one ($C_8H_{14}O$)	203.94	9.01
Octanal ($C_8H_{16}O$)	192.82	9.18
2-Sec-butyl-3-methoxypyrazine ($C_9H_{14}N_2O$)	215.84	8.30
3-Iso-butyl-2-methoxypyrazine ($C_9H_{14}N_2O$)	215.77	8.28
2-Iso-propyl-3-methoxypyrazine ($C_8H_{12}N_2O$)	215.39	8.33
2-Methoxy-3,5-dimethylpyrazine ($C_7H_{10}N_2O$)	217.16	8.11
2-Methylisoborneol ($C_{11}H_{20}O$)	217.79	8.28
Geosmin ($C_{12}H_{22}O$)	205.05	8.35
Guaiacol ($C_7H_8O_2$)	191.50	7.66
4-Ethylguaiacol ($C_9H_{12}O_2$)	198.28	7.29
4-Ethylphenol ($C_8H_{10}O$)	182.32	7.86
Eucalyptol ($C_8H_{10}O$)	213.24	8.28
4-Ethylcatechol ($C_8H_{10}O_2$)	198.28	7.61
4-Methylguaiacol ($C_8H_{10}O_2$)	195.18	7.32
Rotundone ($C_{15}H_{22}O$)	219.70	8.18
Geraniol ($C_{10}H_{18}O$)	212.37	7.77
Hotrienol ($C_{10}H_{16}O$)	208.05	7.73
Linalool ($C_{10}H_{18}O$)	214.27	8.03
Nerol ($C_{10}H_{18}O$)	209.87	7.91

Table 5.3: continued

Molecule name (Formula)	**Proton Affinity** (Kcal/mol)	**Ionization Energy** (eV)
$\alpha-$Terpineol ($C_{10}H_{18}O$)	200.56	7.95
Indole (C_8H_7N)	199.49	7.51
1-Methylindole (C_9H_9N)	203.64	7.30
2-Aminoacetophenone (C_8H_9NO)	214.57	7.61
2-Chloro-6-methylphenol (C_7H_7ClO)	177.47	8.20
2-Octanone ($C_8H_{16}O$)	203.37	8.92
Fenchone ($C_{10}H_{16}O$)	207.11	8.33
Fenchol ($C_{10}H_{18}O$)	198.48	8.31
Trans-2-octen-1-ol ($C_8H_{16}O$)	203.08	8.53
Pentachloroanisole ($C_7H_3Cl_5O$)	180.35	8.44

Table 5.4: Computed values of proton affinity and ionization energy of the VOCs related to sulfur using Gaussian B_3LYP/Aug-cc-PVTZ level of theory.

Molecule name (Formula)	**Proton Affinity** (Kcal/mol)	**Ionization Energy** (eV)
Hydrogen Sulfide (H_2S)	169.14	10.43
Methanethiol (CH_4S)	186.08	9.37
Ethanethiol (C_2H_6S)	190.61	9.16
Dimethyl Sulfide (C_2H_6S)	199.30	8.59
Diethyl Sulfide ($C_4H_{10}S$)	206.31	8.28
Dimethyl Disulfide ($C_2H_6S_2$)	193.66	8.09
Diethyl Disulfide ($C_4H_{10}S_2$)	197.75	7.89
Methyl Thioacetate (C_3H_6OS)	198.47	9.09
3-Mercaptohexan-1-ol ($C_6H_{14}OS$)	196.58	8.62
4-Mercapto-4-methylpentan-2-one ($C_6H_{12}OS$)	198.23	8.50
4-Mercapto-4-methylpentan-2-ol ($C_6H_{14}OS$)	204.77	8.47
Benzothiazole (C_7H_5NS)	220.73	8.55
2-Furanmethanethiol (C_5H_6OS)	199.10	8.05

Table 5.4: continued

Molecule name (Formula)	**Proton Affinity** (Kcal/mol)	**Ionization Energy** (eV)
2-Mercaptoethanol (C_2H_6OS)	193.42	8.98
Benzenemethanethiol (C_7H_8S)	195.26	8.26
2-Mercaptoethyl acetate ($C_4H_8O_2S$)	199.18	9.10
3-mercaptopropyl acetate ($C_5H_{10}O_2S$)	199.60	8.96
Cis-3,6-dimethyl-1,2,4,5-tetrathiane ($C_4H_8S_4$)	196.08	8.03
Prenyl-mercaptan ($C_5H_{10}S$)	198.21	8.06
Trans-3,6-dimethyl-1,2,4,5-tetrathiane ($C_4H_8S_4$)	195.31	8.25
2-Methyl-3-furanthiol (C_5H_6OS)	190.29	7.71
2-Methylthiolane-3-ol ($C_5H_{10}OS$)	207.51	8.16
3-Mercapto-3-methylbutan-1-ol ($C_5H_{12}OS$)	197.74	8.59
Ethyl-3-mercaptopropionate ($C_5H_{10}O_2S$)	196.71	8.90
5-(2-hydroxyethyl)-4-methylthiazole (C_6H_9NOS)	229.67	8.12

Table 5.4: continued

Molecule name (Formula)	**Proton Affinity** (Kcal/mol)	**Ionization Energy** (eV)
2-Methyltetrahydro thiophen-3-one (C_5H_8OS)	196.14	8.57
3-Methylsulfanyl propan-1-ol ($C_4H_{10}OS$)	203.12	8.38
3-Mercaptohexylacatate ($C_8H_{16}O_2S$)	194.86	8.78
Ethylthioacetate (C_4H_8OS)	201.19	8.96