THE PREDICTION OF pK_a VALUES FOR PHENOLIC COMPOUNDS BY THE DFT THEORY

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Abstract - The acid dissociation constant is an important parameter that affects the physicochemical properties of molecules in solution. A set of 20 phenolic compounds were used to establish a model to predict pKa values of phenolic compounds. Calculations in aqueous medium were performed with a polarizable continuum solvent model (PCM) and three hybrid DFT functionals (B3LYP, PBE0, ωB97XD and M062X) with the basis set 6-311++G(d,p). The directly calculated value of $pK_{\rm a}$ gives less accurate results with an average absolute error (MAE) of 1.74 pK_a units when using the ω B97XD functional and phenol as reference compound. In the case of using statistical correction, the accuracy of pK_a is greatly improved. In the case of using statistical correction, the accuracy of pK_a is greatly improved with the lowest MAE value of 0.14 pKa units (M062X; $R^2 = 0.978$). The calculated results of pK_a in this study have the same accuracy as the experimental measurements.

Key words - pK_a ; density functional theory methods (DFT); phenolic.

1. Introduction

The proton transfer reactions are one of the most basic and common types of reactions in chemistry [1]. The ability of a substance to transfer protons in a medium is characterized by its acid dissociation constant (K_a) and is usually reported as a pK_a value. The many chemical compounds act as Brønsted-Lowry acids or bases in aqueous media. Therefore, depending on the pK_a and pH values, these compounds can be ionized to different degrees and thus determine their forms of existence in the aquatic environment. The bioactive molecules from nature as well as drug molecules are usually weak acids or weak bases, so their degree of ionization in the medium affects lipophilicity, solubility, protein binding and mobility across the plasma membrane and thus pK_a affects the absorption, distribution, metabolism, excretion and toxicity properties of compounds [2]. Therefore, the pK_a value is a very important parameter for pharmaceutical compounds as well as other commonly used compounds. Most of the pK_a values are determined experimentally. However, the number of experimental pK_a values is too small compared to the extremely abundant number of chemical compounds. Therefore, there have been many publications using different theoretical approaches to predict pK_a value such as using the QSAR model (quantitative structure - activity relationship) combined with machine learning method [3, 4]; The semiempirical quantum mechanical methods and the density functional theory methods (DFT) [5-7]. The results of these publications show that it is possible to predict pK_a from the theory. However, each family of compounds needs to be approached separately, and the quantitative results of each model must be based on compounds with similar chemical structures.

The subjects in this study were phenolic compounds. They are compounds with one or more hydroxyl groups attached to the aromatic benzene nucleus and are found in most plant tissues [8]. Phenolics are known to have biological activities, such as antibacterial and antiviral properties, anti-inflammatory and antiproliferative activities and especially many phenolics have strong antioxidant activity and are the most abundant source of antioxidants in the human diet [9].

In aqueous media, phenolics are weak acids, which is due to the proton dissociation of the OH group attached to the benzene ring. Depending on the pK_a value and pH of the body's environment, phenolics can exist as neutral molecules or ionic form, or both. Therefore, the acid-base equilibrium of phenolics in the environment affects their bioactivity [10, 11] and pK_a values of phenolics are of the utmost importance in practical applications. In this study, we use DFT theory combined with a linear regression model to predict pK_a of phenolic compounds based on a sample of 20 phenolic compounds with known pK_a from the experiment (Figure 1).



Figure 1. Phenolic compounds used in this study

2. Theoretical and computational methods

2.1. Calculation of pKa

The dissociation of phenolics (ArOH) in aqueous medium (aq) is expressed in terms of Equation (1).

$$\operatorname{ArOH}_{(aq)} + \operatorname{H}_2\operatorname{O}_{(aq)} \rightleftharpoons \operatorname{ArO}_{(aq)}^- + \operatorname{H}_3\operatorname{O}_{(aq)}^+$$
(1)

Acid dissociation constant (K_a) and pK_a are defined according to equations (2) and (3) respectively[12].

$$K_a = [H_3 0^+][Ar 0^-]/[Ar 0H]$$
 (2)

$$pK_a = -\log K_a \tag{3}$$

The value of K_a is calculated based on Equation (4).

$$\Delta G_T^0(1) = -RT \ln K_a \tag{4}$$

Where, $\Delta G_T^0(1)$ is the change in Gibbs energy of acid dissociation, calculated by DFT theory. The disadvantage of this method is that it is difficult to accurately calculate the Gibbs energy of the H₃O⁺ ion because the ion is very strongly hydrated in solution[13]. This can be overcome by using an acid reference (ArOH_{ref}). Consider the following equilibria:

$$ArOH_{(aq)} + ArO_{ref,(aq)}^{-} \rightleftharpoons ArO_{(aq)}^{-} + ArOH_{ref,(aq)}$$
(5)

The pKa value of ArOH is determined according to Equation (6) (detailed description in section 1.1 of supplementary information).

$$pK_{a} = \frac{\Delta G_{T}^{0}(5)}{RT \ln 10} + pK_{a}^{ref}$$
(6)

Where, pK_a^{ref} is the experimental pK_a value the reference phenolics, $ArOH_{ref}$ and $\Delta G_T^0(5)$ is the change in Gibbs energy of reaction on Equation (5), determined by:

$$\Delta G_T^0(5) = G_T^0 (ArOH_{ref}) + G_T^0 (ArO^-) - G_T^0 (ArOH) - G_T^0 (ArO_{ref}^-)$$
(7)

The study used 3 reference phenolic compounds with significantly different pK_a values including phenol ($pK_a = 9.99$), 2-hydroxybenzaldehyde ($pK_a = 8.37$) and 2-cyanophenol ($pK_a = 6.86$). The predicted value of pK_a by direct calculation method (denoted by pK_a^{calc}) is calculated according to Equation (3).

The results are statistically processed as follows: from the pK_a^{calc} values, build a linear regression equation according to Equation (8).

$$pK_a^{exp} = a + b. pK_a^{calc}$$
(8)

Where, pK_a^{exp} is the experimental pK_a of phenolics used in the study sample. The final predicted pK_a after statistical correction (denoted by pK_a^{corr}) is calculated in terms of Equation (9).

$$pK_a^{corr} = \alpha + \beta . pK_a^{calc}$$
⁽⁹⁾

Where, α và β are equal to the values of α and b in Equation (8), respectively.

2.2. The DFT calculation

In this study, four density functional theory (DFT) methods including B3LYP [14], PBE0 [15], ω B97XD [16] and M06-2X [17] combinded with the 6-311++G(d,p) basic set were recommended for predict p K_a values. The choise of these methods was based on the previous studies

because of its accuracy and lower computational cost [18-22]. In addition, the solvent effects were modeled by the polarizable continuum model (PCM) which is the most commonly used solvation model [23, 24].

The stable geometry of the compounds was checked by harmonic frequency calculation to confirm the structures which were minimal on the PES surface and to obtain the thermal and entropy contributions to the Gibbs energy. All calculations were performed at standard conditions in the solution of 1 M and 298.15 K and used Gaussian 16 Revision A.03 software[25].

3. Results and discussion

3.1. Direct calculation of pK_a

The pK_a error between calculation and experiment of 20 phenol compounds when using different DFT functionals and reference compounds is presented in Table S2 (supplementary information: SI) and visualized in Figure 2. The results show that the error pK_a is less dependent on the type of used functional but strongly depends on the reference compound. The 20 phenolic compounds in Figure 2 are numbered in order of increasing pK_a value (see Table S1 in SI). The errors tend to increase as the pK_a of the reference compound is further away from the pK_a of the calculated compound. Specifically, the reference compound 2-cyanophenol with a small pK_a (6.86) will cause large errors for the compound with a large pK_a (compound 7 to 20 have a pK_a between 8.98 and 10.39). In contrast, phenol with large pK_a (9.99) produces small errors for compounds with similar pK_a but large errors for compounds with small pK_a (compound 1 to 6 with pK_a of 6.69 to 8.05). The case of 2hydroxybenzaldehyde has a pK_a (8.37) lower than phenol and greater than 2-cyanophenol, so it generally does not cause too large errors in the regions with large and small pK_a in the sample of the studied compounds. A general trend that does not depend on the functionals or the used reference compounds is that the error is mostly negative for substances with small pK_a and positive for compounds with large pK_a .

The results in Figure 3 show that the mean absolute error is the smallest when using phenol as the reference compound and the largest when using 2-cyanophenol. This is explained by the fact that the majority of phenolics have a p K_a closer to phenol than 2-cyanophenol. For the sample of compounds studied, the best calculation pK_a results were observed by the combination of wB97XD functional and phenol as the reference compound with a MAE value of 1.74. However, the error between calculated and experimental pK_a varied widely from -5.86 (compound 1) to 2.02 (compound 18). The results here indicate that the selection of a reference compound is very important in the theoretical prediction of pK_a value. The closer the pK_a of the reference compound is to the one of interests, the more accurate the result. In general, the pK_a calculated by the direct method using the reference compound has a large error compared with the experimental method, and therefore caution should be exercised when using this method to predict the pK_a of phenolic compounds.





Figure 2. The error differences between pK_a calculated and experimental values without statistical correction



Figure 3. The mean absolute error (MAE) differences between pKa calculated and experimental values without statistical correction

3.2. The Calculated pK_a by statistical correction

The results in section 3.1 show that the pK_a when calculated by the direct method has a large uncertainty and is highly dependent on the reference compound. In this part of the study, we will examine the correlation between the calculated and experimental pK_a values. The results presented in Figure 4 show that there is a strong linear correlation between the calculated (pK_a^{calc}) and experimental pK_a (pK_a^{exp}) with the R^2 coefficient in the range from 0.972 to 0.978. Furthermore, the correlation coefficients and slopes in the regression equations do not depend on the type of reference compound selected. Therefore, the choice of the reference compound does not affect the degree of correlation between the calculated and experimental pK_a values. This means that the error in calculating pK_a after statistical correction will not depend on the type of reference compound and this will be analyzed below.

Based on the correlation between the calculated and experimental pK_a , the predicted pK_a value is statistically

corrected (denoted by pK_a^{corr}) by replacing the quantity pK_a^{exp} in the regression equations with pK_a^{corr} . The equations for calculating pK_a^{corr} when using phenol reference compounds are presented in Table 1. Here, it should be noted that the choice of the reference compound is just a procedure when calculating, has absolutely no effect on the value of the pK_a^{corr} and is therefore the same when using the regression equations of the other reference compounds for the investigation.

Table 1. Equations for calculation of pK_a^{corr} according to pK_a^{calc} of DFT functionals when phenol is reference

Functionals	Equations	R ²
B3LYP	$pK_a^{corr} = 0.306 \times pK_a^{calc} + 6.715$	0.978
PBE0	$pK_a^{corr} = 0.314 \times pK_a^{calc} + 6.450$	0.978
ωB97XD	$pK_a^{corr} = 0.333 \times pK_a^{calc} + 6.617$	0.972
M062X	$pK_a^{\rm corr} = 0.321 \times pK_a^{\rm calc} + 6.099$	0.978

The error between pK_a^{corr} and pK_a^{exp} of 20 phenol compounds when using different DFT functionals is presented in Table S3 (SI) and visualized in Figure 5. The results show that the errors do not depend on the reference compound. Thus, unlike the case of direct pK_a calculation, the error here tends to be uniformly distributed throughout the sample where the pK_a varies over a wide range (from as low as 6.69 for compound 1 to a maximum of 10.39 for compound 20). The most important thing is that the error in calculating pK_a with statistical correction gives much better results than in the case of calculating pK_a directly. The maximum error of the studied phenolics was only 0.4 pK_a units for compound 17 when using the $\omega B97XD$ functional, while the largest error without statistical correction was 6.61 for compound 1 when using the M062X functional combined with phenol as the reference compound. As discussed, the error of the pK_a value after statistical correction is independent of the type of the used reference compound.





Figure 5. The error differences between pK_a calculated and experimental values with statistical correction

The results in Figure 6 show that there is a very small difference in the MAE values when using the B3LYP, PBE0, ω B97XD and M062X functionals. In which, the M062X functional gives the smallest MAE value of 0.14 pK_a units and the largest absolute error when using the M062X functional observed in compound 4 is 0.27 pK_a units. In summary, by using appropriate functionals combined with statistical correction, we are able to calculate the pK_a values of phenolic compounds with an accuracy asymptotic to the experimental measurements.



Figure 6. The mean absolute error (MAE) differences between pK_a calculated and experimental with statistical correction

4. Conclusions

This study presents a reliable procedure for calculating the pK_a of phenolic compounds in aqueous medium. The study sample consisted of 20 phenolic compounds and 3 reference phenolic compounds with experimentally known pK_a . Three hybrid DFT functionals (B3LYP, PBE0, ω B97XD and M062X) with the basis set 6-311++G(d,p) and the polarizable continuum solvent model (PCM) were used to calculate pK_a . The pK_a values calculated directly without statistical processing has a large error $(MAE \ge 1.74 \text{ pK}_{a} \text{ units})$ and the accuracy of the calculation depends strongly on the reference compound. The more accurate the result, the closer the reference compound has a pK_a to the compound of interest. In the sample of the compound studied, the wB97XD functional combined with phenol as the reference compound gave the best results (MAE=1.74). (MAE = 1.74). The pK_a calculation results are greatly improved after statistical processing (MAE = 0.14 when using the M062Xfunctional), with the error asymptotic with the experimental measurements. Furthermore, the pK_a calculation results are independent of the reference

compound. This is the recommended protocol for predicting pK_a values of phenolic compounds.

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SUPPORTING INFORMATION (SI)

S1.1. The expression for calculating pKa based on reference compound The dissociation equation for acid (phenolic: ArOH) in solution:

ArOH(aq) + $H_2O(aq) \rightarrow ArO^-(aq) + H_3O^+(aq)$ (S1) The dissociation equation for the reference phenolic (*ArOH_{ref}*) in

ution:

$$ArOH_{ref}(aq) + H_2O(aq) \rightarrow ArO_{ref}^-(aq) + H_3O^+(aq)$$
 (S2)

Subtract Equation (S2) from Equation (S1) to get:

$$ArOH(a_0) + ArO_{-c}(a_0) \rightarrow ArO^{-}(a_0) + ArOH_{-c}(a_0)$$
 (S3)

$$\Delta G_{\rm T}^{\circ}(S3) = \Delta G_{\rm T}^{\circ}(S1) - \Delta G_{\rm T}^{\circ}(S2) \tag{S4}$$

Where, $\Delta G_{T}^{0}(Si)$ is the standard Gibbs energy of the reactions in terms of Eq (Si). The expression of standard Gibbs energy in terms of acid dissociation constant:

$$\Delta G_T^0(S1) = -RT \ln K_a \tag{S5}$$

$$\Delta G_T^0(S3) = -RT \ln K_a^{ref} \tag{S6}$$

Where, K_a and K_a^{ref} are the acid dissociation constant of ArOH and ArOH_{ref}. Combining equations (S4), (S5) and (S6) get:

$$\Delta G_{\rm T}^0(S3) = -RT \ln \frac{K_a}{K_a^{ref}} \tag{S7}$$

Equation (S7) can be rewritten:

sol

$$-\log K_a = \frac{\Delta G_T^0(3)}{RT \ln 10} - \log K_a^{ref}$$
(S8)

To the definition $pK_a = -\log K_a$, finally get the expression pK_a in terms of pK_a^{ref} :

$$pK_a = \frac{\Delta G_T^0(5)}{RT \ln 10} + pK_a^{ref}$$
(S9)

S1.2. SUPPORT DATA

Table S1. Sequence numbers of compounds and their experimental pK_a values

Table S4. The stable geometry (coordinates xyz) of the compounds is optimized at the theoretical level as M062X/6-311++G(d,p)/PCM(water)

No.	Compound	pK_a^{exp} Ref					
	2-cyanophenol	6.86	[24]				
	2-hydroxylbenzaldehyde	8.37	[24]				
	phenol	9.99	[25]				
1	3,5-dinitrophenol	6.69	[24]				
2	2-fluorophenol	6.86	[26]				
3	4-nitrophenol	7.15	[24]				
4	4-hydroxybenzaldehyde	7.61	[24]				
5	4-cyanophenol	7.95	[24]				
6	4'-Hydroxyacetophenone	8.05	[24]				
7	3-trifluoromethylphenol	8.95	[25]				
8	3-hydroxybenzaldehyde	8.98	[24]				
9	4-phenylphenol	9.55	[24]				
10	3-methoxyphenol	9.65	[25]				
11	4-(2-aminoethyl)phenol	9.77	[24]				
12	4-(hydroxylmethyl)phenol	9.83	[24]				
13	4-hydroxylphenol	9.96	[24]				
14	3-cresol	10.09	[25]				
15	3-ethyl-5-methylphenol	10.1	[24]				
16	4-methoxyphenol	10.1	[24]				
17	4-cresol	10.26	[25]				
18	4-aminophenol	10.3	[25]				
19	3,4-dimethylphenol	10.36	[24]				
20	4-t-butylyphenol	10.39	[24]				

Table S2.	The error between	calculated a	nd experiment	al pK values
when	1 using DFT functi	onals and 3 r	eference comp	ounds

	$\Delta \mathbf{p}K_a = K_a^{calc} - K_a^{exp}$												
Com.		ph	enol		2	-hydro	xylbenza	ldehyde	2-cyanonphenol				
	B3LYF PBE0		0B97XEM062X		B3LYP PBE0 DB97XDM0622			M062X	B3LYPPBE0bB97XDM062X				
1	-6.07	-5.80	-5.86	-6.61	-4.89	-4.87	-4.57	-5.08	-1.98	-1.55	-1.71	-2.40	6.69
2	-1.49	-1.36	-1.30	-1.52	-0.30	-0.43	-0.02	0.01	2.61	2.89	2.84	2.69	6.86
3	-6.63	-6.14	-5.43	-5.77	-5.44	-5.21	-4.14	-4.25	-2.53	-1.90	-1.28	-1.57	7.15
4	-4.12	-4.05	-3.54	-3.57	-2.93	-3.13	-2.26	-2.05	-0.02	0.19	0.60	0.63	7.61
5	-4.45	-4.04	-3.77	-3.93	-3.26	-3.11	-2.48	-2.4	-0.35	0.21	0.38	0.28	7.95
6	-3.24	-3.19	-2.70	-2.86	-2.06	-2.26	-1.41	-1.33	0.85	1.06	1.45	1.35	8.05
7	-1.92	-1.85	-1.73	-2.03	-0.73	-0.93	-0.44	-0.51	2.18	2.39	2.41	2.17	8.95
8	-1.67	-1.67	-1.44	-1.47	-0.48	-0.74	-0.16	0.05	2.43	2.58	2.70	2.73	8.98
9	-0.60	-0.73	-0.38	-0.61	0.59	0.20	0.90	0.92	3.50	3.52	3.76	3.60	9.55
10	0.13	0.13	0.02	-0.07	1.31	1.06	1.31	1.46	4.22	4.37	4.17	4.14	9.65
11	0.76	0.60	0.67	0.7	1.94	1.52	1.95	2.22	4.85	4.84	4.81	4.90	9.77
12	-0.32	-0.21	-0.06	-0.16	0.86	0.72	1.22	1.37	3.77	4.03	4.08	4.05	9.83
13	1.30	1.41	1.32	1.30	2.49	2.34	2.61	2.83	5.40	5.66	5.46	5.51	9.96
14	0.49	0.48	-0.20	0.74	1.68	1.40	1.08	2.26	4.59	4.72	3.94	4.94	10.09
15	1.05	1.04	1.08	0.00	2.24	1.97	2.37	1.52	5.15	5.29	5.22	4.2	10.10
16	1.30	1.40	1.38	1.39	2.49	2.33	2.67	2.92	5.40	5.65	5.52	5.60	10.10
17	1.10	1.43	-0.03	0.95	2.28	2.35	1.26	2.47	5.19	5.67	4.12	5.15	10.26
18	2.05	2.14	2.02	1.77	3.23	3.07	3.31	3.30	6.14	6.39	6.16	5.98	10.30
19	1.14	1.14	1.15	1.06	2.32	2.07	2.44	2.59	5.23	5.38	5.29	5.27	10.36
20	0.56	0.51	0.66	0.49	1.75	1.44	1.95	2.02	4.66	4.76	4.81	4.70	10.39

Table S3. The error between calculated pK values (after statistical correction) and experiment when using DFT functionals and 3 reference compounds

		$\Delta p K_a = p K_a^{corr} - p K_a^{exp}$												
Comp.		ph	enol		2-hy	droxyl	benzalde	hyde	2-cyanonphenol					
	B3LYP	PBE0	ωB97XD	M062X	B3LYP	PBE0	ωB97XD	M062X	B3LYP	PBE0	ωB97XD	M062X		
1	0.21	0.21	0.04	-0.07	0.21	0.21	0.04	-0.07	0.21	0.21	0.04	-0.07		
2	0.22	0.23	0.22	0.19	0.22	0.23	0.22	0.19	0.22	0.23	0.22	0.19		
3	-0.27	-0.21	-0.13	-0.12	-0.27	-0.21	-0.13	-0.12	-0.27	-0.21	-0.13	-0.12		
4	0.17	0.13	0.19	0.27	0.17	0.13	0.19	0.27	0.17	0.13	0.19	0.27		
5	-0.16	-0.10	-0.11	-0.07	-0.16	-0.10	-0.11	-0.07	-0.16	-0.10	-0.11	-0.07		
6	0.14	0.10	0.18	0.20	0.14	0.10	0.18	0.20	0.14	0.10	0.18	0.20		
7	-0.08	-0.10	-0.09	-0.14	-0.08	-0.10	-0.09	-0.14	-0.08	-0.10	-0.09	-0.14		
8	-0.03	-0.06	-0.02	0.02	-0.03	-0.06	-0.02	0.02	-0.03	-0.06	-0.02	0.02		
9	-0.16	-0.04	-0.09	-0.10	-0.10	-0.16	-0.04	-0.09	-0.10	-0.16	-0.04	-0.09		
10	0.06	0.04	0.03	0.01	0.06	0.04	0.03	0.01	0.06	0.04	0.03	0.01		
11	0.17	0.11	0.16	0.18	0.17	0.11	0.16	0.18	0.17	0.11	0.16	0.18		
12	-0.21	-0.19	-0.12	-0.14	-0.21	-0.19	-0.12	-0.14	-0.21	-0.19	-0.12	-0.14		
13	0.20	0.23	0.25	0.24	0.20	0.23	0.25	0.24	0.20	0.23	0.25	0.24		
14	-0.14	-0.15	-0.34	-0.03	-0.14	-0.15	-0.34	-0.03	-0.14	-0.15	-0.34	-0.03		
15	0.03	0.02	0.08	-0.27	0.03	0.02	0.08	-0.27	0.03	0.02	0.08	-0.27		
16	0.10	0.13	0.18	0.17	0.10	0.13	0.18	0.17	0.10	0.13	0.18	0.17		
17	-0.07	0.03	-0.40	-0.08	-0.07	0.03	-0.40	-0.08	-0.07	0.03	-0.40	-0.08		
18	0.19	0.23	0.26	0.16	0.19	0.23	0.26	0.16	0.19	0.23	0.26	0.16		
19	-0.13	-0.13	-0.07	-0.11	-0.13	-0.13	-0.07	-0.11	-0.13	-0.13	-0.07	-0.11		
20	-0.32	-0.34	-0.26	-0.31	-0.32	-0.34	-0.26	-0.31	-0.32	-0.34	-0.26	-0.31		

	р	henol		phenol anion					
Atom	х	у	z	Atom	х	у	Z		
С	0.267299	1.195992	-5E-06	С	0.289747	1.206222	0.000005		
С	-1.12461	1.217336	0	С	-1.09832	1.19765	-6E-06		
С	-1.85186	0.03077	0.000002	С	-1.81929	0	0		
С	-1.17121	-1.18561	0	С	-1.09832	-1.19765	-6E-06		
С	0.218104	-1.22054	0.000002	С	0.289747	-1.20622	0.000005		
С	0.937017	-0.02626	0	С	1.061567	0	0.000046		
Н	0.75677	-2.1606	0.000006	Н	0.828608	-2.14938	-1.1E-05		
0	2.296897	-0.11329	-1.3E-05	0	2.344764	0	-2.5E-05		
Н	2.685609	0.767808	0.000105	Н	-1.63184	-2.14412	-1.9E-05		
Н	-1.72487	-2.11729	0.000001	Н	-1.63184	2.144117	-1.9E-05		
Н	-1.63875	2.171307	0.000001	Н	0.828608	2.149382	-1.1E-05		
Н	0.832071	2.122422	-1.4E-05	Н	-2.90241	0	-0.00001		
Н	-2.93444	0.052489	0.000004						
	2-hydroxy	lbenzaldehyd	le	2	2-hydroxyll	oenzaldehyd	le anion		
Atom	х	У	Z	Atom	х	у	Z		
С	1.270367	1.274811	0.000134	С	1.388297	1.196832	0.000009		
С	2.298235	0.345707	-6.7E-05	С	2.307477	0.178887	0		
С	2.036873	-1.02969	-0.00022	С	1.90815	-1.17773	-0.00006		
С	0.724401	-1.4612	-0.00018	С	0.559912	-1.45121	-4.5E-05		
С	-0.33457	-0.54105	0.000027	С	-0.42403	-0.43675	-0.00003		
С	-0.05683	0.841369	0.000183	С	-0.04078	0.963579	-0.00013		
0	-1.03041	1.766868	0.000402	0	-0.85438	1.92537	0.000146		
Н	-1.89162	1.307769	0.000447	Н	0.220957	-2.4847	-2.6E-05		
Н	0.491167	-2.52106	-0.0003	н	3.366328	0.420646	0.000046		
н	3.323847	0.696004	-0.0001	н	1.712102	2.232736	0.00009		
Н	1.470891	2.339104	0.000262	н	2.64296	-1.97246	-6.1E-05		
Н	2.851663	-1.74155	-0.00038	С	-1.79845	-0.89415	0.000086		
С	-1.70885	-1.03201	0.000078	н	-1.88416	-2.00153	-4.4E-05		
Ĥ	-1.82899	-2.12711	-0.00052	0	-2.82833	-0.23429	-1.7E-05		
0	-2.69393	-0.30946	-0.00029						
	2-cva	nonhenol			2-cvan	ophenol ani	ion		
Atom	x	v	Z	Atom	x	v	Z		
C	-0.46373	-0.40331	_4E_06	C	0 506422	-0.33181	-5 2E-05		
č	0 416849	-1 49449	-2E-06	č	-0 32095	-1 46812	-1.1E-05		
č	1 782194	-1 27945	0.000001	c	-1 69531	-1 34049	-1.4E-05		
c	2 270757	0.030342	0.000001	C	-2 24691	-0.0431	0.000023		
c	1 409742	1 115566	0.000003	C	-1 45437	1 08194	-0.000023		
č	0.030814	0.910015	_1E_06	c	-0.01672	1.013106	_0.00023		
н	1 781396	2 132459	0.000004	н	_1 8999	2 071357	0.00025		
0	-0 76534	1 999128	0.000004	0	0 721937	2.071337	0.000000		
й	-1 70025	1 757923	_0.00002	н	_2 3329	-2 21477	0.000029		
н	2 463892	-2 11946	0.000001	н	-3 32646	0.072565	0.000097		
н	3 339749	0.205697	0.000001	н	0 140035	-2 45028	0.000039		
н	0.009145	-2 49744	-5E-06	C	1 920584	_0.48977	0.000034		
C	-1 87922	-0.60863	_1 3E_05	N	3.069616	-0.61775	0.000034		
N	-3.02509	-0.7275	0.000014		5.007010	0.01770	0.000001		
	3 5_dini	trophenol (1)	0.000011		3 5_dini	tronhenol a	nion		
Atom	5,5 um	v	7	Atom	v.5 unit	v	7		
C	1 21272	1 21/02	0.000282	C	1 208952	1 250979	0.000112		
c	1 16602	0.17025	0.000285	C	1.2000002	0.1106	0.000112		
c	-1.10002	-0.17023	6 7E 05	C	5E 06	-0.1190	2.5E 05		
c	1 17/21/	-0.90011	-0.71-03	C	1 16500	-0.87432	-3.3E=03		
c	1.174314	1 227701	-0.00037	C	1 20885	1 25080	0.00010		
c	0.00002	1.227701	-0.00035	C	-1.20885	1.23707	0.000123		
с u	-0.00992 2 120055	1.91/923	-2.3E-03		0.000000	2.034//2	0.000203		
п 0	2.130833	1./06238	-0.00039	U Ц	2 160054	3.290134 1 7747	0.0001/9		
ц Ц	0.034213	3.203217	-2.70-03	и п	_1 1E 0F	-1.05141	_0.00012		
п	-0.82032	5.055000	0.000217	п	-1.1E-03	-1.93141	-0.00013		
N	-2.10038	_0.01012	0.000342	N	2.747211 _7 11071	-0.05/5/	_7.3E_05		
N	-2.4403 2 462170	-0.21013	_0.000393	0	3 480000	-0.05/50	_0.00021		
0	_3 /70/9	-0.0/950	0.00072	0	2 /10124	-0.2175	0.00007		
0	-3.47048	-0.20297	-0.000007	0	2.410120	-2.0/103	0.000097		
0	-2.39028	-2.12041	-0.00000	0	-3.4609	-0.21/49	_0.000555		
0	2.40014	2 00040	0.000319	c	1 200052	-2.0/103	-0.00033		
c	2.420073	1 250979	0.000003	C	1.200032	1.2390/0	0.000112		
	1.2000JZ	1.2J70/0	0.000112		2 61	onhanal en	ion		
Atom	2–11u0r	opiicitor (2)	~	A +	2-1100f	opinential an	~ ~		
C	X 0.40100	y 0.60002	Z 0.00001	C	X 0.55075	y 0.62012			
C	-0.46189	1 22005	0.00001	C	-0.339/3	1 20502	-7E-00		
C	1 000045	-1.36093	-0.00004 _7 6E 05		1 92975	-1.38383	0.000021		
C	1.500903	0.742704	-7.0E-03	C	1.03023	-0.74103	0.000034		
C	0.622707	1 412442	-J.7E-03	C	1.00076402	1 200/79	0.000043		
C	0.05570/	1.412442	-8E-00	C	0.070483	1.3904/8	2E 04		
U U	-0.33331	2 404551	0.000027	U U	-0.01/4	0./0/800	-2E-00		
п	0.363323	2.494551	0.000000	п	1.71952	2.4/3/13	6.000002		
0	-1./4368	1.345261	0.000075	0	-1./1853	1.43/143	-6./E-05		
н	-2.46824	0.708175	0.000101	H	2.806552	1.1/6421	0.000061		
н	2.772075	1.310088	-0./E-05	н	0.310818	-2.40/94	0.000019		
н	0.707985	-2.40381	-J.1E-05	п	2.754844	-1.31/31	0.0000//		
Н	2.851534	-1.16614	-0.00012	F	-1./5297	-1.30534	-0.00004		
F	-1.65538	-1.3738	0.000047						
	4–nitro	ophenol (3)			4–nitro	ophenol ani	on		
Atom	X	У	Z	Atom	x	у	Z		
C	1.380415	-1.20223	0.000036	C	-1.41593	1.224659	0.000049		
С	-0.00331	-1.21104	0.000125	C	-0.04827	1.221332	0.000105		

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	1 761220	0.00525	1E 06	C	1 990977	0.0060	0.00065
н	1 395203	-2 20879	0.000003	н	1 / 38/3/	_2 21072	0.000239
0	3 096183	-0.3105	-6E-06	0	3 144434	-0.23641	0.000237
н	3 574613	0.526384	-0L-00	н	1 806087	2 072304	0.000191
н	1 857011	2 05605	-5E-06	н	_0 550/6	2.072304	0.000171
11	0.60592	2.05005	-31-00	11	1.01062	1 04902	0.000048
п	-0.00382	2.324303	0.000003	п	-1.01962	-1.94695	0.000081
н	-1.08009	-1.9369	0.000009	C H	-2.39463	0.38459	-0.00031
C	-2.46064	0.393312	0.000012	н	-2./2416	1.442284	0.000297
Н	-2.80029	1.445079	-0.00002	0	-3.2408	-0.5043	0.000395
0	-3.26866	-0.5103	-1.4E-05				
	4–Pheny	lphenol (9)			4–Phen	ylphenol an	ion
Atom	х	у	Z	Atom	Х	у	Z
С	2.410493	-1.13045	0.386516	С	-2.46498	1.157543	0.335881
С	1.020686	-1.12724	0.385272	С	-1.08097	1.14881	0.330453
С	0.296951	0.004565	-0.00037	С	-0.3425	-7.2E-05	0.000139
С	1.015462	1.142193	-0.38732	С	-1.081	-1.14887	-0.33042
С	2.402754	1.152479	-0.39181	С	-2.46501	-1.1576	-0.33572
С	3.104425	0.01264	-0.00387	С	-3.24013	-0.00019	0.000658
Н	2.95451	-2.01569	0.698206	Н	-3.00043	2.061174	0.61151
Н	0.494144	-2.01746	0.71052	н	-0.55289	2.054263	0.616337
Н	2.954076	2.032074	-0.70173	Н	-3.00048	-2.06103	-0.61194
0	4.464836	0.074121	-0.02594	0	-4.51908	0.000168	-0.00052
Н	4.840495	-0.76872	0.25026	н	-0.55295	-2.05422	-0.61667
н	0.482152	2.029027	-0.71098	С	1,13551	-4.2E-05	0.000052
C	_1 1871	0.00021	0.000211	ĉ	1 864396	_1 15197	0 336489
c	_1.00679	1 13/176	0.3944	c	1.864268	1 1510/5	-0.33646
Ċ	_1 90015	_1 13911	_0 30362	c	3 255207	_1 15/12	0 330013
c	_3 20774	1 120742	0.20225	с u	1 322704	_2 05104	0.556704
U U	-3.29//0	1.130/03	0.39323	п	2 255001	-2.03184	0.020/84
н	-1.3/341	2.019066	0.723044	U U	3.433081	1.134205	-0.33103
C	-3.29108	-1.14359	-0.39124	н	1.333406	2.05177	-0.02668
H	-1.36153	-2.01943	-0.7239	c	3.961468	0.000069	-0.0001
C	-3.99593	-0.00853	0.001458	H	3.789738	-2.05852	0.599222
Н	-3.83676	2.016828	0.707821	Н	3.78951	2.058647	-0.5994
Н	-3.82481	-2.03274	-0.70554	Н	5.044921	0.000112	-0.00017
Н	-5.0794	-0.01186	0.001886	С	-2.46498	1.157543	0.335881
С	2.410493	-1.13045	0.386516	С	-1.08097	1.14881	0.330453
С	1.020686	-1.12724	0.385272	С	-0.3425	-7.2E-05	0.000139
С	0.296951	0.004565	-0.00037	С	-1.081	-1.14887	-0.33042
С	1.015462	1.142193	-0.38732				
	3–Methox	yphenol (10)			3-Metho	xyphenol a	nion
Atom	х	у	Z	Atom	х	у	Z
С	1.731493	1.028845	-5E-06	С	1.790703	0.988005	0.000144
Ċ	0.563515	1.777573	0.000003	Ċ	0.638164	1.750552	0.000227
Č	-0.69368	1.174835	0.000019	Č	-0.64219	1.178058	0.000177
c	-0.76705	-0.22021	0.000022	č	-0.71719	-0 21878	-1.1E-05
c	0 397252	_0.99055	0.0000022	č	0 429547	-1.00747	_9 1E_05
c	1.635519	-0.36528	_4E_06	c	1 740438	_0 44739	0.000054
н	0.320751	-2 07137	0.000002	н	0.310336	_2.08604	-0.00026
0	2 735662	-1 1686	_2E_06	0	2 708764	_1.17106	_0.00020
U U	2.735002	-1.1000	0.00012	u U	2.755909	1 464226	0.000158
п	3.333490	-0.03109	-0.00013	п	2.703898	1.404550	0.000138
п	2.702011	1.51057	-1.1E-03	п	1.52227	2.855494	0.000328
п	0.0281	2.639211	0.000002	п	-1.32257	0.00745	0.000245
п	-1.38320	1.787985	0.000031	0	-1.90431	-0.90743	-0.00011
0	-1.92992	-0.92076	0.000043	C H	-3.10165	-0.15301	-0.0001
U U	-3.14488	-0.1868/	-4.6E-05	н	-3.91658	-0.8/434	-0.00023
н	-3.9425	-0.92524	-8.2E-05	н	-3.1/38	0.4/5508	0.891577
н	-3.22466	0.105.05	0.000405	**	2 1 2 2 6 0	0.488.400	0.001.66
H	2 22 4 5 4	0.437687	0.893185	Н	-3.17368	0.475698	-0.89166
	-3.22454	0.437687 0.437655	0.893185	Н	-3.17368	0.475698	-0.89166
Atom	-3.22454 4-(2-aminoe	0.437687 0.437655 thyl)phenol (0.893185 -0.89331 11)	H	-3.17368	0.475698 ethyl)pheno	-0.89166
Atom	-3.22454 4-(2-aminoer x	0.437687 0.437655 thyl)phenol (y	0.893185 -0.89331 11) z	H Atom	-3.17368 1-(2-amino <u>x</u> 1.754461	0.475698 ethyl)pheno y	-0.89166
Atom C	-3.22454 4-(2-aminoer x 1.704712 0.342250	0.437687 0.437655 thyl)phenol (y 1.189525	0.893185 -0.89331 (11) z 0.021236 0.205508	H Atom C	-3.17368 4-(2-amino x 1.754461 0.205018	0.475698 ethyl)pheno y 1.198654	-0.89166 bl anion <u>z</u> 0.011355 0.300127
Atom C C	-3.22454 4-(2-aminoe x 1.704712 0.342369 0.27707	0.437687 0.437655 thyl)phenol (<u>y</u> 1.189525 1.196794 0.010411	0.893185 -0.89331 (11) z 0.021236 0.306608 0.447055	H Atom C C	-3.17368 4-(2-amino x 1.754461 0.395918 0.22006	0.475698 ethyl)pheno y 1.198654 1.19361 0.0055522	-0.89166 bl anion z 0.011355 0.300137 0.442017
Atom C C C	-3.22454 4-(2-aminoet x 1.704712 0.342369 -0.37797 0.311100	0.437687 0.437655 thyl)phenol (y 1.189525 1.196794 0.010411 -1.19505	0.893185 -0.89331 (11) 2 0.021236 0.306608 0.447066 0.280681	H Atom C C C C	-3.17368 4-(2-amino x 1.754461 0.395918 -0.32996 0.380841	0.475698 ethyl)pheno y 1.198654 1.19361 0.005562 -1 18012	-0.89166 J anion 2 0.011355 0.300137 0.443917 0.281051
Atom C C C C	-3.22454 4-(2-aminoe x 1.704712 0.342369 -0.37797 0.311199 1.670677	0.437687 0.437655 thyl)phenol (y 1.189525 1.196794 0.010411 -1.19505 1.22162	0.893185 -0.89331 11) z 0.021236 0.306608 0.447066 0.289681 0.021660	H Atom C C C C C	-3.17368 4-(2-amino x 1.754461 0.395918 -0.32996 0.380841 1.720201	0.475698 ethyl)pheno y 1.198654 1.19361 0.005562 -1.18913 1.20224	-0.89166 Janion 2 0.011355 0.300137 0.443917 0.281961 0.07212
Atom C C C C C C	-3.22454 4-(2-aminoe x 1.704712 0.342369 -0.37797 0.311199 1.670837 2.260822	0.437687 0.437655 thyl)phenol (y 1.189525 1.196794 0.010411 -1.19505 -1.22163 0.23427	0.893185 -0.89331 11) z 0.021236 0.306608 0.447066 0.289681 0.004699 0.12527	H Atom C C C C C C C	-3.17368 4-(2-amino x 1.754461 0.395918 -0.32996 0.380841 1.739204 1.739204	0.475698 ethyl)pheno y 1.198654 1.19361 0.005562 -1.18913 -1.20704 0.00775	-0.89166 2 0.011355 0.300137 0.443917 0.281961 -0.00743 0.12722
Atom C C C C C C C	-3.22454 4-(2-aminoet x 1.704712 0.342369 -0.37797 0.311199 1.670837 2.369883 2.24045	0.437687 0.437655 thylphenol (y 1.189525 1.196794 0.010411 -1.19505 -1.22163 -0.02436 2.123516	0.893185 -0.89331 11) z 0.021236 0.306608 0.447066 0.289681 0.004699 -0.13077 0.0722	H Atom C C C C C C C C	-3.17368 4-(2-amino x 1.754461 0.395918 -0.32996 0.380841 1.739204 2.502381 2.255015	0.475698 ethyl)pheno y 1.198654 1.19361 0.005562 -1.18913 -1.20704 -0.00776 2.141062	-0.89166 bl anion z 0.011355 0.300137 0.443917 0.281961 -0.00743 -0.16278 0.06271
Atom C C C C C C C H	-3.22454 4-(2-aminoet x 1.704712 0.342369 -0.37797 0.311199 1.670837 2.369883 2.24945 2.24945	0.437687 0.437655 (tyl)phenol (y 1.189525 1.196794 0.010411 -1.19505 -1.22163 -0.02436 2.122518	0.893185 -0.89331 11) Z 0.021236 0.306608 0.447066 0.289681 0.004699 -0.13077 -0.0793 -0.0793	H Atom C C C C C C C C C H H	-3.17368 4-(2-amino x 1.754461 0.395918 -0.32996 0.380841 1.739204 2.502381 2.285918 0.12027	0.475698 ethyl)pheno y 1.198654 1.19361 0.005562 -1.18913 -1.20704 -0.00776 2.141092	-0.89166 2 anion 2 0.011355 0.300137 0.443917 0.281961 -0.00743 -0.16278 -0.08641 -0.08641 -0.08641
Atom C C C C C C H H	-3.22454 4-(2-aminoet x 1.704712 0.342369 -0.37797 0.311199 1.670837 2.369883 2.24945 -0.16693 0.26555	0.437687 0.437655 thyl)phenol (y 1.189525 1.196794 0.010411 -1.19505 -1.22163 -0.02436 2.122518 2.148029	0.893185 -0.89331 11) z 0.021236 0.306608 0.447066 0.289681 0.004699 -0.13077 -0.0793 0.424894 0.024894	H Atom C C C C C C C H H H	-3.17368 4-(2-amino x 1.754461 0.395918 -0.32996 0.380841 1.739204 2.502381 2.285918 -0.12196 0.12196	0.475698 ethyl)phene y 1.198654 1.19361 0.005562 -1.18913 -1.20704 -0.00776 2.141092 2.143087	-0.89166 2 0.011355 0.300137 0.443917 0.281961 -0.00743 -0.16278 -0.08641 0.421946 0.308641
Atom C C C C C C H H H	-3.22454 4-(2-aminoet x 1.704712 0.342369 -0.37797 0.311199 1.670837 2.369883 2.24945 -0.16693 -0.22519 -0.22519	0.437687 0.437655 (thylphenol (y 1.1895255 1.196794 0.010411 -1.19505 -1.22163 -0.02436 2.122518 2.148029 -2.13281	0.893185 -0.89331 11) z 0.021236 0.306608 0.447066 0.289681 0.004699 -0.13077 -0.0793 0.424894 0.39611 0.1122	H Atom C C C C C C C H H H H	-3.17368 4-(2-amino x 1.754461 0.395918 -0.32996 0.380841 1.739204 2.502381 2.285918 -0.12196 -0.14873 -0.14873	0.475698 ethyl)phene y 1.198654 1.19361 0.005562 -1.18913 -1.20704 -0.00776 2.141092 2.143087 -2.13382 -1.3382	-0.89166 2 anion 2 0.011355 0.300137 0.443917 0.281961 -0.00743 -0.16278 -0.08641 0.421946 0.389989
Atom C C C C C H H H H H	-3.22454 4-(2-aminoet x 1.704712 0.342369 -0.37797 0.311199 1.670837 2.369883 2.24945 -0.16693 -0.22519 2.201231	0.437687 0.437655 (hyl)phenol (y 1.189525 1.196794 0.010411 -1.19505 -1.22163 -0.02436 2.122518 2.148029 -2.13281 -2.15936	0.893185 -0.89331 11) z 0.021236 0.306608 0.447066 0.289681 0.004699 -0.13077 -0.0793 0.424894 0.39611 -0.1113 -0.1113	H Atom C C C C C C C C H H H H H	-3.17368 4-(2-amino x 1.754461 0.395918 -0.32996 0.380841 1.739204 2.02381 2.285918 -0.12196 -0.14873 2.258665	0.475698 ethyl)pheno y 1.198654 1.19361 0.005562 -1.18913 -1.20704 -0.00776 2.141092 2.143087 -2.13382 -2.15452	-0.89166 2 anion 2 0.011355 0.300137 0.443917 0.281961 -0.00743 -0.16278 -0.08641 0.421946 0.389989 -0.11976
Atom C C C C C H H H H H O	-3.22454 4 -(2-aminoet x 1.704712 0.342369 -0.37797 0.311199 1.670837 2.369883 2.24945 -0.16693 2.24945 -0.16693 0.22519 2.201231 3.704126	0.437687 0.437655 thylphend (y 1.189525 1.196794 0.010411 -1.19505 -1.22163 -0.02436 2.122518 2.148029 -2.13281 -2.15936 -0.10084 -0.10084	0.893185 -0.89331 11) z 0.021236 0.021236 0.02489681 0.004699 -0.13077 -0.0793 0.424894 0.39611 -0.1113 -0.4858	H Atom C C C C C C C H H H H H O O	-3.17368 4(2-amino x 1.754461 0.395918 -0.32996 0.380841 1.739204 2.202381 2.285918 -0.12196 -0.12196 -0.124873 2.258665 3.75984	0.475698 thyl)phene y 1.198654 1.093654 1.03562 -1.18913 -1.20704 -0.00776 2.141092 2.143087 -2.13382 -2.15452 -0.01355	-0.89166 2 0.011355 0.300137 0.443917 0.281961 -0.00743 -0.16278 -0.08641 0.421946 0.389989 -0.11976 -0.43076 -0.43076
Atom C C C C C C H H H H H H H H H	-3.22454 4-(2-aminoet x 1.704712 0.342369 -0.37797 0.311199 1.670837 2.369883 2.24945 -0.16693 -0.22519 -0.22519 2.201231 3.704126 4.078246 4.078246	0.437687 0.437655 thyl)phenol (y 1.189525 1.196794 0.010411 -1.19505 -1.22163 -0.02436 2.122518 2.148029 -2.13281 -2.15936 -0.10084 0.784175	0.893185 -0.8931 11) z 0.021236 0.306608 0.447066 0.289681 0.004699 -0.13077 -0.0793 0.424894 0.39611 -0.1113 -0.40858 -0.47519	H Atom C C C C C C C C C H H H H H O C C	-3.17368 4-(2-amino x 1.754461 0.395918 -0.32996 0.380841 1.739204 2.500381 2.258653 2.258655 3.759984 -1.81692	0.475698 ethyl)pheno y 1.198654 1.19361 0.005562 -1.18913 -1.20704 -0.00776 2.141092 2.143087 -2.13452 -0.01355 0.01531 0.01531	-0.89166 2 0.011355 0.300137 0.443917 0.281961 -0.00743 -0.16278 -0.08641 0.421946 0.389989 -0.11976 -0.43076 0.697887
Atom C C C C C C H H H H O H C	-3.22454 4-(2-aminoe' x 1.704712 0.342369 -0.37797 0.311199 1.670837 2.369883 2.24945 -0.16693 -0.22519 2.201231 3.704126 4.078246 -1.86369 -0.8639	0.437687 0.437655 thyl)phenol (y 1.189525 1.196794 0.010411 -1.19505 -1.22163 -0.02436 2.122518 2.148029 -2.13281 -2.15936 -0.10084 0.784175 0.03036	0.893185 -0.89331 11) z 0.021236 0.306608 0.447066 0.289681 0.004699 -0.13077 -0.0793 0.424894 0.39611 -0.1113 -0.42858 -0.47519 0.702333	H Atom C C C C C C C C C H H H H H O C C H	-3.17368 4-(2-amino) x 1.754461 0.395918 -0.32996 0.380841 1.739204 2.502381 2.285918 -0.12196 -0.14873 2.258665 3.75998 -1.81692 -2.10428	0.475698 ethyl)phene y 1.198654 1.19361 0.005562 0.005562 2.143087 -2.1382 -2.15452 -0.01551 -0.87299 -0.01571 -0.87299	-0.89166 2 anion 2 0.011355 0.300137 0.443917 0.281961 -0.00743 -0.16278 -0.08641 0.421946 0.389989 -0.11976 -0.43076 0.697887 1.272566
Atom C C C C C C C H H H H C H	-3.22454 4-(2-aminoeu x 1.704712 0.342369 -0.37797 0.311199 1.670837 2.369883 2.24945 -0.16693 -0.22519 2.201231 3.704126 4.078246 -1.86369 -2.15108	0.437687 0.437655 (hyl)phenol (y 1.189525 1.196794 0.010411 -1.19505 -1.22163 -0.02436 2.122518 2.148029 -2.13281 -2.15936 -0.10084 0.784175 0.03036 -0.84724	0.893185 -0.8931 11) z 0.021236 0.306608 0.447066 0.289681 0.004699 -0.13077 -0.0793 0.424894 0.39611 -0.1113 -0.40858 -0.47519 0.702233 1.29059	H Atom C C C C C C C H H H H O C H H H	-3.17368 4-(2-amino x 1.754461 0.395918 -0.329518 -0.329548 1.739204 2.502381 2.285918 -0.12196 -0.14273 2.258665 3.759984 -1.81692 -2.10428 -2.10428 -2.09776	0.475698 ethylphene y 1.198654 1.19361 0.005562 -1.18913 -1.20704 -0.00776 2.141092 2.143087 -2.13382 -2.15452 -0.01355 0.01551 -0.87279 0.887719	-0.89166 2 anion 2 0.011355 0.300137 0.443917 0.281961 -0.00743 -0.16278 -0.08641 0.421946 0.389989 -0.11976 -0.43076 0.697887 1.272566 1.295667
Atom C C C C C C H H H O H C H H	-3.22454 4-(2-aminoeu x 1.704712 0.342369 -0.37797 0.311199 1.670837 2.369883 2.24945 -0.16693 2.26198 2.201231 3.704126 4.078246 -1.86369 -2.15108 -2.15108 -2.13754	0.437687 0.437655 thylphenol (y 1.189525 1.196794 0.010411 -1.196794 0.010411 -1.196794 0.02436 2.122518 2.148029 2.13281 -2.15936 -0.10084 0.784175 0.03036 -0.84724 0.915485	0.893185 -0.89331 11) 2 0.021236 0.306608 0.447066 0.289681 0.044699 -0.13077 0.424894 0.39611 -0.01793 0.424894 0.39611 -0.1113 -0.40858 -0.47519 0.702333 1.29059 1.282501	H Atom C C C C C C C H H H H H H C H H C	-3.17368 4-(2-amino x 1.754461 0.395918 -0.32996 0.380841 1.739204 2.502381 2.285918 -0.12196 -0.14873 2.258665 3.759984 -1.81692 -2.10428 -2.07076 -2.63039	0.475698 ethyl)phene y 1.198654 1.9361 0.005562 -1.18913 -1.20704 -0.00776 2.141092 2.143087 -2.13382 -2.15452 -0.01355 0.01531 -0.87279 0.039002	-0.89166 2 0.011355 0.300137 0.443917 0.281961 -0.00743 -0.08641 0.421946 0.389989 -0.11976 -0.43076 0.697887 1.272566 1.2963677 -0.59717
Atom C C C C C C C H H H C H H C	-3.22454 4-(2-aminee' x 1.704712 0.342369 -0.37797 0.311199 1.670837 2.369883 2.24945 -0.16693 -0.22519 2.201231 3.704126 4.078246 -1.86369 -2.15108 -2.15108 -2.15108 -2.15108	0.437687 0.437655 thyl)phenol (y 1.189525 1.196794 0.010411 -1.19505 -1.22163 -0.02436 2.122518 2.148029 -2.13281 -2.15936 -0.10084 0.784175 0.03036 -0.84724 0.915485 0.034386	$\begin{array}{c} 0.893185 \\ -0.89331 \\ \hline 111 \\ \hline \\ \hline \\ 2 \\ 0.021236 \\ 0.306608 \\ 0.447066 \\ 0.289681 \\ 0.004699 \\ -0.13077 \\ -0.0793 \\ 0.424894 \\ 0.39611 \\ -0.01113 \\ -0.0753 \\ 0.424894 \\ 0.39611 \\ -0.113 \\ -0.40558 \\ -0.47519 \\ 0.702333 \\ 1.29059 \\ 1.282501 \\ -0.60303 \\ \end{array}$	H Atom C C C C C C C C H H H H O C C H H H C H	-3.17368 4-(2-amino) x 1.754461 0.395918 -0.32996 0.380841 1.739204 2.205918 -0.12196 -0.14873 2.258665 3.759984 -1.81692 -2.10428 -2.0976 -2.63039 -2.32813	0.475698 ethyl)phene y 1.198654 1.198654 1.09361 0.09362 -1.18913 -1.20704 -0.00776 2.141092 2.141092 -2.15452 -0.01355 0.01531 -0.87299 0.887719 0.039002 -0.81576	-0.89166 2 anion 2 0.011355 0.300137 0.443917 0.281961 -0.00743 -0.16278 -0.08641 0.421946 0.389989 -0.11976 -0.43076 0.697887 1.272566 1.296367 -0.59717 -1.21773
Atom C C C C C C C H H H H C H H C H	-3.22454 4-(2-aminoe x 1.704712 0.342369 -0.37797 0.311199 1.670837 2.369883 2.24945 -0.16693 -0.22519 2.201231 3.704126 4.078246 -1.86369 -2.15108 -2.15108 -2.13754 -2.66156 -2.35645	0.437687 0.437655 thyl)phenol (y 1.189525 1.196794 0.010411 -1.19505 -1.22163 -0.02436 2.122518 2.148029 -2.13281 -2.15936 -0.10084 0.784175 0.03036 -0.84724 0.915485 0.034386 -0.83154	0.893185 -0.89331 11) z 0.021236 0.306608 0.447066 0.289681 0.004699 -0.13077 -0.0793 0.424894 0.39611 -0.1113 -0.424894 0.424894 0.39611 -0.113 1.29059 1.282501 -0.60303 -1.20629	H Atom C C C C C C C C C C H H H H H C H H H H H H	-3.17368 4.(2-amino) x 1.754461 0.395918 -0.32996 0.380841 1.739204 2.2685918 -0.12196 -0.12496 -0.14873 2.258665 3.75984 -1.81692 -2.10428 -2.00776 -2.3039 -2.32813 -2.328324	0.475698 ethyl)phene y 1.198654 1.19361 0.005562 -1.18913 -1.20704 -0.00776 2.141092 2.143087 -2.13382 -2.15452 -0.015531 -0.87719 0.039002 -0.81576 0.946312	-0.89166 2 anion 2 0.011355 0.300137 0.443917 0.281961 -0.00743 -0.16278 -0.08641 0.421946 0.389989 -0.11976 -0.43076 -0.697887 1.272566 1.296367 -0.59717 -1.21773 -1.15577
Atom C C C C C C C C H H H C H H C H H	-3.22454 4 -(2-aminoeu x 1.704712 0.342369 -0.37797 0.311199 1.670837 2.369883 2.24945 -0.16693 -0.22519 2.201231 3.704126 4 .078246 4 .078246 4 .078246 4 .078246 4 .078246 4 .213754 -2 .66156 -2 .35645 -2 .40564	0.437687 0.437655 thylphenol (y 1.189525 1.196794 0.010411 -1.19505 -1.22163 -0.02436 2.122518 2.148029 2.13281 -2.15936 -0.10084 0.784175 0.03036 -0.84724 0.915485 0.034386 -0.83154 0.931429	0.893185 -0.8931 11) z 0.021236 0.306608 0.447066 0.289681 0.004699 -0.13077 -0.0793 0.424894 0.39611 -0.1113 -0.40858 -0.47519 0.702333 1.29059 1.282501 -0.60303 -1.20629 -1.20629 -1.2078	H Atom C C C C C C C C C C C C C C H H H H C H H H H N	-3.17368 4-(2-amino x 1.754461 0.395918 -0.32996 0.380841 1.739204 2.285918 -0.12196 -0.142196 -0.142196 -0.142196 -0.142196 -0.142196 -0.142196 -0.142196 -0.142196 -0.142196 -0.142196 -0.14219 -	0.475698 ethylphene y 1.198654 1.19361 0.005562 -1.18913 -1.20704 -0.00776 2.141092 2.143087 -2.13382 -2.15452 -0.01355 0.01551 -0.87279 0.887719 0.039002 -0.81576 0.946312 0.056841	-0.89166 2 anion 2 0.011355 0.300137 0.443917 0.281961 -0.00743 -0.06241 0.421946 0.389989 -0.11976 -0.43076 0.697887 1.272566 1.296367 -0.59717 -1.21773 -1.15577 -0.30563
Atom C C C C C C C C H H H C H H C H H N	-3.22454 4 -(2-aminoet x 1.704712 0.342369 -0.37797 0.311199 1.670837 2.369883 2.24945 -0.16693 0.22519 2.201231 3.704126 4.078246 -1.86369 -2.15108 -2.15108 -2.13754 -2.66156 -2.35645 -2.40564 -4.09914	0.437687 0.437655 thyl)phenol (y 1.189525 1.196794 0.010411 -1.19505 -1.22163 -0.02436 2.122518 2.148029 -2.13281 -2.15936 -0.10084 0.784175 0.03036 -0.84724 0.915485 0.034386 -0.83154 0.931429 0.063573	0.893185 -0.89331 11) 2 0.021236 0.306608 0.447066 0.289681 0.004699 -0.13077 0.424894 0.39611 -0.1113 -0.40858 -0.47519 0.702333 1.29059 1.29059 1.29059 -0.60303 -1.20629 -1.17368 -0.32042	H Atom C C C C C C C C C H H H H O C H H H C H H N H	-3.17368 4-(2-amino) x 1.754461 0.395918 -0.32996 0.380841 1.739204 2.265918 2.285918 -0.12196 -0.14873 2.258665 3.759984 -1.81692 -2.10428 -2.0073 -2.3039 -2.32813 -2.3324 -4.06878	0.475698 ethyl)phene y 1.198654 1.198654 1.093662 -0.138913 -1.20704 -0.00776 2.143087 -2.13382 -2.143087 -2.13382 -0.01355 0.01531 -0.87299 0.887719 0.887719 0.887719 0.837012 -0.81576 0.946312 0.056841 -0.81389	-0.89166 2 anion 2 0.011355 0.300137 0.443917 0.281961 -0.00743 -0.16278 -0.08641 0.421946 0.389989 -0.11976 -0.43076 0.697887 1.272566 1.292667 -0.59717 -1.21773 -1.5577 -0.30563 0.147032
Atom C C C C C C C C H H H C H H C H H N H	-3.22454 4-(2-aminoev x 1.704712 0.342369 -0.37797 0.311199 1.670837 2.369883 2.24945 -0.16693 -0.22519 2.201231 3.704126 4.078246 -1.86369 -2.15108 -2.15108 -2.15108 -2.35645 -2.35645 -2.35645 -2.40564 4.09914 -4.37651	0.437687 0.437655 thyl)phenol (y 1.189525 1.196794 0.010411 -1.19505 -1.22163 -0.02436 2.122518 2.148029 -2.13281 -2.13281 -2.15936 -0.10084 0.784175 0.03036 -0.84724 0.915485 0.034386 -0.83154 0.931429 0.063573 -0.80683	0.893185 -0.89331 11) z 0.021236 0.306608 0.447066 0.289681 0.004699 -0.13077 -0.0793 0.424894 0.39611 -0.1113 -0.424894 0.39611 -0.47519 0.702333 1.29059 1.282501 -0.60303 -1.20629 -1.17368 -0.32042 0.124243	H Atom C C C C C C C C C H H H H H C H H H H	-3.17368 4-(2-amino) x 1.754461 0.395918 -0.32906 0.380841 1.739204 2.285918 -0.12196 -0.14873 2.258655 3.75984 -1.81692 -2.10428 -2.09776 -2.63039 -2.32813 -2.38324 -4.06878 -4.32246 -4.59967	0.475698 ethyl)phene y 1.198654 1.19361 0.005562 -1.18913 -1.20704 -0.00776 2.141092 2.143087 -2.13382 -2.15452 -0.01551 -0.87299 0.87719 0.039002 -0.81576 0.946312 0.056841 -0.81389 0.094076	-0.89166 2 anion 2 0.011355 0.300137 0.443917 0.281961 -0.00743 -0.16278 -0.08641 0.421946 0.389989 -0.11976 -0.43076 0.697887 1.272566 1.296367 -0.59717 -1.21773 -1.15577 -0.30563 0.147032 -1.16998
Atom C C C C C C C H H H C H H C H H H N H H	-3.22454 4-(2-aminoe x 1.704712 0.342369 -0.37797 0.311199 1.670837 2.369883 2.24945 -0.16693 -0.22519 2.201231 3.704126 4.078246 -1.86369 -2.15108 -2.15108 -2.13754 -2.66156 -2.35645 -2.40564 -4.09914 -4.37651 -4.62334	0.437687 0.437655 thyl)phenol (y 1.189525 1.196794 0.010411 -1.19505 -1.22163 -0.02436 2.122518 2.148029 -2.13281 -2.13281 -2.13281 -2.13284 0.784175 0.03036 -0.84724 0.915485 0.034386 -0.83154 0.931429 0.063573 -0.80683 0.115202	0.893185 -0.8931 11) z 0.021236 0.306608 0.447066 0.289681 0.004699 -0.13077 -0.0793 0.0289681 0.004699 -0.13077 -0.0793 0.424894 0.39611 -0.1113 -0.40858 -0.47519 0.702333 1.29059 1.282501 -0.60303 -1.20629 -1.1368 -0.124243 -0.124243 -1.1879	H Atom C C C C C C C C C C C C C C C C C C C	-3.17368 4.(2-amino) x 1.754461 0.395918 -0.32996 0.380841 1.739204 2.502381 2.285918 -0.12196 -0.14873 2.258665 3.75998 -0.12196 -1.81692 -2.10428 -2.0776 -2.63039 -2.32813 -2.38124 -4.06878 -4.33246 -4.59967	0.475698 ethyl)phene y 1.198654 1.19361 0.00556 2.143087 -2.13382 -2.15452 -0.01355 0.01551 -0.87709 0.837012 0.05841 -0.81389 0.04076	-0.89166 2 anion 2 0.011355 0.300137 0.443917 0.281961 -0.00743 -0.16278 -0.08641 0.421946 0.389989 -0.11976 -0.43076 -0.697887 1.272566 1.296367 -0.59717 -1.21773 -1.15577 -0.30563 0.147032 -1.16998
Atom C C C C C C C C C C C C C C C C C C C	-3.22454 4-(2-aminoe) x 1.704712 0.342369 -0.37797 0.311199 1.670837 2.369883 2.24945 0.16693 -0.22519 2.201231 3.704126 4.078246 -1.86369 -2.15108 -2.15108 -2.15108 -2.15108 -2.15108 -2.35645 -2.40564 -4.09914 -4.37651 -4.62334 4-(hydroxylm	0.437687 0.437655 thyl)phenol (y 1.189525 1.196794 0.010411 -1.19505 -1.22163 -0.02436 2.122518 2.148029 -2.13281 -2.15936 -0.10084 0.784175 0.03036 -0.84724 0.784175 0.03036 -0.84724 0.915485 0.034386 -0.83154 0.931429 0.063573 -0.80683 0.115202 ethyl)phenol	0.893185 -0.8931 11) z 0.021236 0.306608 0.447066 0.289681 0.004699 -0.13077 -0.0793 0.424894 0.39611 -0.1113 -0.424894 0.424894 0.424894 0.424894 0.424894 0.424894 0.424894 0.424894 0.424894 0.424894 0.424894 0.29059 1.282501 -0.60303 -1.20629 -1.17368 -0.32042 0.124243 0.124243 0.124243	H Atom C C C C C C C C C C C C C H H H H C H H H H H H C C Atom Atom Atom Atom Atom Atom Atom Atom	-3.17368 4.(2-amino) x 1.754461 0.395918 -0.32996 0.380841 1.739204 2.502381 2.285918 -0.12196 -0.12196 -0.14873 2.258665 3.759984 -1.81692 -2.10428 -2.09776 -2.32813 -2.38324 -4.06878 -4.33246 -4.59967 -(hydroxylr	0.475698 ethyl)phend y 1.198654 1.19361 0.005562 -1.18913 -1.20704 -0.00776 2.141092 2.143087 -2.13382 -2.15452 -0.01551 -0.87719 0.035002 -0.81776 0.946312 0.056841 -0.81389 0.094076 entyl)phendix	-0.89166 2 anion 2 0.011355 0.300137 0.443917 0.281961 -0.00743 -0.16278 -0.08641 0.421946 0.389989 -0.11976 -0.43076 -0.43076 0.697887 1.272566 1.296367 -0.59717 -1.21773 -1.15577 -0.30563 0.147032 -1.16998 tol anion
Atom C C C C C C C C C C C C C C C C C C C	-3.22454 4-(2-aminoet x 1.704712 0.342369 -0.37797 0.311199 1.670837 2.369883 2.24945 -0.16693 2.201231 3.704126 4.078246 4.078246 -2.86369 -2.15108 -2.15108 -2.15754 -2.66156 -2.35645 -2.40564 -4.09914 -4.62334 4-(hydroxylm x	0.437687 0.437655 thyl)phenol (y 1.189525 1.196794 0.010411 -1.19505 -1.22163 -0.02436 0.122518 2.148029 -2.13281 -2.15936 -0.10084 0.784175 0.03036 -0.84724 0.915485 0.034386 -0.83154 0.9315429 0.063573 -0.80683 0.115202 ethyl)phenol y	0.893185 -0.89331 11) 2 0.021236 0.306608 0.447066 0.289681 0.0447066 0.289681 0.0447086 0.447066 0.447066 0.447066 0.447068 0.447086 0.447086 0.447086 0.447086 0.447086 0.447086 0.428581 -0.40858 -0.47519 0.702333 -1.282501 -0.60303 -1.282501 -0.60303 -1.282501 -0.60303 -1.282501 -0.32042 0.32042 -1.17368 -0.32042 -1.1879 (12)	H Atom C C C C C C C C C C C C C C C C C C C	-3.17368 4.(2-amino x 1.754461 0.395918 -0.32996 0.380841 1.739204 2.502381 2.285918 -0.12196 -0.14287 2.258665 3.759984 -1.81692 -2.10428 -2.09776 -2.63039 -2.32813 -2.32813 -4.06878 -4.33246 -4.69878 -4.33246 -4.69967 x	0.475698 ethylphene y 1.198654 1.19361 0.005562 -1.18913 -1.20704 -0.00776 2.141092 2.143087 -2.13382 -2.15452 -0.01551 -0.81576 0.036021 -0.81576 0.946312 0.056841 -0.81889 0.0946312 0.0946512 0.0946552 0.0946552 0.0946552 0.09	-0.89166 2 anion 2 0.011355 0.300137 0.443917 0.281961 -0.0743 -0.16278 -0.08641 0.421946 0.389989 -0.11976 -0.43076 -0.43076 1.272566 1.296367 -0.59717 -1.21773 -1.5577 -0.30563 0.147032 -1.16998 totanion z
Atom C C C C C C C C C C C C C C C C C C C	-3.22454 4-(2-aminee' x 1.704712 0.342369 -0.37797 0.311199 1.670837 2.369883 2.24945 -0.16693 -0.22519 2.201231 3.704126 4.078246 -1.86369 -2.15108 -2.15108 -2.15108 -2.15108 -2.35645 -2.40564 -4.09914 -4.37651 -4.62334 4-(hydroxylm x 1.195917 x	0.437687 0.437655 thyl)phenol (y 1.189525 1.196794 0.010411 -1.19505 -1.22163 -0.02436 2.122518 2.148029 -2.13281 -2.15936 -0.10084 0.784175 0.03036 -0.84724 0.915485 0.034386 -0.83154 0.931429 0.063573 -0.80683 0.115202 ethyl)phenol y 1.193772 2.193762 -0.10084 -0.10084 -0.8154 -0.115202 -0.115	0.893185 -0.89311 z 0.021236 0.306608 0.447066 0.289681 0.004699 -0.13077 0.424894 0.39611 -0.01793 0.424894 0.39611 -0.1113 -0.40858 -0.47519 0.702333 1.282501 -0.60303 -1.20629 -1.17368 -0.32042 0.124243 -1.1879 (12) z 0.004572	H Atom C C C C C C C C C C C C C C C C C C C	-3.17368 4-(2-amino x 1.754461 0.395918 -0.32996 0.380841 1.739204 2.205918 2.285918 -0.12196 -0.14873 2.258665 3.759984 -1.81692 -2.0428 -2.09769 -2.32813 -2.38324 -4.33246 -4.35967 -4.359767 -4.35977 -4.359777 -4.3597777 -4.35977	0.475698 ethyl)phene y 1.198654 1.198654 1.198654 1.198654 1.1987 -2.13813 -1.20704 -0.003502 2.141092 2.143087 -2.13382 -2.15452 -0.01355 0.01531 -0.87719 0.887719 0.887719 0.887719 0.887719 0.039002 -0.81576 0.946312 0.056841 -0.03839 0.094076 methyl)phet y 1.20646	-0.89166 2 anion 2 0.011355 0.300137 0.443917 0.281961 -0.00743 -0.16278 -0.08641 0.421946 0.389989 -0.11976 -0.431946 0.697887 1.272566 1.296367 -0.59717 -1.21773 -1.15577 -0.30563 0.147032 -1.16998 tol anion 2 -0.01896 -0.01896
Atom C C C C C C C C C C H H H C H H H C H H H K M C C C C C C C C C C C C C C C C C C	-3.22454 4-(2-aminoe x 1.704712 0.342369 -0.37797 0.311199 1.670837 2.369883 2.24945 -0.16693 -0.22519 2.201231 3.704126 4.078246 -1.86369 -2.15108 -2.15108 -2.13754 -2.66156 -2.35645 -2.40564 -4.09914 -4.37651 -4.62334 4-(hydroxylm x 1.195917 -0.18303 -0.18303 -0.18303 -0.18303 -0.18303 -0.1622 -0.18303 -0.1622 -0.18303 -0.18303 -0.18303 -0.18303 -0.18303 -0.18303 -0.18303 -0.18303 -0.18303 -0.18303 -0.18303 -0.18303 -0.1622 -	0.437687 0.437655 thyl)phenol (y 1.189525 1.196794 0.010411 -1.19505 -1.22163 -0.02436 2.122518 2.148029 -2.13281 -2.15936 -0.10084 0.784175 0.03036 -0.84724 0.91548 0.034386 -0.83154 0.931429 0.063573 -0.80683 0.115202 ethyl)phenol y 1.193772 1.228527	0.893185 -0.89331 11) z 0.021236 0.306608 0.447066 0.289681 0.004699 -0.13077 -0.0793 0.424894 0.39611 -0.1713 0.424894 0.39611 -0.47519 0.702333 1.20529 -1.7368 -0.32042 0.124243 -1.1879 (12) z 0.004572 -0.18017	H Atom C C C C C C C C C C C C C C C C C C C	-3.17368 4.(2-amino) x 1.754461 0.395918 -0.32906 0.380841 1.739204 2.502381 2.285918 -0.12196 -0.14873 2.258665 3.75998 -1.81692 -2.10428 -2.09776 -2.63039 -2.32813 -2.38324 -4.06878 -4.33246 -4.05878 -4.33246 -4.59967 x x 1.21561 -0.15665	0.475698 ethyl)phene y 1.198654 1.19361 0.005562 0.005562 2.143087 -2.13382 -2.15452 -0.01551 -0.87299 0.035701 -0.87299 0.035719 0.039002 -0.81576 0.946312 0.056841 -0.81387 0.094076 ethyl)phen methyl)phen y 1.20646 1.194852	-0.89166 2 anion 2 0.011355 0.300137 0.443917 0.443917 0.281961 -0.00743 -0.16278 -0.08641 0.421946 0.389989 -0.11976 -0.43076 0.697887 1.272566 1.296367 1.272566 1.296367 -0.59717 -1.21773 -1.15577 -0.30563 0.147032 -1.16998 -0.147032 -1.16998 -0.1896 -0.21341
Atom C C C C C C C C C C C C C C C C C C C	-3.22454 4-(2-aminoe) x 1.704712 0.342369 -0.37797 0.311199 1.670837 2.369883 2.24945 2.201231 3.704126 4.078246 -1.86369 -2.15108 -2.15108 -2.15108 -2.15108 -2.15108 -2.15108 -2.40564 -4.09914 -4.07651 -4.62334 4-(hydroxylm x 1.195917 -0.18303 -0.92272	0.437687 0.437655 thyl)phenol (y 1.189525 1.196794 0.010411 -1.19505 -1.22163 -0.02436 2.122518 2.148029 -2.13281 -2.15936 -0.10084 0.784175 0.03036 -0.84724 0.784175 0.03036 -0.84724 0.931429 0.063573 0.043573 0.015202 ethyl)phenol y 1.193772 1.228527 0.055158	0.893185 -0.8931 11) z 0.021236 0.306608 0.447066 0.289681 0.004699 -0.13077 -0.0793 0.024894 0.39611 -0.1113 -0.424894 0.424894 0.424894 0.424894 0.424894 0.424894 0.424894 0.424894 0.424894 0.424894 0.424894 0.124243 -1.1879 (12) z 0.00457 -0.18017 -0.30785	H Atom C C C C C C C C C C C C H H H H H C H H H H H C H H H C	-3.17368 -(2-amino) x 1.754461 0.395918 -0.32906 0.380841 1.739204 2.502381 2.285918 -0.12196 -0.14873 2.258665 3.759984 -1.81692 -2.10428 -2.09776 -2.32813 -2.38324 -4.06878 -4.33246 -4.59967 -(hydroxylr x 1.21561 -0.15665 -0.87983	0.475698 ethylphene y 1.198654 1.19361 0.005562 -1.18913 -1.20704 -0.00776 2.141092 2.143087 -2.13382 -2.15452 -0.015531 -0.87719 0.035701 -0.81576 0.946312 0.056841 -0.81389 0.094076 ethylphen y 1.20664 1.194852 -2E-06	-0.89166 2 anion 2 0.011355 0.300137 0.443917 0.281961 -0.00743 -0.16278 -0.08641 0.421946 0.389989 -0.11976 -0.43076 -0.43076 -0.697887 1.272566 1.296367 -0.59717 -1.21773 -1.15577 -0.30563 0.147032 -1.16998 tol anion 2 -0.01896 -0.21341 -0.31493
Atom C C C C C C C C C C C C H H H H C H H H C H H H C	-3.22454 4-(2-aminoet x 1.704712 0.342369 -0.37797 0.311199 1.670837 2.369883 2.24945 -0.16693 2.201231 3.704126 4.078246 4.078246 -2.86369 -2.15108 -2.15108 -2.15108 -2.15108 -2.15108 -2.15108 -2.35645 -2.40564 -4.09914 -4.62334 4-(hydroxylm x 1.195917 -0.18303 -0.92272 -0.2485	0.437687 0.437655 thyl)phenol (y 1.189525 1.196794 0.010411 -1.19505 -1.22163 -0.02436 2.122518 2.148029 -2.13281 -2.15936 -0.10084 0.784175 0.03036 -0.83154 0.934386 -0.83154 0.934386 -0.83154 0.915485 0.034386 -0.83154 0.915485 0.034386 -0.83154 0.915485 0.115202 thylphenol y 1.193772 1.228527 0.055158 -1.16686	0.893185 -0.89311 2 0.021236 0.306608 0.447066 0.289681 0.004699 -0.13077 0.424894 0.39611 -0.0793 0.424894 0.39611 -0.0793 0.424894 0.39611 -0.40858 -0.47519 0.702333 -1.282501 -0.60303 -1.282501 -0.60303 -1.23042 0.124243 -1.13768 -0.32042 0.124243 -1.1379 2 0.004572 -0.18017 -0.37085 -0.24442	H Atom C C C C C C C C C C C C C C C C C C C	-3.17368 4-(2-amino) x 1.754461 0.395918 -0.32996 0.380841 1.739204 2.285918 2.285918 -0.12196 -0.14873 2.258665 3.759984 -1.81692 -2.10428 -2.09776 -2.63039 -2.32813 -2.38324 -4.05878 -4.33246 -4.59967 -0.15661 -0.15664	0.475698 ethyl)phene y 1.198654 1.19361 0.005564 -1.18913 -1.20704 -0.00776 2.141092 2.141092 2.141092 2.143087 -2.15382 -0.013531 -0.87719 0.887719 0.039002 -0.81576 0.046312 0.056841 -0.81389 0.094076 methyl)phen y 1.20646 1.194852 -2.E-06 -1.19485	-0.89166 2 anion 2 0.011355 0.300137 0.443917 0.281961 -0.00743 -0.16278 -0.08641 0.421946 0.389989 -0.11976 -0.43076 0.697887 1.272566 1.296367 -0.59717 -1.21773 -1.15577 -0.30563 0.147032 -1.16998 tol anion 2 -0.01896 -0.21341 -0.21341 -0.21341 -0.21341 -0.21341
Atom C C C C C C C C C C C C C C C C C C C	-3.22454 4-(2-aminoe) x 1.704712 0.342369 -0.37797 0.311199 1.670837 2.369883 2.24945 -0.16693 -0.22519 2.201231 3.704126 4.078246 -1.86369 -2.13754 -2.66156 -2.35645 -2.35645 -2.40564 -4.09914 -4.37651 -4.62334 4-(hydroxylm) x 1.195917 -0.18303 -0.92272 -0.2485 1.125308	0.437687 0.437655 thyl)phenol (y 1.189525 1.196794 0.010411 -1.19505 -1.22163 -0.02436 2.122518 2.148029 -2.13281 -2.15936 -0.10084 0.784175 0.03036 -0.84724 0.915485 0.034386 -0.84724 0.915485 0.034386 -0.83154 0.931429 0.063573 -0.80683 0.115202 ethyl)phenol y 1.193772 1.228527 0.055158 -1.16686 -1.22027	0.893185 -0.89331 11) z 0.021236 0.306608 0.447066 0.289681 0.004699 -0.13077 -0.0793 0.424894 0.39611 -0.0793 0.424894 0.39611 -0.1113 -0.40858 -0.47519 0.702333 1.292051 1.282501 -0.60303 -1.27368 -0.32042 0.124243 -1.1879 (12) z 0.004572 -0.28442 -0.28442 -0.28442 -0.28442 -0.28442 -0.28442 -0.28457 -0.28457 -0.28577 -0.30785 -0.28577 -0.28577 -0.28577 -0.5877	H Atom C C C C C C C C C C C C C H H H H H O C C H H H H	-3.17368 4.(2-amino) x 1.754461 0.395918 -0.32996 0.380841 1.739204 2.265918 2.285918 -0.12196 -0.14873 2.258665 3.759984 -0.12196 -0.14873 2.258665 3.759984 -2.09776 -2.63039 -2.32813 -2.38324 -4.06878 -4.35246 -4.59967 x 1.21561 -0.15665 -0.87983 -0.15664 1.215613	0.475698 ethyl)phene y 1.198654 1.19361 0.005562 -1.18913 -1.20704 -0.007562 2.141092 2.141092 -2.15452 -0.01355 0.01531 -0.87299 0.039002 -0.81576 0.946312 0.056841 -0.813879 0.094076 -0.813576 -0.814576 -0.	-0.89166 2 anion 2 0.011355 0.300137 0.443917 0.281961 -0.00743 -0.16278 -0.08641 0.421946 0.389989 -0.11976 -0.43076 0.697887 1.272566 1.296367 -0.59717 -1.21773 -1.15577 -0.30563 0.147032 -1.16998 aligned -0.13441 -0.21341 -0.21341 -0.1895
Atom C C C C C C C C C C C C H H H C H H H C H H H C	-3.22454 4-(2-aminoe) x 1.704712 0.342369 -0.37797 0.311199 1.670837 2.369883 2.24945 -0.16693 -0.2519 2.201231 3.704126 4.078246 -1.86369 -2.15108 -2.15108 -2.13754 -2.66156 -2.35645 -2.40564 -4.09914 x 1.195917 -0.18303 -0.92272 -0.2485 1.25308 1.849149	0.437687 0.437655 thyl)phenol (y 1.189525 1.196794 0.010411 -1.19505 -1.22163 -0.02436 2.122518 2.148029 -2.13281 -2.13281 -2.15936 -0.10084 0.784175 0.03036 -0.84724 0.915485 0.034386 -0.83154 0.931429 0.063573 -0.80683 0.115202 ethyl)phenol y 1.193772 1.228527 0.0551588 -1.16686 -1.22027 -0.03458	0.893185 -0.8931 11) z 0.021236 0.306608 0.447066 0.289681 0.004699 -0.13077 -0.0793 0.0289681 0.004699 -0.13077 -0.0793 0.424894 0.39611 -0.1113 -0.40858 -0.47519 0.702333 1.20659 -1.282501 -0.60303 -1.20629 -1.1368 -0.124243 -0.124243 -0.124243 -0.124242 -0.03857 -0.03877 0.0066207	H Atom C C C C C C C C C C C C C C H H H H H	-3.17368	0.475698 ethyl)phene y 1.198654 1.19361 0.00562 2.143087 -2.13382 -2.15452 -0.01355 0.01551 -0.81756 0.946312 0.05841 -0.81766 0.946312 0.058418 -0.81789 0.094076 1.20646 1.194852 -2E-06 -1.19485 -1.20646 0.000001	-0.89166 2 anion 2 0.011355 0.300137 0.443917 0.281961 -0.00743 -0.16278 -0.08641 0.421946 0.389989 -0.11976 -0.43076 -0.43076 0.697887 1.272566 1.296367 -0.59717 -1.21773 -1.15577 -0.30563 0.147032 -1.16998 tol anion 2 - -0.1998 -0.11998 -0.11998 -0.11998 -0.11998 -0.11998 -0.11996 -0.21341 -0.31493 -0.2134 -0.11895 0.090656

56							
C	-0.01468	1 221494	0.000088	C	-0.04827	-1 22133	-0.00012
c	1.366757	1.226605	-4E-06	c	-1.41593	-1.22466	-0.00012
С	2.066928	0.01572	-0.00003	C	-2.18911	0	-0.0004
Н	1.930702	-2.13564	0.000017	Н	-1.96212	2.161265	0.000279
Н	1.920936	2.156206	-5.8E-05	Н	-1.96212	-2.16127	-0.00012
0	3.412645	0.086423	-0.00012	0	-3.44395	0	0.000263
Н	3.802924	-0.79557	-0.00013	H	0.50891	-2.14952	-0.00012
н	-0.57436	2.146549	0.00011	H	0.50891	2.149523	0.000283
H N	-0.55198	-2.14200	0.000176	N O	2.007059	1.076207	0.000201
0	-2.71296	-1.08287	-0.00025	õ	2.672161	-1.07621	-5.6E-05
õ	-2.7247	1.061131	-0.00015	-			
	4-hydroxyb	enzaldehyde	(4)	4	4-hydroxyb	enzaldehyd	e anion
Atom	х	у	z	Atom	х	у	z
С	1.209812	1.186794	-1E-06	С	1.253863	1.197874	-0.0001
С	-0.16978	1.330689	0.000003	С	-0.1135	1.32923	-8.5E-05
С	-1.00178	0.210065	0.000007	С	-0.96597	0.204337	-0.00023
С	-0.43481	-1.07113	0.000006	С	-0.37075	-1.07836	-5.9E-05
С	0.936677	-1.22769	0.000003	С	0.991055	-1.23103	-6.8E-05
C II	1.761339	-0.09535	-1E-06	С 11	1.8898//	-0.0969	-0.00065
п 0	3.096183	-2.20879	-6F-06	п 0	3 144434	-2.21972	0.000239
н	3.574613	0.526384	-4E-06	н	1.896087	2.072304	0.000191
Н	1.857911	2.05605	-5E-06	н	-0.55946	2.321321	0.000048
Н	-0.60582	2.324363	0.000003	Н	-1.01962	-1.94893	0.000081
Н	-1.08669	-1.9369	0.000009	С	-2.39463	0.38459	-0.00031
С	-2.46064	0.393312	0.000012	Н	-2.72416	1.442284	0.000297
Н	-2.80029	1.445079	-0.00002	0	-3.2408	-0.5043	0.000395
0	-3.26866	-0.5103	-1.4E-05		4		
Atom	4–cyano	ophenol (5)	2	Atom	4–cyan	ophenol and	ion
C	-1 01819	_1 20085	0.000024	C	1 060103	1 21662	_2E_06
c	0.366615	-1.20842	0.0000024	c	-0.3148	1.21246	-9E-06
Č	1.071509	-0.0013	-1.4E-05	Ċ	-1.03397	-1.8E-05	0.0001
С	0.379093	1.215837	-1.5E-05	С	-0.31478	-1.21248	0.00002
С	-1.00331	1.223901	0.000004	С	1.060124	-1.21662	0.000026
С	-1.7043	0.015432	0.000023	С	1.832777	0.000009	0.000333
Н	-1.55596	2.154782	0.000003	Н	1.601924	-2.1564	-0.00014
О Ц	-3.0536	0.086238	0.00004	о ц	3.097804	0.00002	-0.00039
п н	-3.4409	-0.79003	-3 1E-05	п	-0.86022	2 150455	-0.00008
н	0.92784	-2 149355	0.000006	н	1 601886	2.156409	-0.00011
н	-1.5683	-2.13476	0.000039	C	-2.45425	-3.5E-05	0.000075
С							
	2.504053	-0.01002	-3.4E-05	Ν	-3.61099	0.000034	0.000048
N	2.504053 3.65582	-0.01002 -0.01729	-3.4E-05 -0.00005	Ν	-3.61099	0.000034	0.000048
N	2.504053 3.65582 4'-hydroxya	-0.01002 -0.01729 cetophenone	-3.4E-05 -0.00005	N 4	-3.61099	0.000034	0.000048
N Atom	2.504053 3.65582 4'-hydroxya x -1.49694	-0.01002 -0.01729 cetophenone y -1.18142	-3.4E-05 -0.00005 (6) z -0.00003	N 4 Atom	-3.61099	0.000034 acetophenor y	0.000048 ne anion z 0.000052
N Atom C C	2.504053 3.65582 4'-hydroxya x -1.49694 -0.11381	-0.01002 -0.01729 cetophenone y -1.18142 -1.23932	-3.4E-05 -0.00005 (6) z -0.00003 -0.00003	N Atom C C	-3.61099 -hydroxya x 1.541957 0.169436	0.000034 acetophenor y 1.196946 1.248036	0.000048 ae anion z 0.000052 -0.0001
N Atom C C C C	2.504053 3.65582 4'-hydroxya x -1.49694 -0.11381 0.656148	-0.01002 -0.01729 cetophenone y -1.18142 -1.23932 -0.0718	-3.4E-05 -0.00005 (6) z -0.00003 -0.00006 -0.00006	N Atom C C C	-3.61099 -3.61099 -hydroxyz x 1.541957 0.169436 -0.62155	0.000034 acetophenor y 1.196946 1.248036 0.077809	0.000048 a anion z 0.000052 -0.0001 -4.9E–05
N Atom C C C C C	2.504053 3.65582 4²-hydroxya x -1.49694 -0.11381 0.656148 0.002477	-0.01002 -0.01729 cetophenone y -1.18142 -1.23932 -0.0718 1.165687	-3.4E-05 -0.00005 (6) z -0.00003 -0.00006 -0.00006 -1.7E-05	N Atom C C C C C C	-3.61099 -3.61099 	0.000034 xeetophenor y 1.196946 1.248036 0.077809 -1.15999	0.000048 ae anion z 0.000052 -0.0001 -4.9E-05 0.000042
N Atom C C C C C C C	2.504053 3.65582 4'-hydroxya x -1.49694 -0.11381 0.656148 0.002477 -1.38125	-0.01002 -0.01729 cetophenone y -1.18142 -1.23932 -0.0718 1.165687 1.23822	-3.4E-05 -0.00005 (6) z -0.00003 -0.00006 -0.00006 -1.7E-05 0.000018	N Atom C C C C C C C	-3.61099 -3.61099 	0.000034 acetophenor y 1.196946 1.248036 0.077809 -1.15999 -1.23281	0.000048 ae anion Z 0.000052 -0.0001 -4.9E-05 0.000042 0.000204
N Atom C C C C C C C	2.504053 3.65582 4'-hydroxya x -1.49694 -0.11381 0.656148 0.002477 -1.38125 -2.13312 -2.13312	-0.01002 -0.01729 cetophenone y -1.18142 -1.23932 -0.0718 1.165687 1.23822 0.06309	-3.4E-05 -0.00005 (6) z -0.00003 -0.00006 -0.00006 -1.7E-05 0.000018 0.000011	N Atom C C C C C C C C	-3.61099 -3.61099 	0.000034 xcetophenor y 1.196946 1.248036 0.077809 -1.15999 -1.23281 -0.05462	0.000048 te anion z -0.0001 -4.9E-05 0.000042 0.000204 0.000204
N Atom C C C C C C C C H	2.504053 3.65582 4'-hydroxya x -1.49694 -0.11381 0.656148 0.002477 -1.38125 -2.13312 -2.08786 0.290551	-0.01002 -0.01729 cetophenone y -1.18142 -1.23932 -0.0718 1.165687 1.23822 0.06309 -2.09112 2.19842	-3.4E-05 -0.00005 (6) z -0.00003 -0.00006 -0.00006 -1.7E-05 0.000018 0.000011 -3.9E-05 0.1E.05	N Atom C C C C C C C C H H	-3.61099 -3.61099 X 1.541957 0.169436 -0.62155 0.056784 1.431214 2.259722 2.127994 0.23785	0.000034 xcetophenor y 1.196946 1.248036 0.077809 -1.15999 -1.23281 -0.05462 2.110604 2.207321	0.000048 z 0.000052 -0.0001 -4.9E-05 0.000042 0.000204 0.000204 0.000264 -7.9E-05 0.000204
N Atom C C C C C C C C H H H	2.504053 3.65582 4'-hydroxya -0.11381 0.656148 0.002477 -1.38125 -2.13312 -2.08786 0.389551 -1.8974	-0.01002 -0.01729 cetophenone y -1.18142 -1.23932 -0.0718 1.165687 1.23822 0.06309 -2.09112 -2.19846 2.192112	-3.4E-05 -0.00005 (6) z -0.00003 -0.00006 -0.00006 -1.7E-05 0.000018 0.000011 -3.9E-05 -9.1E-05 -9.1E-05 0.000052	N Atom C C C C C C C C H H H	-3.61099 	0.000034 x x 1.196946 1.248036 0.077809 -1.15999 -1.23281 -0.05462 2.110604 2.207381 -2.19646	0.000048 z anion z 0.000052 -0.0001 -4.9E-05 0.0000204 0.000204 0.000264 -7.9E-05 -0.00028
N Atom C C C C C C C C H H H O	2.504053 3.65582 4'-hydroxya -0.11381 0.656148 0.002477 -1.38125 -2.13312 -2.08786 0.389551 -1.89374 -3.48124	-0.01002 -0.01729 cetophenone y -1.18142 -1.23932 -0.0718 1.165687 1.23822 0.06309 -2.09112 -2.19846 2.192112 0.188369	-3.4E-05 -0.00005 (6) z -0.00003 -0.00006 -1.7E-05 0.000018 0.000011 -3.9E-05 -9.1E-05 0.000052	N Atom C C C C C C C H H H O	-3.61099 	0.000034 x 1.196946 1.248036 0.077809 -1.15999 -1.23281 -0.05462 2.110604 2.207381 -2.19604 -2.19209	0.000048 z 0.000052 -0.0001 -4.9E-05 0.000042 0.000204 0.000464 -7.9E-05 -0.00028 0.000185 0.000185
N Atom C C C C C C C C H H H O H	2.504053 3.65582 4'-hydroxya x -1.49694 -0.11381 0.656148 0.002477 -1.38125 -2.13312 -2.08786 0.389551 -1.89374 -3.48124 -3.90017	-0.01002 -0.01729 cetophenone y -1.18142 -1.23932 -0.0718 1.165687 1.23822 0.06309 -2.09112 -2.19846 2.192112 0.188369 -0.67965	-3.4E-05 -0.00005 (6) z -0.00003 -0.00006 -0.00006 -1.7E-05 0.000011 -3.9E-05 -9.1E-05 0.000052 0.000052 0.000047	N Atom C C C C C C C H H H H O H	-3.61099 -3.61099 -1.541957 0.169436 -0.62155 0.056784 1.431214 2.259722 2.127994 -0.33785 1.930128 3.52411 -0.51174	0.000034 icetophenor y 1.196946 1.248036 0.077809 -1.15999 -1.23281 -0.05462 2.110604 2.207381 -2.19646 -0.11209 -2.0846	0.000048 z anion z 0.000052 -0.0001 -4.9E-05 0.000042 0.000044 0.00044 0.00044 0.000456 -7.9E-05 -0.00028 0.000056 -1.9E-05
N Atom C C C C C C C C C H H H H O H	2.504053 3.65582 4'-hydroxya x -1.49694 -0.11381 0.656148 0.002477 -1.38125 -2.13312 -2.08786 0.389551 -1.89374 -3.48124 -3.90017 0.570782	-0.01002 -0.01729 cetophenone y -1.18142 -1.23932 -0.0718 1.165687 1.23822 0.06309 -2.09112 -2.19846 2.192112 0.188369 -0.67965 2.087825	-3.4E-05 -0.00005 (6) z -0.00003 -0.00006 -0.00006 -1.7E-05 0.000018 0.000011 -3.9E-05 0.000052 0.000044 0.000041	N Atom C C C C C C C H H H O H C	-3.61099 <u>P-hydroxys</u> 1.541957 0.169436 -0.62155 0.056784 1.431214 2.259722 2.127994 -0.33785 1.930128 3.52411 -0.51174 -0.51174	0.000034 xcetophenor y 1.19694 1.248036 0.077809 -1.23281 -0.05462 2.110604 2.207381 -2.19646 -0.11209 -2.0846 0.181486	0.000048 z anion z 0.000052 -0.0001 -4.9E-05 0.000042 0.00042 0.00044 -7.9E-05 -0.00028 0.000056 -1.9E-05 -0.0019
N Atom C C C C C C C C C C H H H O H H C C	2.504053 3.65582 4'-hydroxya x -1.49694 -0.11381 0.656148 0.002477 -1.38125 -2.13312 -2.08786 0.389551 -1.89374 -3.48124 -3.90017 0.570782 2.142371	-0.01002 -0.01729 cctophenone y -1.18142 -1.23932 -0.0718 1.165687 1.23822 0.06309 -2.09112 -2.19846 2.192112 0.188369 -0.67965 2.087825 -0.18596	-3.4E-05 -0.00005 (6) z -0.00003 -0.00006 -0.00006 -1.7E-05 0.000011 -3.9E-05 0.000044 0.000047 -0.00001 -9.7E-05	N Atom C C C C C C C H H H O H C C	-3.61099 P-hydroxy2 x 1.541957 0.169436 -0.62155 0.056784 2.259722 2.127994 -0.33785 1.930128 3.52411 -0.51174 -2.07804 -2.289832	0.000034 y 1.196946 1.248036 0.077809 -1.23281 -0.05462 2.110604 2.207381 -2.19646 -0.11209 -2.0846 0.181486 -1.09506	0.000048 z 0.000052 -0.0001 -4.9E-05 0.000042 0.00044 0.00044 -7.9E-05 -0.00028 0.000185 0.000056 -1.9E-05 -1.9E-05 -0.00019 -0.00011
Atom C C C C C C C C C H H H H C C C C C C	2.504053 3.65582 4'-hydroxya x -1.49694 -0.11381 0.656148 0.002477 -1.38125 -2.13312 -2.08786 0.389551 -1.89374 -3.48124 -3.90017 0.570782 2.142371 2.963256	-0.01002 -0.01729 cctophenone y -1.18142 -1.23932 -0.0718 1.165687 1.23822 0.06309 -2.09112 -2.19846 2.192112 0.188369 -0.67965 2.087825 -0.18596 1.080238	-3.4E-05 -0.00005 (6) z -0.00003 -0.00006 -0.00006 -1.7E-05 0.000018 0.000011 -3.9E-05 -9.1E-05 0.000052 0.000044 0.000047 -0.00001 -9.7E-05 0.000022	N Atom C C C C C C C C H H H H C C C H H H H	-3.61099 P-hydroxy x 1.541957 0.169436 -0.62155 0.056784 1.431214 2.259722 2.127994 -0.33785 3.52411 -0.51174 -2.07804 -2.89832 -3.95526	0.000034 icetopheno y 1.196946 1.248036 0.077809 -1.15999 -1.32381 -0.05462 2.110604 2.207381 -2.19646 -0.11209 -2.0846 0.181486 -1.09506 -0.83674	0.000048 z 0.000052 -0.0001 -4.9E-05 0.000042 0.000042 0.000204 0.000264 -7.9E-05 -0.00028 0.000185 0.000185 0.000185 0.00019 -0.00019 -0.00011 -0.00019
N Atom C C C C C C C C C C C C C C C C C C C	2.504053 3.65582 4'-bydroxya -1.49694 -0.11381 0.656148 0.002477 -1.38125 -2.13312 -2.08786 0.389551 -1.89374 -3.48124 -3.48124 -3.48124 2.142371 2.963256 4.019275	-0.01002 -0.01729 cetophenone y -1.18142 -1.23932 -0.0718 1.165687 1.23822 0.06309 -2.09112 -2.19846 2.192112 0.188369 -0.67965 2.087825 -0.18596 1.080238 0.820419 + .062021	-3.4E-05 -0.00005 (6) z -0.00003 -0.00006 -1.7E-05 0.000018 0.000018 0.000018 0.000012 0.000052 0.000044 0.0000047 -0.00001 -9.7E-05 0.000002 0.000002	N Atom C C C C C C C C C H H H H C C C H H H H C C H H H C	-3.61099 '-hydroxyz x 1.541957 0.169436 -0.62155 0.056784 1.431214 2.259722 2.127994 -0.33785 1.930128 3.52411 -0.51174 -2.07804 -2.89832 -3.95526 -2.67251	0.000034 xcetophenory y 1.196946 1.248036 0.077809 -1.32981 -0.05462 2.110604 2.207381 -2.19646 -0.11209 -2.0846 0.181486 -1.09506 -0.83674 -1.70012 -1.70012	0.000048 z anion z 0.000052 -0.0001 -4.9E-05 0.000042 0.000204 0.000204 0.000264 -7.9E-05 -0.00028 0.000185 0.000185 0.00019 -0.00011 -0.00023 -0.00023 -0.88073 0.00026
N Atom C C C C C C C C C C C C C C C C C C C	2.504053 3.65582 4'-hydroxya -1.49694 -0.11381 0.656148 0.002477 -1.38125 -2.13312 -2.08786 0.389551 -1.89374 -3.48124 -3.48124 -3.90017 0.570782 2.142371 2.963256 4.019275 2.733813 2.73375	-0.01002 -0.01729 cctophenone y -1.18142 -1.23932 -0.0718 1.165687 1.23822 -0.0718 1.165687 1.23822 -2.09112 -2.19846 2.192112 -2.19846 2.087825 -0.18596 1.080238 0.820419 1.683292 1.683292 1.683292	-3.4E-05 -0.00005 (6) z -0.00003 -0.00006 -1.7E-05 0.000018 0.000011 -3.9E-05 0.000012 0.000047 -0.00001 -9.7E-05 0.000014 -9.7E-05 0.000012 0.000001 -9.7E-05 0.000001 -9.7E-05 0.000001 -9.7E-05 0.000001 -9.7E-05 0.000001 -9.7E-05 0.000001 -9.7E-05 0.000001 -9.7E-05 0.000001 -9.7E-05 0.000001 -9.7E-05 0.000001 -9.7E-05 0.000001 -9.7E-05 0.00001 -0.0	N Atom C C C C C C C C H H H O H C C C H H H O H C C C C	-3.61099 '-hydroxya x 1.541957 0.169436 -0.62155 0.056784 1.431214 2.259722 2.127994 -0.3785 1.930128 3.52411 -0.51174 -2.89832 -3.95526 -2.67251 -2.67266 2.67266	0.000034 xcetophenor y 1.196946 1.248036 0.077809 -1.23281 -0.05462 2.110604 2.207381 -2.19646 -0.11209 -2.0846 0.181486 -1.09506 -0.83674 -1.70012 -1.69991 1.25218	0.000048 z 0.000052 -0.0001 -4.9E-05 0.000042 0.000204 0.000204 0.000264 -7.9E-05 -0.00028 0.000185 0.000056 -1.9E-05 -0.00011 -0.00011 -0.00023 -0.88073 0.880696 0.00032
N Atom C C C C C C C C C C C C C C C C C C C	2.504053 3.65582 4'-hydroxya x -1.49694 -0.11381 0.656148 0.002477 -1.38125 -2.13312 -2.08786 0.389551 -1.89374 -3.48124 -3.90017 0.570782 2.142371 2.963256 4.019275 2.733813 2.73375 2.681218	-0.01002 -0.01729 cctophenone y -1.18142 -1.23932 -0.0718 1.165687 1.23822 0.06309 -2.09112 -2.19846 2.192112 0.188369 -0.67965 2.087825 -0.18596 1.080238 0.820419 1.683292 1.683186 -1.27712	-3.4E-05 -0.00005 (6) z -0.00003 -0.00006 -1.7E-05 0.000018 0.000011 -3.9E-05 0.000047 -0.00004 0.000047 -0.00001 -9.7E-05 0.000001 -9.7E-05 0.0000031 -0.88129 0.881351 0.00017 -0.00017 -0.88129 0.881351 0.00017 -0.00017 -0.88129 -0.881351 0.00017 -0.00017 -0.00017 -0.00017 -0.00017 -0.0000000000 -0.00000000000000000000	N Atom C C C C C C C C C H H H O H C C C C H H H O H C C C C	-3.61099 '-hydroxya x 1.541957 0.169436 -0.62155 0.056784 1.431214 -2.259722 2.127994 -0.33785 1.930128 3.52411 -0.51174 -2.07804 -2.67832 -3.95526 -2.67251 -2.67266 -2.65853	0.000034 icetophenor y 1.196946 1.248036 0.077809 -1.52981 -0.05462 2.110604 2.207381 -2.19646 0.181486 -1.09506 -1.09506 -0.83674 -1.70012 -1.69991 1.265718	0.000048 z 0.000052 -0.0001 -4.9E-05 0.000042 0.000204 0.000464 -7.9E-05 -0.00028 0.000056 -1.9E-05 -0.00018 -0.00019 -0.00019 -0.00013 0.880696 -0.00023 -0.88073 0.880696 -0.00023 -0.0002 -0.0002
Atom C C C C C C C C C C C C C C C C C C C	2.504053 3.65582 4'-hydroxya x -1.49694 -0.11381 0.656148 0.002477 -1.38125 -2.13312 -2.08786 0.389551 -1.89374 -3.48124 -3.90017 0.570782 2.142371 2.963256 4.019275 2.733813 2.73375 2.733813 2.73375 2.681218 3-trifluorom	-0.01002 -0.01729 cetophenone y -1.18142 -1.23932 -0.0718 1.165687 1.23822 0.06309 -2.09112 -2.19846 2.192112 0.188369 -0.67965 2.087825 -0.18596 1.080238 0.820419 1.683292 1.683186 0.820419 1.683292 1.683186 -2.7712 	-3.4E-05 -0.00005 (6) z -0.00003 -0.00006 -0.00006 -0.00006 0.000011 -3.9E-05 0.000012 0.000041 -9.7E-05 0.000001 -9.7E-05 0.000001 -9.7E-05 0.000001 -0.88129 0.881351 0.00014 (7)	N Atom C C C C C C C C C H H H C C H H H O O H H H O O C C C C	-3.61099 -3.61099 x 1.541957 0.169436 -0.62155 0.056784 1.431214 2.259722 2.127994 -0.33785 1.930128 3.52411 -0.3174 -2.07804 -2.89832 -3.95526 -2.67251 -2.67256 -2.67853	0.000034 y 1.196946 1.248036 0.077809 -1.23281 -0.05462 2.110604 2.207381 -2.19646 -0.11209 -2.0846 0.181486 -1.09506 -0.8874 -1.70012 -1.69991 1.265718 methylphen	0.000048
Atom C C C C C C C C C C C C C C C C C C C	2.504053 3.65582 4'-hydroxya x -1.49694 -0.11381 0.656148 0.002477 -1.38125 -2.13312 -2.08786 0.389551 -1.89374 -3.48124 -3.90017 0.570782 2.142371 2.963256 4.019275 2.733813 2.73375 2.681218 3-trifluorom x	-0.01002 -0.01729 cetophenone y -1.18142 -1.23932 -0.0718 1.165687 1.23822 0.06309 -2.09112 -2.19846 2.192112 0.188369 -0.67965 2.087825 -0.18596 1.080238 0.820419 1.683292 1.683186 -1.27712 tethylphenol y	-3.4E-05 -0.00005 (6) z -0.00003 -0.00006 -0.00006 -0.00006 0.000011 -3.9E-05 0.000012 0.000044 0.000004 -9.7E-05 0.000001 -9.7E-05 0.000001 -9.7E-05 0.000001 -9.7E-05 0.000001 -0.88129 0.881351 0.000124 (7) z_	A Atom C C C C C C C C C C C C C C H H H O O H H H O H H C C C H H H O A Atom	-3.61099 X -hydroxyz x 1.541957 0.169436 -0.62155 0.056784 1.431214 2.259722 2.127994 -0.33785 1.930128 3.52411 -0.51174 -2.07804 -2.89832 -3.95526 -2.67256 -2.67256 3-trifluoron x	0.000034 y 1.196946 1.248036 0.077809 -1.23281 -0.05462 2.110604 2.207381 -2.19646 -0.11209 -2.0846 0.181486 -1.09506 -0.181486 -1.09506 -1.69991 1.265718 methylphene y	0.000048 z anion z 0.000052 -0.0001 -4.9E-05 0.000042 0.00044 -7.9E-05 -0.00028 0.000185 0.000185 0.000185 -0.00019 -0.00011 -0.00011 -0.00013 0.880696 -0.00023 bl anion z
Atom C C C C C C C C C C C C C C C C C C C	2.504053 3.65582 4'-hydroxya x -1.49694 -0.11381 0.656148 0.002477 -1.38125 -2.13312 -2.08786 0.389551 -1.89374 -3.48124 -3.48124 -3.90017 0.570782 2.142371 2.963256 4.019275 2.733813 2.73375 2.681218 3-trifluorom x -2.42285	-0.01002 -0.01729 cetophenone y -1.18142 -1.23932 -0.0718 1.165687 1.23822 0.06309 -2.09112 -2.19846 2.192112 0.188369 -0.67965 2.087825 -0.18596 1.080238 0.820419 1.683292 1.683186 -1.27712 rethylphenol y 0.816182	-3.4E-05 -0.00005 (6) z -0.00003 -0.00006 -0.00006 -0.00006 0.000011 -3.9E-05 0.000012 0.000044 0.000047 -0.1E-05 0.000042 0.000047 -0.00001 -9.1E-05 0.000042 0.000047 -0.00001 -9.7E-05 0.000002 0.000002 0.000002 0.000001 -9.7E-05 0.000002 0.0000002 0.0000002 0.000002 0.0000000000	N 4 Atom C C C C C C C C C C C C C C C C C C C	-3.61099 Y-hydroxy2 x 1.541957 0.169436 -0.62155 0.056784 1.431214 2.259722 2.127994 -0.33785 1.930128 3.52411 -0.51174 -2.07804 -2.89832 -3.95526 -2.67251 -2.67253 3-trifluorom x -2.47733	0.000034 v y 1.196946 1.248036 0.077809 -1.23281 -0.05462 2.110604 2.207381 -2.19646 -0.11209 -2.0846 0.181486 -0.181486 -0.181486 -1.09506 -0.81847 v 0.748347	0.000048 z anion z 0.000052 -0.0001 -4.9E-05 0.000042 0.00044 0.00044 -7.9E-05 -0.00028 0.000185 0.000185 0.000185 0.00019 -0.0001 -0.0001 -0.0001 -0.0001 -0.0001 -0.00023 olanion z 0
Atom C C C C C C C C C C C C C C C C C C C	2.504053 3.65582 4'-hydroxya x -1.49694 -0.11381 0.656148 0.002477 -1.38125 -2.13312 -2.08786 0.389551 -1.89374 -3.48124 -3.90017 0.570782 2.142371 2.963256 4.019275 2.733813 2.73375 2.681218 3-trifluorom x -2.42285 -1.47795	-0.01002 -0.01729 cetophenone y -1.18142 -1.23932 -0.0718 1.165687 1.23822 0.06309 -2.09112 -2.19846 2.192112 0.188369 -0.67965 2.087825 -0.18596 1.080238 0.820419 1.683292 1.683186 -1.27712 v y 0.816182 1.833437	-3.4E-05 -0.00005 (6) z -0.00003 -0.00006 -0.00006 -0.000018 0.000011 -3.9E-05 0.000021 0.000044 0.000044 0.000044 0.000047 -0.00001 -9.7E-05 0.000002 0.000002 0.000002 0.000001 -9.7E-05 0.000002 0.000002 0.000012 (7) z 0 0 0 0 0 0 0 0 0 0 0 0 0	N Atom C C C C C C C C C C C C C	-3.61099	0.000034 icetopheno y 1.196946 1.248036 0.077809 -1.125999 -1.23281 -0.05462 2.110604 2.207381 -2.19646 -0.11209 -2.0846 0.181486 0.181486 -0.181486 -0.83674 -1.69991 1.265718 icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene icetylphene 	0.000048 z 0.000052 -0.0001 -4.9E-05 0.000042 0.000042 0.000042 0.000204 0.000464 -7.9E-05 -0.00028 0.000185 0.0000185 0.00019 -0.00011 -0.00023 -0.88073 0.88076 -0.00023 ol anion z 0 0.000001
Atom C C C C C C C C C C C C C C C C C C C	2.504053 3.65582 4'-hydroxya x -1.49694 -0.11381 0.656148 0.002477 -1.38125 -2.08786 0.389551 -1.89374 -3.48124 -3.90017 0.570782 2.142371 2.963256 4.019275 2.733813 2.73375 2.681218 3-trifluorom x -2.42285 -1.47795 -0.11665 0.275721	-0.01002 -0.01729 cetophenone y -1.18142 -1.23932 -0.0718 1.165687 1.23822 0.06309 -2.09112 -2.19846 2.192112 0.188369 -0.67965 2.087825 -0.18596 1.080238 0.820419 1.683186 -1.27712 tethylphenol y 0.816182 1.833437 1.541426 0.202425	-3.4E-05 -0.00005 (6) z -0.00003 -0.00006 -0.00006 -0.000018 0.000011 -3.9E-05 0.000052 0.000044 0.000044 0.000047 -0.00001 -9.7E-05 0.000002 0.000002 0.000002 (7) z 0 0 0 0 0 0 0 0 0 0 0 0 0	N Atom C C C C C C C C C C C C C	-3.61099 P-hydroxy2 x 1.541957 0.169436 -0.62155 0.056784 1.431214 2.259722 2.127994 -0.33785 3.52411 -0.51174 -2.07804 -2.87832 -3.95526 -2.67251 -2.67826 3-2.67826 3-2.67853 -2.67853 -2.67853 -2.678560 -0.155603 -0.17899 0.27679	0.000034 icctophenor y 1.196946 1.248036 0.077809 -1.15999 -1.23281 -0.05462 2.110604 2.207381 -0.05462 2.110604 -2.207381 -2.18446 -0.11209 -2.0846 0.181486 -0.83674 -1.09506 -0.83674 -1.69991 1.265718 icctophenor y 0.748347 0.748347 0.748347 0.748347 0.748347 0.748347 0.748347 0.748347 0.748347 0.748347 0.748347 0.748347 0.748347 0.748347 0.748347 0.748347 0.748347 0.748347 0.748347 0.12027 0.1207 0.12027 0.12	0.000048 z 0.000052 -0.0001 -4.9E-05 0.000042 0.000042 0.000044 0.000204 0.000204 0.000204 0.000185 0.0000185 0.00019 -0.00011 -0.00011 -0.00013 0.88073 0.88073 0.880696 -0.00023 olamon z 0 0.000001 -1E-06 25 or
Atom C C C C C C C C C C C C C C C C C C C	2.504053 3.65582 4'-hydroxya x -1.49694 -0.11381 0.656148 0.002477 -1.38125 -2.13312 -2.08786 0.389551 -1.89374 -3.48124 -3.90017 0.570782 2.142371 2.963256 4.019275 2.733813 2.73375 2.681218 3-trifluoron x -2.42285 -1.47795 -0.11665 0.275724 -0.65317	-0.01002 -0.01729 cetophenone y -1.18142 -1.23932 -0.0718 1.165687 1.23822 0.06309 -2.09112 -2.19846 2.192112 0.188369 -0.67965 2.087825 -0.18596 1.080238 0.820419 1.683292 1.683186 -1.27712 cethylphenol y 0.816182 1.833437 1.541426 0.028486 -0.9763	-3.4E-05 -0.00005 (6) z -0.00003 -0.00006 -1.7E-05 0.000018 0.000011 -3.9E-05 0.000012 0.000012 0.000047 -0.00001 -9.7E-05 0.000001 -9.7E-05 0.000012 0.000001 -0.88129 0.881351 0.0000124 (7) z 0 0 0 -1E-06 -1E-06	N Atom C C C C C C C C C C C C C	-3.61099 '-hydroxyz x 1.541957 0.169436 -0.62155 0.056784 1.431214 2.259722 2.127994 -0.33785 3.52411 -0.51174 -2.07804 -2.67853 -2.67251 -2.67251 -2.67853 -2.67853 -2.67853 -1.55603 -1.55603 -0.17899 0.22657 -0.67527 -0.5507 -0.67527 -0.5507 -0.67527 -0.5507 -0.67527 -0.5507 -0.67527 -0.5507 -0.67527 -0.5507 -0.67577 -0.67527 -0.67527 -0.67527 -0.675777 -0.67577 -0.67577 -0.675777 -0.675777 -0.675777 -0.675777 -0.675777 -0.675777 -0.675777 -0.675777 -0.6757777 -0.6757777 -0.6757777 -0.6757777 -0.67577777777777777777777777777777777777	0.000034 iccetophenor y 1.196946 1.248036 0.077809 -1.15999 -1.23281 -0.05462 2.110604 2.207381 -2.19646 -0.11209 -2.0846 0.181486 -1.09506 -0.83674 -1.09501 i.265718 i.265718 i.265718 i.780708 1.532906 0.199997 -0.855290	0.000048 z 0.000052 -0.0001 -4.9E-05 0.000042 0.000204 0.000204 0.000204 0.00026 -7.9E-05 -0.00028 0.000185 0.00019 -0.00019 -0.00011 -0.00023 -0.88073 0.880696 -0.00023 ol anion z 0 0.000001 -1E-06 -2E-06 -3E-06
Atom C C C C C C C C C C C C C C C C C C C	2.504053 3.65582 4'-hydroxya x -1.49694 -0.11381 0.656148 0.002477 -1.38125 -2.13312 -2.08786 0.389551 -1.89374 -3.48124 -3.90017 0.570782 2.142371 2.963256 4.019275 2.733813 2.73375 2.681218 3-trifluorom x -2.42285 -1.42795 -0.11665 0.275724 -0.65317 -2.08966	-0.01002 -0.01729 cetophenone y -1.18142 -1.23932 -0.0718 1.165687 1.23822 0.06309 -2.09112 -2.19846 2.192112 0.188369 -0.67965 2.087825 -0.18596 1.080238 0.820419 1.683292 1.683186 -1.27712 tethylphenol y 0.816182 1.541426 0.208486 -0.208486 -0.208486 -0.208486 -0.82632 -0.51705	-3.4E-05 -0.00005 (6) z -0.00003 -0.00006 -1.7E-05 0.000011 -3.9E-05 0.000012 -3.9E-05 0.000047 -0.00001 -9.7E-05 0.000001 -9.7E-05 0.000001 -9.7E-05 0.000001 (7) z 0 0 0 0 0 0 0 -1E-06 -1E-06 0 0 0	N 4 Atom C C C C C C C C C C H H H O H C C C C C	-3.61099 -3.61099 -3.61099 x 1.541957 0.169436 -0.62155 0.056784 1.431214 2.259722 2.127994 1.431214 2.259722 2.127994 -0.33785 1.930128 3.52411 -0.51174 -2.07804 -2.89832 -3.95526 -2.67251 -2.67251 -2.67251 -2.67253 -1.55603 x -2.47733 -1.55603 -0.17899 0.22657 -0.67637 -2.0884	0.000034 y 1.196946 1.248036 0.077809 -1.23281 -0.05462 2.110604 2.207381 -2.19646 0.181486 -0.11209 -2.08460 0.181486 -0.83674 -1.70012 -1.69991 1.265718 ncthylphene y 0.748347 1.532906 0.199997 -0.63317 -0.63317	0.000048 z 0.000052 -0.0001 -4.9E-05 0.000042 0.000204 0.000204 0.000204 0.000204 0.000204 -7.9E-05 -0.00018 0.0000185 0.000018 -1.9E-05 -0.00011 -0.00011 -0.00023 olimin z 0 0.0000001 -1E-06 -2E-06 -3E-06 -6E-06
Atom C C C C C C C C C C C C C C C C C C C	2.504053 3.65582 4'-hydroxya x -1.49694 -0.11381 0.656148 0.002477 -1.38125 -2.13312 -2.08786 0.389551 -1.89374 -3.48124 -3.90017 0.570782 2.142371 2.963256 4.019275 2.733813 2.73375 2.681218 3-trifluorom x -2.42285 -1.47795 0.275724 -0.65317 -2.00896 -3.4816	-0.01002 -0.01729 cetophenone y -1.18142 -1.23932 -0.0718 1.165687 1.23822 0.06309 -2.09112 -2.19846 2.192112 0.188369 -0.67965 2.087825 -0.18596 1.080238 0.820419 1.683186 -1.27712 tethylphenol y 0.816182 1.531426 0.208486 -0.208486 -0.82632 -0.51705 1.051905	-3.4E-05 -0.00005 (6) z -0.00003 -0.00006 -0.00006 -0.00006 0.000011 -1.7E-05 0.000018 0.000012 -3.9E-05 0.000004 0.000004 -9.7E-05 0.0000012 0.0000012 (7) z 0 0 0 0 0 0 0 0 0 0 0 0 0	N 4 Atom C C C C C C C C C C C C H H H O H C C C C	-3.61099 -3.61099 -3.61099 x 1.541957 0.169436 -0.62155 0.056784 1.431214 2.259722 2.127994 -0.33785 1.930128 3.52411 -0.31785 -3.95526 -2.67281 -2.67281 -2.67285 -2.672853 -1.55603 -0.17899 0.22657 -0.67637 -2.08881 -3.54057 -2.67281 -3.54057	0.000034 xectophenol y 1.196946 1.248036 0.077809 -1.23281 -0.05462 2.110604 2.207381 -2.19646 -0.11209 -2.0846 0.181486 -1.09506 -0.88178 y 0.748347 1.780708 1.532906 0.199997 -0.63317 0.968618	0.000048
Atom C C C C C C C C C C C C C C C C C C C	2.504053 3.65582 4'-hydroxya x -1.49694 -0.11381 0.656148 0.002477 -1.38125 -2.1312 -2.08786 0.389551 -1.89374 -3.48124 -3.90017 0.570782 2.142371 2.963256 4.019275 2.733813 2.73375 2.681218 3-trifluorom x -2.42285 -1.47795 -0.11665 0.275724 -0.65317 -2.00896 -3.4816 -1.80698	-0.01002 -0.01729 cetophenone y -1.18142 -1.23932 -0.0718 1.165687 1.23822 0.06309 -2.09112 -2.19846 2.192112 0.188369 -0.67965 2.087825 -0.18596 1.080238 0.820419 1.683292 1.683186 -1.27712 v 0.816182 1.833437 1.541426 0.208486 -0.82632 -0.51705 1.051905 2.86506	-3.4E-05 -0.00005 (6) z -0.00003 -0.00006 -0.00006 -0.00006 0.1.7E-05 0.000018 0.000011 -3.9E-05 0.000052 0.000044 0.000001 -9.1E-05 0.000002 0.0000012 (7) z 0 0 0 0 0 0 0 0 0 0 0 0 0	N 4 Atom C C C C C C C C C C C C C C C C C C C	-3.61099 Y-hydroxy2 x 1.541957 0.169436 -0.62155 0.056784 1.431214 2.259722 2.127994 -0.33785 1.930128 3.52411 -0.51174 -2.07804 -2.89832 -3.95526 -2.67266 -2.65853 3-1.55603 -0.17899 0.22657 -0.67637 -2.08881 -3.54057 -1.90853	0.000034 v v 1.196946 1.248036 0.077809 -1.23281 -0.05462 2.110604 2.207381 -2.19646 -0.11209 -2.0846 0.181486 -1.09506 -0.83674 -1.70012 -1.69991 1.265718 v v v 0.748347 1.780708 1.532906 0.199997 -0.85529 -0.63317 0.9968618 2.807241	0.000048 2 anion 2 0.000052 -0.0001 -4.9E-05 0.000042 0.000204 0.000464 -7.9E-05 -0.00028 0.000185 0.0000185 0.0000185 0.000019 -0.00011 -0.00011 -0.00011 -0.00013 0.880696 -0.00023 0 anion 2 0 0 0.000001 -1E-06 -2E-06 -3E-06 -6E-06 0.000003 0.000004
Atom C C C C C C C C C C C C C H H H H O H H C C C H H H O M C C C C C C C C C C C C C C C C C C	2.504053 3.65582 4'-hydroxya x -1.49694 -0.11381 0.656148 0.002477 -1.38125 -2.13312 -2.08786 0.389551 -1.89374 -3.48124 -3.90017 0.570782 2.142371 2.963256 4.019275 2.733813 2.73375 2.681218 3-trifluorom x -2.42285 -1.47795 -0.11665 0.275724 -0.65317 -2.00896 -3.4816 -1.80698 -0.34321	-0.01002 -0.01729 cetophenone y -1.18142 -1.23932 -0.0718 1.165687 1.23822 0.06309 -2.09112 -2.19846 2.192112 0.188369 -0.67965 2.087825 -0.18596 1.080238 0.820419 1.683292 1.683186 -1.27712 v 0.816182 1.833437 1.541426 0.208486 -0.82632 -0.51705 1.051905 2.86506 -1.86492	-3.4E-05 -0.00005 (6) z -0.00006 -0.00006 -0.00006 -1.7E-05 0.000018 0.000011 -3.9E-05 0.000052 0.000044 0.000044 0.000047 -0.00011 -9.7E-05 0.000002 0.000001 -0.881351 0.000124 (7) z 0 0 0 0 0 0 0 0 0 0 0 0 0	N 4 Atom C C C C C C C C C C C C C C C C C C C	-3.61099	0.000034 icetophenor y 1.196946 1.248036 0.077809 -1.23281 -0.05462 2.110604 2.207381 -2.19646 -0.11209 -2.0846 0.181486 -1.09506 -0.83674 -1.70012 -1.69991 1.265718 icetylphene y 0.748347 1.780708 1.532908 0.199997 -0.85529 -0.63317 0.966618 2.807241 -1.88065	0.000048
Atom C C C C C C C C C C C C C C C C C C C	2.504053 3.65582 4'-hydroxya x -1.49694 -0.11381 0.656148 0.002477 -1.38125 -2.08786 0.389551 -1.89374 -3.48124 -3.90017 0.570782 2.142371 2.963256 4.019275 2.733813 2.73375 2.681218 3-trifluorom x -2.42285 -1.47795 -0.11665 0.275724 -0.5317 -2.00896 -3.4816 -1.80698 -0.34321 -2.88238	-0.01002 -0.01729 ectophenone y -1.18142 -1.23932 -0.0718 1.165687 1.23822 0.06309 -2.09112 -2.19846 2.192112 0.188369 -0.67965 2.087825 -0.18596 1.080238 0.820419 1.683292 1.683186 61.27712 tethylphenol y 0.816182 1.833437 1.541426 0.08486 0.208486 0.208486 0.208487 1.541426 0.08481 0.51905 2.86506 -1.85589 -1.55589	-3.4E-05 -0.00005 (6) z -0.00003 -0.00006 -0.00006 -1.7E-05 0.000018 0.000018 0.000018 0.000012 0.000044 0.000044 0.000047 -9.1E-05 0.000002 0.000004 0.000001 -9.7E-05 0.000002 0.000001 -0.881251 0.000124 (7) z 0 0 0 0 0 0 0 0 0 0 0 0 0	N Atom C C C C C C C C C C C C C	-3.61099	0.000034 icctophenor y 1.196946 1.248036 0.077809 -1.152921 -0.05462 2.110604 2.207381 -2.19646 -0.11209 -2.0846 0.181486 0.181486 -0.181486 -0.83674 -1.09506 -0.83674 1.265718 i.265718 i.265718 0.748347 1.780708 1.532906 0.199997 -0.85529 -0.63317 0.968618 2.807241 -1.80865 -1.58813	0.000048
Atom C C C C C C C C C C C C C C C C C C C	2.504053 3.65582 4'-hydroxya x -1.49694 -0.11381 0.656148 0.002477 -1.38125 -2.13312 -2.08786 0.389551 -1.89374 -3.48124 -3.48124 -3.48124 -3.90017 0.570782 2.142371 2.963256 4.019275 2.733813 2.733813 2.73375 2.681218 3-trifluorom x -2.42285 -1.47795 -0.11665 0.275724 -0.65317 -2.00896 -3.4816 -1.80698 -0.34321 -2.88238 -3.78991 -2.88238 -3.78991 -2.88238 -3.78991 -2.88238 -3.78991 -2.88238 -3.78991 -2.88238 -3.78991 -2.88238 -3.78991 -2.68227 -2.88238 -3.78991 -2.68227 -2.68227 -2.88238 -3.78991 -2.68227 -2.68228 -3.78991 -2.68227 -2.68228 -3.78991 -3.7891 -3	-0.01002 -0.01729 cetophenone y -1.18142 -1.23932 -0.0718 1.165687 1.23822 0.06309 -2.09112 -2.19846 2.192112 -2.19846 2.087825 -0.18596 1.080238 0.820419 1.683292 1.683186 -1.27712 v 0.816182 1.833437 1.541426 0.208486 -0.82632 -0.51705 1.051905 2.86506 -1.86492 -1.235589 -1.235589 -1.23259 -1.235589 -1.23259	-3.4E-05 -0.00005 (6) z -0.00003 -0.00006 -1.7E-05 0.000011 -3.9E-05 0.000012 0.000044 0.000047 -0.00001 -9.7E-05 0.000013 -0.88129 0.000031 -0.88129 0.0000124 (7) z 0 0 0 0 0 0 0 0 0 0 0 0 0	N 4 Atom C C C C C C C C H H H O H C C C C C C C	-3.61099	0.000034 icctophenor y 1.196946 1.248036 0.077809 -1.15399 -1.23281 -0.05462 2.110604 2.207381 -2.19646 -0.11209 -2.0846 -0.181486 -1.09506 -0.83674 -1.09506 -0.83674 -1.09991 1.265718 iccty1phene y 0.748347 0.748347 0.198997 -0.85529 -0.65317 0.968618 2.807241 -1.88055 -1.58813 2.339918 8.339918	0.000048
Atom C C C C C C C C C C C C C C C C C C C	2.504053 3.65582 4'-hydroxya x -1.49694 -0.11381 0.656148 0.002477 -1.38125 -2.13312 -2.08786 0.389551 -1.89374 -3.48124 -3.90017 0.570782 2.142371 2.963256 4.019275 2.733813 2.73375 2.681218 3-trifluorom x -2.42285 -1.47795 -0.11665 0.275724 -0.65317 -2.00896 -3.4816 -1.80698 -0.34321 -2.88238 -3.78991 0.619369 1.720144	-0.01002 -0.01729 cetophenone y -1.18142 -1.23932 -0.0718 1.165687 1.23822 0.06309 -2.09112 -2.19846 2.192112 0.188369 -0.67965 2.087825 -0.18596 1.080238 0.820419 1.683292 1.683186 -1.27712 tethylphenol y 0.816182 1.541426 0.208486 -0.208486 -0.2084862 -0.51705 1.051905 2.86506 -1.86492 -1.35589 -1.23259 2.333783 0.16175	$\begin{array}{c} -3.4E-05\\ -0.00005\\ \hline \hline \\ \hline \\$	N 4 Atom C C C C C C C C C C C C H H H O H C C C C	-3.61099 -3.61099 -3.61099 -3.61099 -3.61093 -0.62155 0.056784 1.431214 2.259722 2.127994 -0.33785 1.930128 3.52411 -0.31785 -3.95526 -2.67251 -2.67251 -2.67251 -2.67256 -2.675853 -1.55603 -0.17899 0.22657 -0.67637 -2.08881 -0.31907 -2.93573 0.540344 1.688313 2.24220 -2.93573 -2.94257 -2.94583 -2.94257 -2.94583 -3.54057 -1.90853 -0.31907 -2.93573 0.540344 1.688313 2.24220 -2.94573 -2.94573 -2.94573 -2.94573 -2.94573 -2.94573 -2.94573 -2.94573 -2.9454 -2.94573 -2.94573 -2.9454 -2.94573 -2.9454 -2.94573 -2.9454 -2.94573 -2.9454 -2.94573 -2.9454 -2.94573 -2.9454 -2.94573 -2.9454 -2.945 -2.94 -2.945	0.000034 ccetophenol y 1.196946 1.248036 0.077809 -1.23281 -0.05462 2.110604 2.207381 -2.19646 -0.11209 -2.0846 0.181486 -1.09506 -0.83674 -1.70012 -1.69991 1.265718 ccthylphenol y 0.748347 1.780708 1.532906 0.199997 -0.63317 0.968618 2.807241 -1.88065 -1.58813 2.339918 -0.14822 0.87241 -1.58805 -1.58813 2.33918 -0.14822 0.87241 -1.58805 0.158813 2.33918 -0.14822 0.87241 -1.58813 2.33918 -0.14822 0.87241 -1.58813 2.33918 -0.14822 0.87241 -1.58813 2.33918 -0.14822 0.87241 -1.58813 2.33918 -0.14822 0.87241 -1.58813 -0.14822 0.87241 -1.58813 -0.14822 0.87241 -1.58813 -0.14822 0.87241 -1.58813 0.87241 -1.58813 -0.14822 0.87241 -1.58813 -0.1482 0.87241 -1.58813 -0.1482 0.87241 -1.58813 -0.1482 0.87241 -1.58813 -0.1482 0.87241 -1.58813 -0.1482 0.87241 -1.58813 -0.1482 0.87241 -1.58813 -0.1482 0.87241 -1.58813 -0.1482 0.87241 -1.58813 -0.1482 0.87241 -1.58813 -0.1482 0.87241 -1.5881 -0.1482 0.87241 -1.5881 -0.1482 0.8724 -0.872 -0.8724 -0.8724 -0.8724 -0.8724 -0.872 -0.872	0.000048
Atom C C C C C C C C C C C C C C C C C C C	2.504053 3.65582 4'-hydroxya x -1.49694 -0.11381 0.656148 0.002477 -1.38125 -2.13312 -2.08786 0.389551 -1.89374 -3.48124 -3.90017 0.570782 2.142371 2.963256 4.019275 2.733813 2.73375 2.681218 3-trifluorom x -2.42285 -1.47795 -0.11665 0.275724 -0.65317 -2.00896 -3.4816 -1.80698 -0.34321 -2.88238 -3.78991 0.619369 1.729144 2.059506	-0.01002 -0.01729 cetophenone y -1.18142 -1.23932 -0.0718 1.165687 1.23822 0.06309 -2.09112 -2.19846 2.192112 0.188369 -0.67965 2.087825 -0.18596 1.080238 0.820419 1.683186 -1.27712 v 0.816182 1.83437 0.28456 -0.82632 -0.51705 2.86506 -1.86492 -1.85589 2.33783 -0.16175 2.30782 -0.016175 -0.01172 -0.0112 -0.0172 -0.0102 -0.0112 -0.012 -0.012 -0.012 -0.012 -0.012 -0.012 -0.012 -0.012 -0.012 -0.0	-3.4E-05 -0.00005 (6) z -0.00003 -0.00006 -0.00006 -0.00006 0.000011 -1.7E-05 0.000018 0.000015 -9.1E-05 0.0000052 0.000044 0.0000017 -0.000011 -9.7E-05 0.0000012 (7) z 0 0 0 0 -1E-06 0 0 0 -1E-06 0 0 -1E-06 0 0 -1E-06 0 0 -1E-06 0 0 -1E-06 0 0 -1E-06 0 0 -1E-06 0 0 0 -1E-06 0 0 0 -1E-06 0 0 0 -1E-06 0 0 0 -1E-06 0 0 0 0 -1E-06 0 0 0 0 -1E-06 0 0 0 -1E-06 0 0 0 0 -1E-06 0 0 0 0 -1E-06 0 0 0 0 -1E-06 0 0 0 0 0 0 0 0 0 0 0 0 0	N 4 Atom C C C C C C C C C C C C C C C C C C C	-3.61099 -3.61099 x 1.541957 0.169436 -0.62155 0.056784 1.431214 2.259722 2.127994 -0.33785 1.930128 3.52411 -0.5114 -2.07804 -2.07804 -2.07804 -2.07804 -2.67251 -2.67251 -2.67251 -2.67257 -0.67637 -2.08881 -3.54057 -1.90853 -0.31907 -2.93573 0.540344 1.683813 2.042402 2.04240 2.04240 2.04240 2.04240 2.04240 2.04240 2.04240 2.04240 2.04240 2.04240 2.04240 2.04240 2.04240 2.04240 2.0424 2.04240 2.04240 2.04240 2.0424 2.0424 2.0424 2.0424 2.0424 2.042 2.0424 2.0424 2.0424 2.042 2.0424 2.0424 2.042 2.042 2.042 2.042 2.04 2.04	0.000034 tectophenol y 1.196946 1.248036 0.077809 -1.23281 -0.05462 2.110604 2.207381 -2.19646 -0.11209 -2.0846 0.181486 -1.09506 -0.83674 -1.70012 -1.69991 1.265718 t.532906 0.199997 -0.85529 -0.63317 0.9968618 2.807241 -1.88065 -1.58813 2.339918 -0.14082 -0.87613 -0.8761 -0.88 -0.88 -0.886 -0.886 -0.88 -0.88 -0.886 -0.88 -0.8	0.000048 z anion z 0.000052 -0.0001 -4.9E-05 0.000042 0.000204 0.00024 0.000464 -7.9E-05 -0.00028 0.000185 0.000185 0.00019 -0.00011 -0.00011 -0.00013 0.880696 -0.00023 olanion z 0 0.000001 -1E-06 -3E-06 -3E-06 -6E-06 0.000003 0.000004 -3E-06 0.000002 0 0 -1.07541 10754 10754 10754 10754 10754 10754 10754 10754 10754 10754 10754 100 10754 1075 1075 1075
Atom C C C C C C C C C C C C H H H O H H C C C C	2.504053 3.65582 4'-hydroxya x -1.49694 -0.11381 0.656148 0.002477 -1.38125 -2.13312 -2.08786 0.389551 -1.89374 -3.48124 -3.90017 0.570782 2.142371 2.963256 4.019275 2.733813 2.73375 2.681218 3-trifluorom x -2.42285 -1.47795 -0.11665 0.275724 -0.65317 -2.00896 -3.4816 -1.80698 -0.34321 -2.88238 -3.78991 0.619369 1.729144 2.059506	-0.01002 -0.01729 cetophenone y -1.18142 -1.23932 -0.0718 1.165687 1.23822 0.06309 -2.09112 -2.19846 2.192112 0.188369 -0.67965 2.087825 -0.18596 1.080238 0.820419 1.683292 1.683186 -1.27712 0.816182 1.833437 1.541426 0.208486 -0.82632 -0.816182 1.65169 1.55589 -1.35589 -1.35589 -1.35589 -1.3259 2.333783 -0.16175 -0.90113 -0.90113	-3.4E-05 -0.00005 (6) z -0.00003 -0.00006 -0.00006 -0.00006 0.000011 -3.9E-05 0.000012 0.000044 0.000041 -9.1E-05 0.0000012 0.0000011 -0.88129 0.881351 0.000012 (7) z 0 0 0 -1E-06 0 0 0 -1E-06 0 0 0 -1E-06 0 0 0 -1E-06 0 0 0 -1E-06 0 0 0 -1E-06 0 0 0 -1E-06 0 0 0 0 -1E-06 0 0 0 0 -1E-06 0 0 0 0 -1E-06 0 0 0 0 0 0 0 0 0 0 0 0 0	N 4 Atom C C C C C C C C C C C C C	-3.61099	0.000034 v v 1.196946 1.248036 0.077809 -1.23281 -0.05462 2.110604 2.207381 -2.19646 -0.11209 -2.0846 -0.11209 -2.084 0.181486 -1.09506 -0.83674 -1.70012 -1.69991 1.265718 v v v 0.748347 1.780708 1.532906 0.199997 -0.85529 -0.63317 0.968618 2.339918 2.339918 -1.88065 -1.58813 2.339918 -0.14082 -0.87613 -0.8761 -0.8761 -0.8761 -0.8761 -0.8761 -0.8761 -0.8761 -0.8761 -0.8761 -0.8	0.000048
Atom C C C C C C C C C C H H H O H H C C C C	2.504053 3.65582 x -1.49694 -0.11381 0.656148 0.002477 -1.38125 -2.08786 0.389551 -1.89374 -3.48124 -3.90017 0.570782 2.142371 2.963256 4.019275 2.733813 2.73375 2.681218 3-trifluorom x -2.42285 -1.47795 -0.11665 0.275724 -1.47795 -0.11665 0.275724 -1.47795 -0.11665 0.275724 -1.47795 -0.11665 0.275724 -1.80698 -3.4816 -1.80698 -0.34321 -2.88238 -3.78991 0.619369 1.729144 2.059506 2.537605	-0.01002 -0.01729 cetophenone y -1.18142 -1.23932 -0.0718 1.165687 1.23822 0.06309 -2.09112 -2.19846 2.192112 0.188369 -0.67965 2.087825 -0.18596 1.080238 0.820419 1.683292 1.683186 -1.27712 nethylphenol y 0.816182 1.833437 1.541426 0.208486 -0.82632 -0.51705 1.051905 1.051905 1.051905 1.25589 -1.35589 -0.6175 -0.90114 -0.90133783 -0.9015307	$\begin{array}{c} -3.4E{-}05\\ -0.00005\\ \hline 0.00005\\ \hline 0.00003\\ -0.00006\\ -0.00006\\ -0.00006\\ -0.00006\\ 0.000011\\ -3.9E{-}05\\ 0.000018\\ 0.000011\\ -3.9E{-}05\\ 0.000052\\ 0.000044\\ 0.000047\\ -9.1E{-}05\\ 0.000042\\ 0.000047\\ -9.1E{-}05\\ 0.000012\\ 0.000012\\ \hline 0.000012\\ \hline 0\\ -0.88129\\ 0.881351\\ 0.000012\\ \hline 0\\ -0.88129\\ 0.881351\\ 0.000012\\ \hline 0\\ 0\\ -0.88129\\ 0.881351\\ 0.000012\\ \hline 0\\ 0\\ -1E{-}06\\ 0\\ 0\\ -1E{-}06\\ 0\\ 0\\ 0\\ -1E{-}06\\ 0\\ 0\\ -1E{-}06\\ 0\\ 0\\ -1E{-}06\\ 0\\ -1E{-}06\\ 0\\ -1E{-}06\\ 0\\ -1E{-}06\\ -0\\ -10.7569\\ -9E{-}06 \end{array}$	N Atom C C C C C C C C C	-3.61099	0.000034 icetophenor y 1.196946 1.248036 0.077809 -1.23281 -0.05462 2.110604 2.207381 -2.19646 -0.11209 -2.0846 0.181486 -1.09506 -0.83674 -1.70012 -1.69991 1.265718 icetylphenor y 0.748347 1.780708 1.532906 0.199997 -0.85529 -0.63317 0.968618 2.389781 -1.58813 2.339918 -0.14082 -0.87613 -0.87611 0.93821	0.000048 z anion z 0.000052 -0.0001 -4.9E-05 0.000042 0.00024 0.00044 -7.9E-05 -0.00018 0.000185 0.000018 -0.00019 -0.00019 -0.00011 -0.00023 -0.88073 0.880696 -0.00023 bl anion z 0 0.000001 -1E-06 -2E-06 -3E-06 -6E-06 0.000004 -3E-06 0.000004 -3E-06 0.000002 0 0 -1.07541 1.075421 -1.1E-05 -1.1E-05 -0.00002 -0.00002 -0.000002 -0.000002 -0.000002 -0.000004 -3E-06 -0.000004 -3E-06 0.000004 -3E-06 0.00004 -3E-0
Atom C C C C C C C C C C H H H O H H C C C C	2.504053 3.65582 4'-hydroxya x -1.49694 -0.11381 0.656148 0.002477 -1.38125 -2.08786 0.389551 -1.89374 -3.48124 -3.90017 0.570782 2.142371 2.963256 4.019275 2.733813 2.73375 2.681218 3-trifluorom x -2.42285 -1.47795 -0.11665 0.275724 -0.11665 0.275724 -0.65317 -2.00896 -3.4816 -1.80698 -0.34321 -2.88238 -3.78991 0.619369 1.729144 2.059506 2.537605 4-hydroxybr	-0.01002 -0.01729 cetophenone y -1.18142 -1.23932 -0.0718 1.165687 1.23822 0.06309 -2.09112 -2.19846 2.192112 0.188369 -0.67965 2.087825 -0.18596 1.080238 0.820419 1.683292 1.683186 -1.27712 rethylphenol y 0.816182 1.833437 1.541426 0.0816182 1.833437 1.541426 0.208486 0.208486 0.208486 0.208487 1.55589 -1.35589 -1.35589 -1.35589 -1.35589 -1.35589 -1.323783 -0.61675 -0.90114 -0.90113 0.905307 renzaldehyde	-3.4E-05 -0.00005 (6) z -0.00003 -0.00006 -0.00006 -0.00006 0.000011 -3.9E-05 0.000012 0.000044 0.000044 0.000047 -9.1E-05 0.000002 0.0000011 -9.7E-05 0.000002 0.0000012 (7) z 0 0 0 0 0 -0.881351 0.000124 (7) 2 0 0 0 0 -0.881351 0.000012 (7) -0.881351 0.000012 (7) -0.881351 0.000012 (7) -0.881351 0.000012 (7) -0.881351 0.000012 (7) -0.8816 0 0 0 -1.E-06 0 0 -1.E-06 0 0 -1.E-06 0 0 -1.E-06 0 0 -1.E-06 0 0 -1.E-06 0 (8) -1.E-06 0 -1.E-06 0 0 -1.E-06 0 (8) -1.E-06 0 0 -1.E-06 0 -1.E-06 0 0 0 (8) -1.E-06 0 0 0 0 (8) -1.E-06 0 0 (8) -1.E-06 0 0 (8) -1.E-06 0 (8) -1.E-06 0 (8) (8) (8) (8) (8) (8) (8) (8)	N 4 Atom C C C C C C C C C C C C C C C C C C C	-3.61099	0.000034 icetophenor y 1.196946 1.248036 0.077809 -1.23281 -0.05462 2.110604 2.207381 -2.19646 -0.11209 -2.0846 0.181486 -1.09506 -0.83674 -1.70012 -1.69991 1.265718 icetophenor y 0.748347 1.780708 1.532909 -0.63317 0.968618 2.3897241 -1.88065 -1.58813 2.339918 -0.14082 -0.87611 0.93821 enzaldebyd	0.000048 te anion z 0.000052 -0.0001 -4.9E-05 0.000042 0.00024 0.000464 -7.9E-05 -0.00028 0.000185 0.000056 -1.9E-05 -0.00019 -0.00011 -0.00023 0.88073 0.88073 0.88073 0.88073 0.88073 0.88073 0.88073 0.88073 0.000001 -1E-06 -3E-06 -3E-06 -3E-06 -6E-06 0.000002 0 0 -1.07541 1.075421 -1.1E-05 te anion
Atom C C C C C C C C C C H H H O H H C C C C	2.504053 3.65582 4'-hydroxya x -1.49694 -0.11381 0.656148 0.002477 -1.38125 -2.1312 -2.08786 0.389551 -1.89374 -3.48124 -3.90017 0.570782 2.142371 2.963256 4.019275 2.733813 2.73375 2.681218 3-trifluoron x -2.42285 -1.47795 -0.11665 0.275724 -0.65317 -2.0896 -3.4816 -1.80698 -3.4816 -1.80698 -3.4816 -1.80698 -3.4828 -3.78991 0.61369 -2.88238 -3.78991 0.61369 2.537605 4-hydroxybd x	-0.01002 -0.01729 cetophenone y -1.18142 -1.23932 -0.0718 1.165687 1.23822 0.06309 -2.09112 -2.19846 2.192112 0.188369 -0.67965 2.087825 -0.18596 1.080238 0.820419 1.683186 -1.27712 rethylphenol y 0.816182 1.833437 1.541426 0.028486 -0.82632 -0.51705 1.051905 2.86506 -1.85589 -1.23259 2.333783 -0.16175 -0.90114 -0.90113 0.905307 enzaldehyde y	-3.4E-05 -0.00005 (6) z -0.00003 -0.00006 -1.7E-05 0.000018 0.000011 -3.9E-05 0.000012 0.000042 0.000044 (7) z 0.00001 -9.7E-05 0.000011 -9.7E-05 0.000012 0.000012 0.000012 0.000012 0.000124 (7) z 0 0 0 0 0 0 0 0 0 0 0 0 0	N Atom C C C C C C C C C	-3.61099	0.000034 tectophenor y 1.196946 1.248036 0.077809 -1.23281 -0.05462 2.110604 2.207381 -2.19646 -0.11209 -2.0846 0.181486 -0.181486 -0.83674 -1.70012 -1.69991 1.265718 t.532906 0.199997 -0.83529 -0.63317 0.968618 2.807241 -1.88065 -1.58813 2.339918 -0.14082 -0.876611 0.93821 tenzaldehyd y	0.000048
Atom C C C C C C C C C C C C H H H O H H C C C C	2.504053 3.65582 4'-hydroxya x -1.49694 -0.11381 0.656148 0.002477 -1.38125 -2.13312 -2.08786 0.389551 -1.89374 -3.48124 -3.90017 0.570782 2.142371 2.963256 4.019275 2.733813 2.73375 2.681218 3-trifluorom x -2.42285 -1.47795 -0.11665 0.275724 -0.65317 -2.08966 -3.4816 -1.80698 0.34321 -2.88238 -3.78991 0.619369 1.729144 2.059506 2.059509 2.537605 4-hydroxybr x 1.209812	-0.01002 -0.01729 cetophenone y -1.18142 -1.23932 -0.0718 1.165687 1.23822 0.06309 -2.09112 -2.19846 2.192112 0.188369 -0.67965 2.087825 -0.18596 1.080238 0.820419 1.683292 1.683186 -1.27712 rethylphenol y 0.816182 1.833437 1.541426 0.208486 -0.82632 -0.51705 1.051905 2.86506 -1.86492 -1.55589 -1.23259 2.333783 -0.16175 -0.90114 -0.90113 0.905307 enzaldehyde y 1.186794	-3.4E-05 -0.00005 (6) z -0.00006 -0.00006 -0.00006 -1.7E-05 0.000011 -3.9E-05 0.000012 -0.9-005 0.000047 -0.00001 -9.7E-05 0.000001 -9.7E-05 0.000011 -0.88129 0.000001 -0.88129 0.0000124 (7) z 0 0 0 0 0 0 0 -1E-06 0 0 0 -1E-06 0 0 0 -1E-06 0 0 -1E-06 0 0 -1E-06 0 0 -1E-06 0 0 -1E-06 0 -1E-06 0 -1E-06 0 -1E-06 0 0 -1E-06 0 -1E-06 0 -1E-06 0 -1E-06 0 -1E-06 0 -1E-06 0 -1E-06 0 -1E-06 0 -1E-06 0 -1E-06 0 -1E-06 -1	N 4 Atom C C C C C C C C C C C H H H O H C C C C	-3.61099 -3.61099 -3.61099 -3.61099 -3.61099 -3.62155 0.169436 -0.62155 0.056784 1.431214 2.259722 2.127994 1.431214 -2.07804 -2.879251 -3.95526 -3.95526 -2.67251 -2.67251 -2.67251 -2.67251 -2.67251 -2.67253 -1.95603 -1.55603 -0.17809 0.22657 -0.07637 -2.93873 0.540344 1.683813 2.042402 2.042404 2.483701 -2.93873 0.540344 2.483701 -2.042404 2.483701 -3.54057 -1.90853 -0.31907 -2.93873 0.540344 2.483701 -3.54054 -3.54057 -3.90853 -3.54057 -3.90853 -3.54057 -3.90853 -3.54054 2.483701 -3.54034 -3.5405 -3.5405 -3.54 -3.5405	0.000034 v 1.196946 1.248036 0.077809 -1.23281 -0.05462 2.110604 2.207381 -2.19646 0.181486 -0.11209 -2.0846 0.181486 -1.09506 -0.83674 -1.70012 -1.69991 1.265718 nethylphen y 0.748347 1.780708 1.532906 0.199997 -0.63317 0.968618 2.807241 -1.88065 -1.58813 2.339918 -0.14082 -0.87613 -0.87613 0.93821 enzaldehyd y 1.197874	0.000048
Atom C C C C C C C C C C C C C C C C C C C	2.504053 3.65582 4'-hydroxya x -1.49694 -0.11381 0.656148 0.002477 -1.38125 -2.13312 -2.08786 0.389551 -1.89374 -3.48124 -3.90017 0.570782 2.142371 2.963256 4.019275 2.733813 2.73375 2.681218 3-trifluorom x -2.42285 -1.47795 -0.11665 0.275724 -0.65317 -2.00896 -3.4816 -1.80698 -0.34321 -2.88238 -3.78991 0.619369 1.729144 2.059506 2.059509 2.537605 4-hydroxybr x 1.209812 -0.16978	-0.01002 -0.01729 cetophenone y -1.18142 -1.23932 -0.0718 1.165687 1.23822 0.06309 -2.09112 -2.19846 2.192112 0.188369 -0.67965 2.087825 -0.18596 1.080238 0.820419 1.683292 1.683186 -1.27712 tethylphenol y 0.816182 1.833437 1.541426 0.208486 -0.208486 -0.2084862 -0.51705 2.86506 -1.86492 -1.55589 -1.23259 2.333783 -0.16175 -0.90114 -0.90113 0.905307 enzaldehyd y 1.186794 1.330689 -0.21925	-3.4E-05 -0.00005 (6) z -0.00003 -0.00006 -1.7E-05 0.000018 0.000011 -3.9E-05 0.000042 0.000047 -0.00001 -9.7E-05 0.0000012 0.000041 -0.000012 (7) z 0 0 0 0 0 0 0 0 0 0 0 0 0	N 4 Atom C C C C C C C C C C C C C C C C C C C	-3.61099 -3.61099 x 1.541957 0.169436 -0.62155 0.056784 1.431214 2.259722 2.127994 -0.33785 1.930128 3.52411 -0.31785 1.930128 3.52411 -0.51174 -2.07804 -2.89832 -3.95526 -2.67251 -2.67251 -2.67251 -2.67251 -2.67251 -2.67251 -2.67253 -1.55603 -0.17899 0.22657 -0.67637 -2.98581 2.042404 2.483701 -2.93573 -0.31907 -2.93573 -0.31907 -2.93573 -0.31907 -2.93573 -0.31907 -2.93573 -0.31907 -2.93573 -0.31907 -2.93573 -0.31907 -2.93573 -0.31907 -2.93573 -0.31907 -2.93573 -0.34044 2.483701 -4.1404rosybb x 1.253863 -0.1135 -0.1789 -0.1789 -0.135	0.000034 ccetophenor y 1.196946 1.248036 0.077809 -1.23281 -0.05462 2.110604 2.207381 -2.19646 0.181486 -0.01209 -2.0846 0.181486 -1.09506 -0.83674 -1.70012 -1.69991 1.265718 ccetophenor y 0.748347 1.780708 1.532906 0.199997 -0.63317 .1.532906 0.968618 2.807241 -1.88065 -1.58813 2.339918 -0.14082 -0.87613 -0.87613 0.93821 cenzaldechyd y 1.197874 1.32923 0.021252	0.000048 z anion z 0.000052 -0.0001 -4.9E-05 0.000042 0.000044 -7.9E-05 -0.00028 0.000185 0.000185 0.00018 -1.9E-05 -0.00019 -0.00011 -0.00011 -0.00013 0 0.000001 -1.9E-05 -0.00023 ol anion z 0 0.0000001 -1E-06 -2E-06 -3E-06 -6E-06 0.000003 0.000004 -3E-06 -6E-06 0.000002 0 0 -1.07541 1.075421 -1.1E-05 z -0.0001 -8.5E-05 -0.0001 -8.5E-05 0.00001 -8.5E-05 0.0001 -8.5E-05 0.0002 -0.0001 -8.5E-05 0.00001 -8.5E-05 0.00001 -8.5E-05 0.0001 -8.5E-05 0.0002 0 -0.0001 -8.5E-05 0.0001 -8.5E-05 0.0001
Atom C C C C C C C C C C C C C C C C C C C	2.504053 3.65582 4'-hydroxya x -1.49694 -0.11381 0.656148 0.002477 -1.38125 -2.13312 -2.08786 0.389551 -1.89374 -3.48124 -3.90017 0.570782 2.142371 2.963256 4.019275 2.733813 2.73375 2.681218 3-trifluorom x -2.42285 -1.47795 -0.11665 0.275724 -0.65317 -2.00896 -3.4816 -1.80698 -0.34321 -2.88238 -3.78991 0.619369 1.729144 2.059506 2.059509 2.537605 4-hydroxyb x 1.209812 -0.16978 -0.0178 -0.0	-0.01002 -0.01729 cetophenone y -1.18142 -1.23932 -0.0718 1.165687 1.23822 0.06309 -2.09112 -2.19846 2.192112 0.188369 -0.67965 2.087825 -0.18596 1.080238 0.820419 1.683292 1.683186 -1.27712 v 0.816182 1.83437 0.816182 1.83437 0.816182 1.83437 0.816182 1.651905 2.86506 -1.86492 -1.55589 -1.23259 2.33783 -0.16175 2.86506 -1.86492 -1.85589 -1.23259 2.33783 -0.16175 -0.90114 -0.90113 0.905307 enzaldehyde y 1.86794 1.330689 0.210065 -1.07112	-3.4E-05 -0.00005 (6) z -0.00003 -0.00006 -0.00006 -0.00006 0.000011 -1.7E-05 0.000052 0.000044 0.000047 -0.000011 -9.7E-05 0.000004 0.000047 -0.000012 0.000041 -9.7E-05 0.000001 -9.7E-05 0.0000012 (7) z 0 0 0 0 -1E-06 0 0 0 -1E-06 0 0 -1.7E-06 0 0 0 -1.7E-06 0 0 -1.7E-06 0 0 -1.7E-06 0 0 -1.7E-06 0 0 -1.7E-06 0 0 -1.7E-06 0 0 -1.7E-06 0 0 -1.7E-06 0 0 -1.7E-06 0 0 -1.7E-06 0 0 -1.7E-06 0 0 -1.7E-06 0 0 -1.7E-06 0 -1.7E-06 0 -1.075699 -9E-06 (8) -1.275699 -9E-06 0 0 0 0 0 0 0 0 0 0 0 0 0	N 4 Atom C C C C C C C C C C C C C C C C C C C	-3.61099 -3.61099 x 1.541957 0.169436 -0.62155 0.056784 1.431214 2.259722 2.127994 -0.33785 1.930128 3.52411 -0.5114 -2.07804 -2.07804 -2.07804 -2.07804 -2.67251 -2.67251 -2.67251 -2.67257 -0.67637 -2.07881 -3.54057 -0.07637 -1.90853 -0.31907 -2.9373 0.540344 1.683813 2.042402 2.042404 2.042657 -0.96597 -0.96597 -0.96597 -0.96597 -0.96597 -0.96597 -0.96597 -0.96597 -0.96597 -0.9705	0.000034 cectophenor y 1.196946 1.248036 0.077809 -1.23281 -0.05462 2.110604 2.207381 -2.19646 -0.11209 -2.0846 0.181486 -1.09506 -0.83674 -1.70012 -1.69991 1.265718 rethylphend y 0.748347 1.780708 1.532906 0.199997 -0.63512 -0.63317 0.968618 2.807241 -1.88065 -1.58813 2.339918 -0.14082 -0.87613 -0.87613 -0.87613 -0.87611 0.93821 rethylphend y 1.197874 1.32923 0.204337 -1.0722	0.000048

ISSN	1859-1531	- THE	UNIVER	SITY	OF DAN	ANG - J	OURNAL	OF SCIE	NC	E AND	TECHNOL	LOGY, V	'OL. 2	0, NO. 6	.1, 2022	
0	3.195814	-0.13957	0.243038	0	3.249284	0.000002	0.268227	Н		-4.16642	-0.03639	-8.5E-05	Н	-3.00307	-1.10991	-0.
н	3.590746	0.736411	0.308533	Н	1.748835	2.150163	0.049333	Н		-3.05384	-1.10185	-0.89301				
н	1.762077	2.114455	0.098142	Н	-0.68975	2.139943	-0.29248	<u> </u>		4–cı	resol (17)			4-cı	resol anion	
п Н	-0.80866	-2.09088	-0.22739	С	-2.36738	-2.13993 -3E-06	-0.29247	Ator	n	X 0.7515	y 1 10151	Z	Atom	X 0.780177	y 1 201204	0
c	-2.41679	0.094239	-0.46104	н	-2.69149	0.888132	-1.02278	C		-0.7313	-1.19131	-0.00067	c	-0.60038	1.201294	-0. -0
Н	-2.72517	1.059707	-0.87358	Н	-2.69149	-0.88815	-1.02277	C		1.376097	-0.01233	-0.0038	c	-1.33649	0.000039	-(
Н	-2.74489	-0.69602	-1.14364	0	-2.98686	0.000005	0.829147	С		0.665067	1.192351	-0.00358	С	-0.6004	-1.18988	-0.
0	-3.00491	-0.10138	0.8274	Н	-3.94139	-1E-06	0.704419	С		-0.72293	1.217238	-0.00069	С	0.78913	-1.20129	-0.
H	-3.96123	-0.117/3	0.721941		1 herdua		nian	_ C		-1.43586	0.019215	0.001308	C	1.563811	0.000005	0.0
Atom	4-iiyuroxyi	ipnenoi (15) 7	Atom	4-iiyuro	xyipiienoi a	2	— н О		-1.2651/	2.1554/3	-0.00141	н	1.322679	-2.14/68	-0.
C	0.7173	1.190085	0	C	0.760605	1.197961	0.000104	— 0 Н		-3.17907	-0.78915	0.003105	н	1.322735	2.147681	-0.
C	-0.67286	1.216374	0.000002	С	-0.62985	1.211812	-3E-06	Н		-1.30166	-2.12678	-0.00151	н	-1.13368	2.138231	-0.
С	-1.39414	0.027018	0	С	-1.35049	0.021658	0.000048	Н		1.162851	-2.14889	-0.00652	Н	-1.13372	-2.13819	-0
С	-0.7173	-1.19009	-4E-06	С	-0.65635	-1.18361	-2.4E-05	Н		1.208871	2.131777	-0.00649	С	-2.84585	-2.2E-05	0.0
C	0.672858	-1.21637	0	С	0.736545	-1.20115	0.00011	С		2.883306	-0.01782	0.004685	H	-3.23541	-0.00285	1.0
н	1.394139	-2 15985	0	н	1.322001	-2 15427	-0.000874	н		3 272117	-1 02965	-0 11586	н	-3 2509	-0.88157	-0. -0
0	2.759533	-0.11337	0.000001	0	2.812537	-0.0229	-0.00045	Н		3.283579	0.59921	-0.80287		5.2507	0100107	0.
Н	3.144958	0.768888	0.000005	Н	1.302993	2.138732	-0.00016			4–amin	ophenol (18)			4-aminop	henol anion	(18)
Н	1.274122	2.121055	0	Н	-1.17038	2.153412	-0.00018	Ator	n	х	у	z	Atom	х	у	
H	-1.20519	2.15985	0.000005	Н	-1.20744	-2.12091	-0.00023	C		-0.72407	-1.18861	-0.00068	С	0.766452	1.197245	-0.
п 0	-1.27413	-2.12103	-0.00001	н	-2.75515	-0 79806	-0.00017	С		0.667509	-1.19993	-0.00699	С	-0.62554	1.193053	-0.
н	-3.14495	-0.7689	0.000088		5.07025	0.79000	0.000170	C		0.687824	-0.00771	-0.00885	C	-0.6255	-2.8E-05	-0. -0
	3-cres	ol (14)			3-с	resol anion		c		-0.70092	1.21413	-0.00031	c	0.766481	-1.19724	-0.
Atom	х	у	z	Atom	х	у	Z	С		-1.41395	0.019032	0.002167	С	1.541759	0.000022	0.0
С	1.319554	1.017981	-0.00019	С	-1.38923	0.963063	0.000257	Н		-1.2422	2.152935	0.004249	Н	1.296783	-2.14522	0.0
C C	0.161501	1.786894	-5.3E-05	C	-0.25604	1.76073	0.000065	0		-2.78303	0.092681	0.009362	0	2.834445	0.000028	0.0
C	-1.20636	-0.20754	0.000214	C	1.162313	-0.18748	-0.00028	Н		1.232524	2.137602	-0.01117	Н	-1.16242	2.138655	-0.
č	-0.04401	-0.97905	0.0003	Č	0.025642	-0.99171	-0.00039	Н		1.193228	-2.14869	-0.01051	Н	1.296713	2.145254	0.0
С	1.207993	-0.37216	-2.6E-05	С	-1.30362	-0.46745	0.000113	Н		-1.27066	-2.12596	0.00355	Ν	-2.77605	-0.00016	-0.
Н	-0.10005	-2.06266	0.000531	Н	0.137331	-2.07384	-0.00074	N		2.798259	-0.01908	-0.08037	Н	-3.17495	-0.81865	0.3
О Н	2.299419	-1.19048	-5.4E-05	0 н	-2.34416	-1.2201	0.000047	Н		3.232542	0.805047	0.313669	Н	-3.17492	0.819828	0.3
н	2.297961	1.486558	-0.00034	н	-0.36851	2.841481	0.000074			3.4-dimet	thvlnhenol (19	0.507550 N		3.4-dimet	hvlphenol a	nion
Н	0.24229	2.867719	-7.5E-05	С	2.531858	-0.82703	0.00034	Ator	n	x	у	z	Atom	x	у	
С	-2.55391	-0.88263	-0.00025	Н	2.672291	-1.45279	0.885561	С		-1.27768	-1.25256	0	С	-1.32323	-1.2502	-7.
н	-2.6/156	-1.5123/	-0.88512	H U	2.005052	-1.46962	-0.8/3/1	С		0.075912	-1.58292	-2E-06	C	0.028663	-1.575	-1.
н	-3.36076	-0.14966	0.007734	Н	1.907458	1.840764	-0.00053	C		0.686134	-0.60922	-4E-06 -3E-06	C	1.035398	-0.606/	-9.
Н	-1.98878	1.796163	0.000399					_ c		-0.66547	1.077533	-1E-06	c	-0.71813	1.074459	-8.
	3-ethyl-5-met	thylphenol	(15)		3-ethyl-5-n	nethylphen	ol anion	C		-1.64558	0.08709	0	С	-1.7692	0.10486	-0.
Atom	X	y	Z	Atom	X	y	Z	H		-2.03475	-2.02938	0.000001	Н	-2.07212	-2.03713	0.0
C	-0.36391	-1.20239	-0.23195 -0.36412	C	0.330765	0.01812	-0.2273	н		0.359574	-2.03025	-4E-06 -1E-06	н	-1.00608	-2.02440	0.0
c	-0.16438	1.19557	-0.24486	č	0.167064	-1.14818	-0.24162	0		-2.94974	0.494861	0.000003	0	-3.0143	0.433417	0.0
С	1.205773	1.101344	0.002437	С	-1.20732	-1.05356	0.00911	Н		-3.53322	-0.27133	-5E-06	С	2.49506	-0.98859	-2.
C	1.786406	-0.16049	0.130935	С	-1.80208	0.195617	0.145995	C		2.528174	-0.99235	0.000003	Н	3.021656	-0.60027	0.8
С	1.002372	-1.3032	0.013608	С	-1.06/29	0.264636	0.033834	н		3.044257	-0.59583	0.8/89/6	н н	2.60/59/	-2.0/446	-4. _0
0	1.628373	-2.50915	0.144736	0	-1.62243	2.569882	0.158313	Н		3.044292	-0.59574	-0.87891	C	1.677856	1.832733	0.0
Н	0.990382	-3.22315	0.040879	Н	0.930588	2.165976	-0.32085	С		1.731184	1.82889	0	Н	2.326897	1.759564	0.8
Н	-0.96808	-2.10234	-0.32197	Н	0.638103	-2.12209	-0.34379	Н		2.377323	1.749966	0.878606	Н	2.327066	1.759728	-0.
Н	-0.62336	2.174159	-0.34877	C	-2.04638	-2.30782	0.094222	Н		2.377323	1.749973	-0.87861	Н	1.215322	2.820521	0.0
н	2.060846	2.330043	0.126542	н	-2.95134	-2.13962 -2.63705	-0.90247	H		1.2/188 4_t_buts	2.81/198 /lynhenol (20)	0.000004		4_t_buts	dynhenol ar	ion
н	2.848187	2.341259	-0.63076	Н	-1.48684	-3.12785	0.549293	Ator	n	x	y v	z	Atom	x	v v	
Н	1.464623	3.241294	0.005885	С	2.428353	-0.08513	-0.57239	С		-1.76299	-1.18119	-0.00002	С	-1.81073	-1.1921	-4
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н	-2.00238	-0.67977	-1.1492	С	2.791309	0.819/18	-1.00/08	С		0.351464	0.035563	-6.4E-05	С	0.308764	0.034176	-1.
C	-3.20289	0.218446	0.758754	н	2.852677	-1.19216	1.24854	C		-0.38454	1.222848	-6E-06	C	-0.44/26	1.211572	
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Atom	4-metnoxy	pnenol (16) 7	Atom	4-metho	xypnenoi a	nion	_ H		0.121633	2.179809	-2E-06	H	0.052797	2.174585	0.0
C	1.325919	1.164601	-3E-06	C	1.378173	1.161723	-6.5E-05	0		-3.83501	0.06825	0.000021	0	-3.88836	-0.01928	0.0
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C	-0.41629	-1.00828	0.000029	C	-0.36029	-1.00408	0.000163	C		2.490218	1.404708	0.000927	H	2.140164	1.977597	0.8
C	0.963079	-1.21291	0.000014 _2E_06	C	1.021693	-1.20908	0.000085	H		2.195072	1.970187	0.888621	Н Ч	2.140079	1.977972	-0.
н	1.365444	-2.21881	0.000014	н	1.404714	-2.22524	0.000088	Н		3.58001	1.326367	0.000619	C	2.348496	-0.73254	1.2
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H U	2.001155	2.013632	-1.2E-05	H U	-0.40036	2.372386	-4.6E-05	H		3.46886	-0.77564	1.263053	H	2.016799	-0.22072	2.1
Н	-1.07154	-1.86864	0.000043	п 0	-2.22841	0.59815	0.000246	H C		2.375977	-0.23282	-1.25469	Н	2.348339	-1.75922	-1.
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Ĥ	-3 05394	-1.10192	0.892883	Ĥ	-4 13063	-0.0587	-0.00047	н		3 469096	-0 77374	-1 2639				

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