SUPPORTING INFORMATION FOR:

A Photo-Basic D-A Fluorophore with a High Intramolecular Charge-Transfer as Model Strategy for Designing Organic Proton-Coupled Electron-Transfer Modulators: An Analysis based on Steady-State Fluorescence, Isotopic Effect and Theoretical Study

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I. General Experimental Details

1. Materials and Instruments. The N^1-(4-phenyl)-2-(trifluoromethyl)-8-methoxybenzo[*b*][1,8]naphthyridin-4(1*H*)-one **3k** (Chart 1C) was employed as high CT-dye, the N^1-phenyl-2-(trifluoromethyl)-benzo[*b*][1,8]naphthyridin-4(1*H*)-one **3g** was used as the low CT-dye (Figure 1A-B). These derivatives were previously prepared by our group following a synthetic strategy of successive steps.[1-2] The fluorescent profile of the mentioned pK_a-probes were previously studied by our group[3] and some key photophysical properties are listed in Table S1. All selected phenols were purchased from commercial sources (Sigma-Aldrich, Fluka or Merck) and they were used without further purification. Ethanol was purchased from Droguería Industrial Uruguaya as rectified ethanol (95 %). Ultrapure grade water was obtained by filtration of deionized water with Milipore system. All tested phenols were dissolved in ethanol. Absorption and fluorescence spectra as well as photophysical data were obtained from a Thermo Scientific Varioskans Flash Multimode instrument for air-equilibrated solutions at 25ºC.

2. Quenching study by using phenol/phenolates. A group of thirty-three phenols with a variety of pK_a values from 0.4 to 10.35 and structurally varied was selected for the study (Table 1). The solution stocks of phenols were prepared in ethanol. The solution of phenolate ions were prepared from estequiometric titration with sodium hydroxide to reach final point in aqueous solution. The final solution for fluorescence measurements consisted of ethanol-water (8:2). It is important to mention that ethanol: water (8:2) ratio led the highest fluorescence intensity for the dye **3k**.[3] For a final volume of 200 μL, solution containing phenols consisted of 120 μL of the fluorescent probe **3k** or **3g** in ethanol solution (final concentration from 10, 20 or 100 μM), 40 μL of quencher solution (in ethanol) and 40 μL of water. For phenolate measurements, solution containing phenols consisted of 160 μL of the fluorescent probe **3k** or **3g** in ethanol solution (final concentration from 10, 20 or 100 μM) and 40 μL of phenolate solution (in water). The majority of the fluorescence measurements were performed at a 20 μM concentration of the high CT-probe **3k**. Lower concentration of the probe by about from 5 to 10 μM were applied for weak-acidic phenols. Higher concentrations ($\geq$ 30 μM) were needed for the low CT-probe **3g** by their discrete quenching response and lower fluorescence intensities. The emission spectra were collected upon 370 nm excitation. The Stern-Volmer plots

were constructed from corresponding fluorescence ratio (I/I_0) *vs.* acid concentration plots in to determine K_{SV} constant according to following equation:[4-5]

$$\frac{I}{I_0} = 1 + K_{SV}[Q] \qquad (1)$$

Where I_0 represents the fluorescence intensity of the compound solution in absence of the quencher, I is the fluorescence intensity of the compound solution upon increasing concentration of the quencher, [Q] is the concentration of the quencher. Examples of emission spectra upon different acid concentrations as well as their corresponding Stern-Volmer plots are found in Figure S1-S8 of the Supporting Information. All graphics and further calculations relative to plots were performed in Origin 2021b software.[6]

3. Isotopic effect. Kinetic isotope effects (KIE) were measured by using eight key phenols (picric acid, 2-hdyroxybenzaldehyde, 4-hydroxybenzaldehyde, phenol, 2-isopropylphenol, 4-chlorophenol, 4-methoxyphenol, 2-aminophenol, 3-hydroxyphenol and 4-acetamidophenol). The quenching experiments were performed by adding phenol and deuterated methanol (MeOD) (5-10% of the total volume). The quenching experiment was carried out according to quenching protocol described herein and their corresponding Stern-Volmer constants were calculated from the equation 1.

4. Theoretical Calculation. All DFT calculations were carried out in Gaussian09[7] package at the B3LYP level[8] in combination the 6-31G(d,p)[9] basis set. Calculations were performed either on personal notebooks or on Copernicus Cluster at the computational center at Science Faculty (Universidad Central Venezuela, Caracas, Venezuela). Optimization of the geometry was performed for the ground and excited states of the probe **3k** as well as for the ground state of all tested phenols. HOMO-LUMO energy levels and Mulliken charges were extracted from their optimized geometries. Calculations were done in gas phase and zero point energy corrections were not included in all the calculations. Phenol data for the H-O bond dissociation free energies (BDFE) were extracted from the reference 45.[10] Previously, we found that the B3LYP/6-31G(d,p) gave good estimations for structural parameters and absorption/emission profile of the N^1-aryl-2-(trifluoromethyl)benzo[*b*][1,8]naphthyridin-4(1*H*)-ones, being a convenient approach for providing reasonably results for describing electronic states.[3] All calculation outputs can be found in Supporting Information material. From LUMO-HOMO orbital levels, the

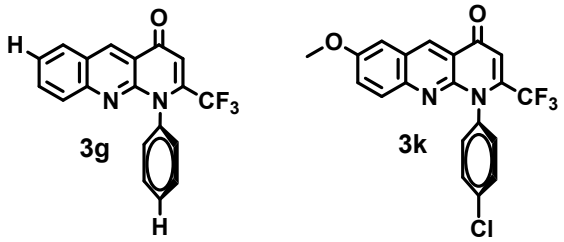
Gibbs free energy can be calculated by using the Rehm-Weller relation as follows in equation (2):[11]

$$\Delta G_{cs} = E_{ox} - E_{red} - E_{0,0} + C = E_{LUMO(PhOH)} - E_{LUMO\ (Dye)} - E_{0,0} + C \quad (2)$$

where $E_{1/2\ ox}$ and $E_{1/2\ red}$ are half-wave oxidation potential of the donor and half-wave reduction potential of the acceptor, respectively; C is the solvent dependent Coulombic interaction energy (which can be neglected in moderately polar environment); whereas $E_{0,0}$ represent the energy of the zero-zero transition to the lowest excited singlet state of the donor molecule. A wavelength of 400 nm was considered for the excitation of steady state measurement, while, a wavelength of 476 nm was considered for time-resolved measurements, for the *N′*-(4-chlorophenyl)-2-(trifluoromethyl)benzo[*b*][1,8]naphthyridin-4(1*H*)-one **3k** in the present investigation. Then, $E_{0,0} = (E_{abs} - E_{em})/2 = (3.0996\text{-}2.6047)/2 = 0.24745$ eV.

II. Photophysical Data for Probes **3g** and **3k**

Table S1. Fluorescence properties for the *N′*-aryl 2-(trifluoromethyl)benzo[*b*][1,8]naphthyridin-4(1*H*)-ones **3g** and **3k** in ethanol.[3]



	λ_{exc}[a]	λ_{em}[a]	Lifetimes (ns)[b]	Stoke shift (cm^{-1})[c]	Q.Y.[d]
3k	324/**420**	404/**476**	**14.20**; 6.73 (79.26; 20.74%)	56	0.24
3g	324/**400**	**426**/476	**8.13**; 2.27; 0.44 (37.6; 32.3; 30.2%)	26	0.052

[a]Maxima lengths (excitation or emission) is reflected in black bold. [b]Lifetimes with respective abundance percent, more details can be found in lifetime data section. [c]Stoke shift calculated from difference between maxima λ_{em} and λ_{abs}. [d]Q.Y.: quantum yield that was calculated from Rhodamine 6G.

III. Experimental Quenching Results

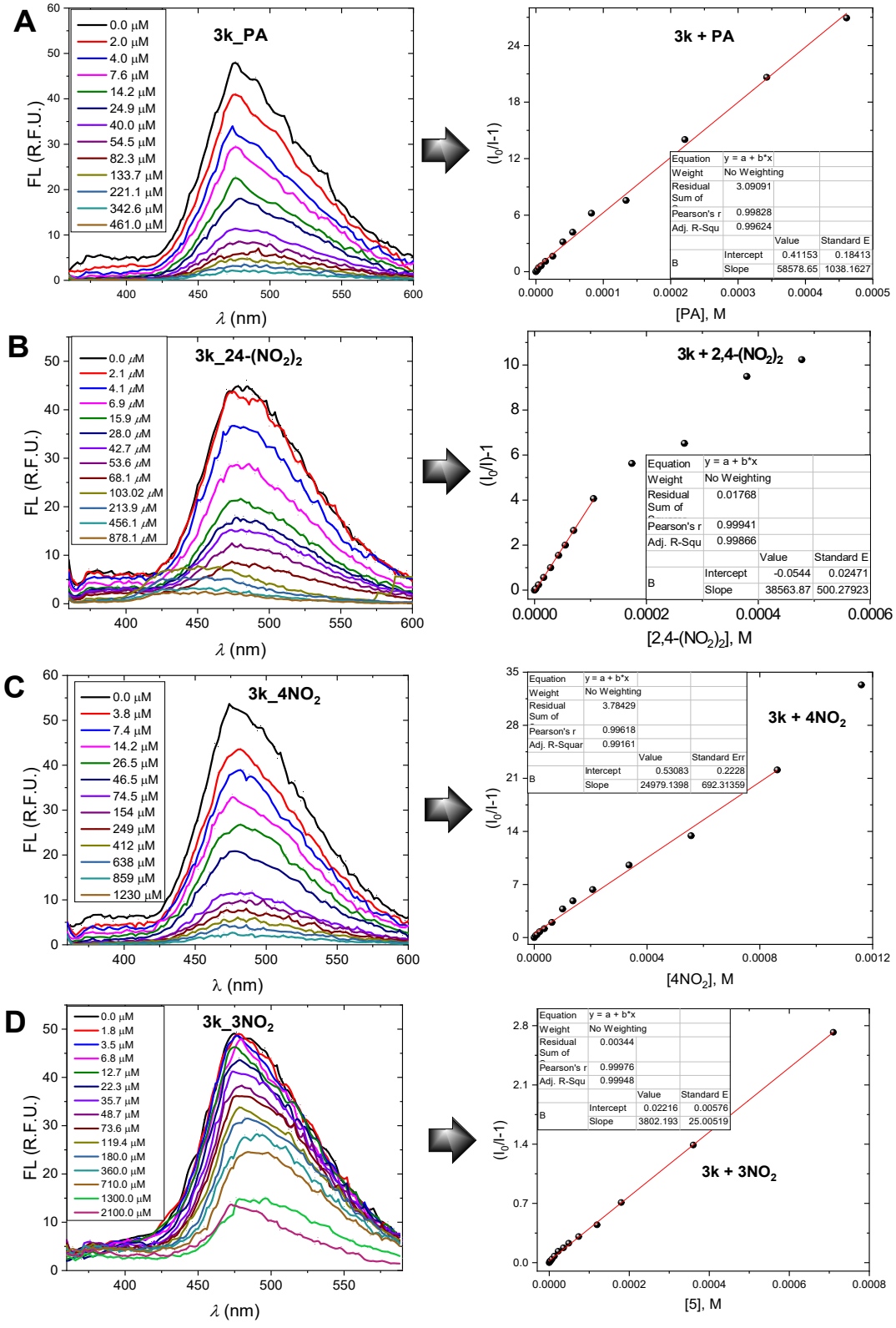


Figure S1. Emission spectra (left) for compounds **3k** in ethanol in presence of different

phenols: PA (**A**), 2,4-dinitrophenol (**B**), 4-nitrophenol (**C**) and 3-nitrophenol (**D**) and their corresponding Stern-Volmer plots (right).

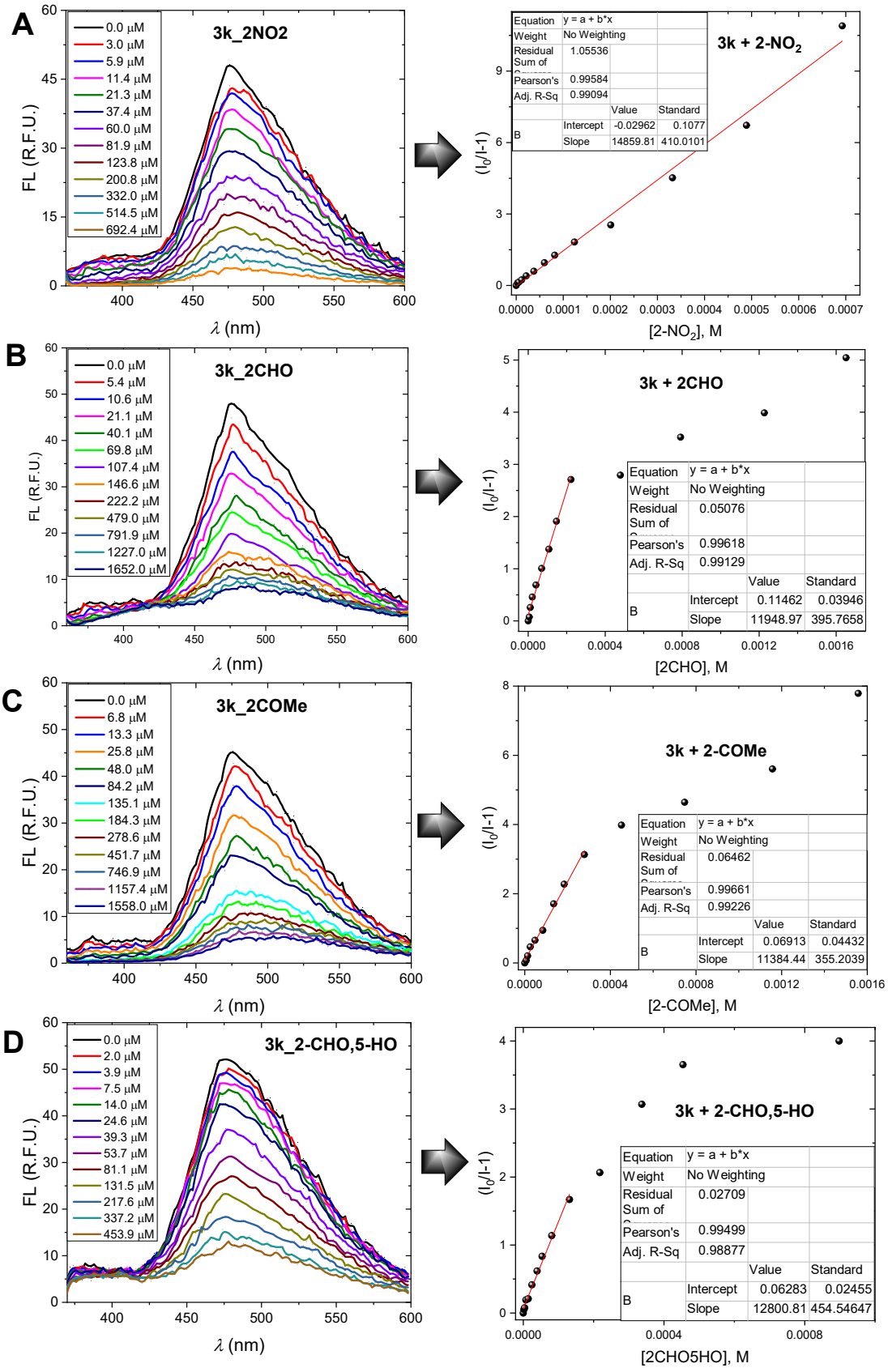


Figure S2. Emission spectra (left) for compounds **3k** in ethanol in presence of different phenols: 3-nitrophenol (**A**), 2-salicyaldehyde (**B**), 2-hydroxyacetophenone (**C**) and 2,4-dihydroxyl-benzaldehyde (**D**) and their corresponding Stern-Volmer plots (right).

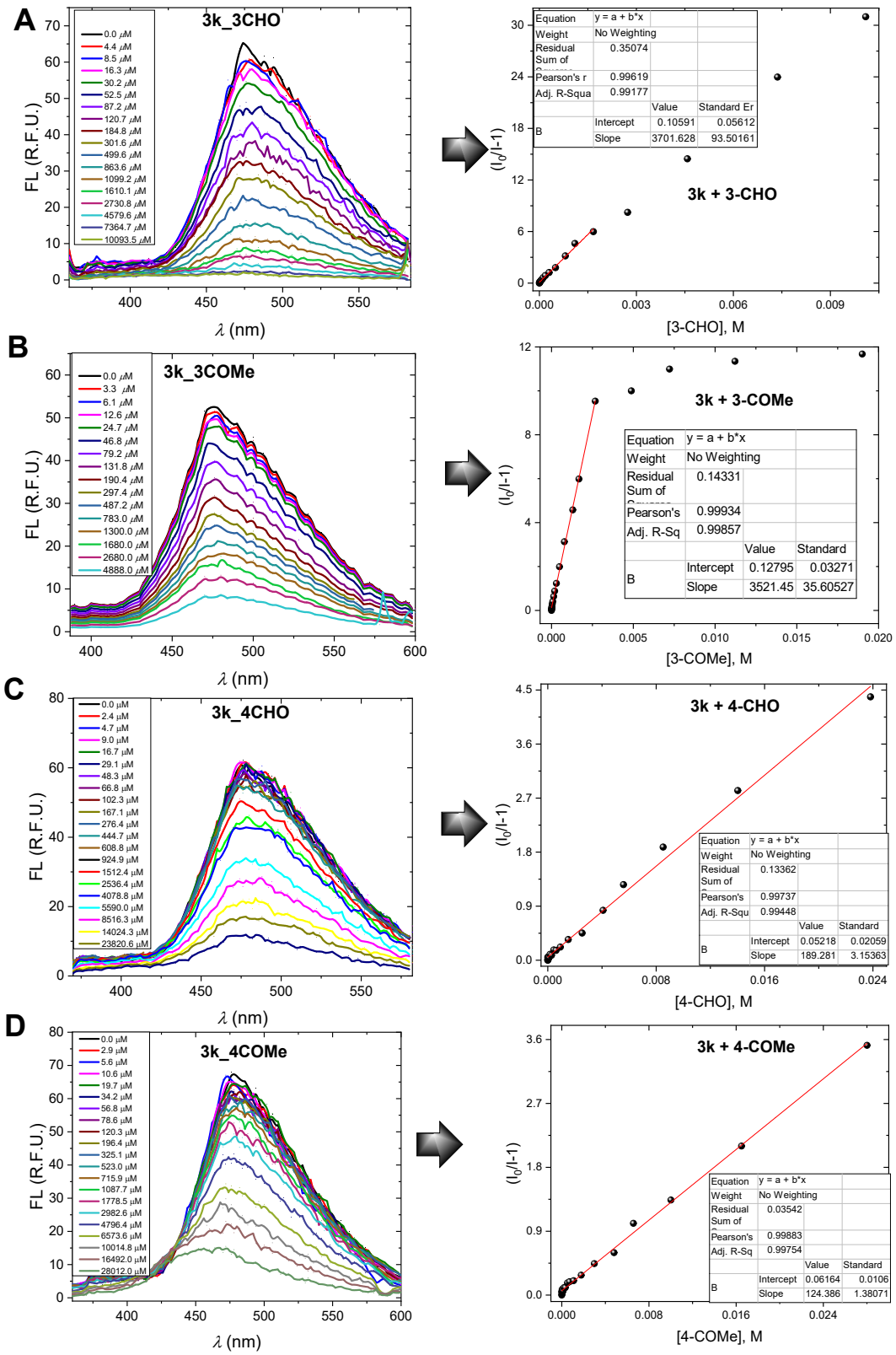


Figure S3. Emission spectra (left) for compounds **3k** in ethanol in presence of different phenols: 3-hydroxybenzaldehyde (**A**), 3-hydroxyacetophenone (**B**), 4-hydroxybenzaldehyde (**C**) and 4-hydroxylacetophenone (**D**) and their corresponding Stern-Volmer plots (right).

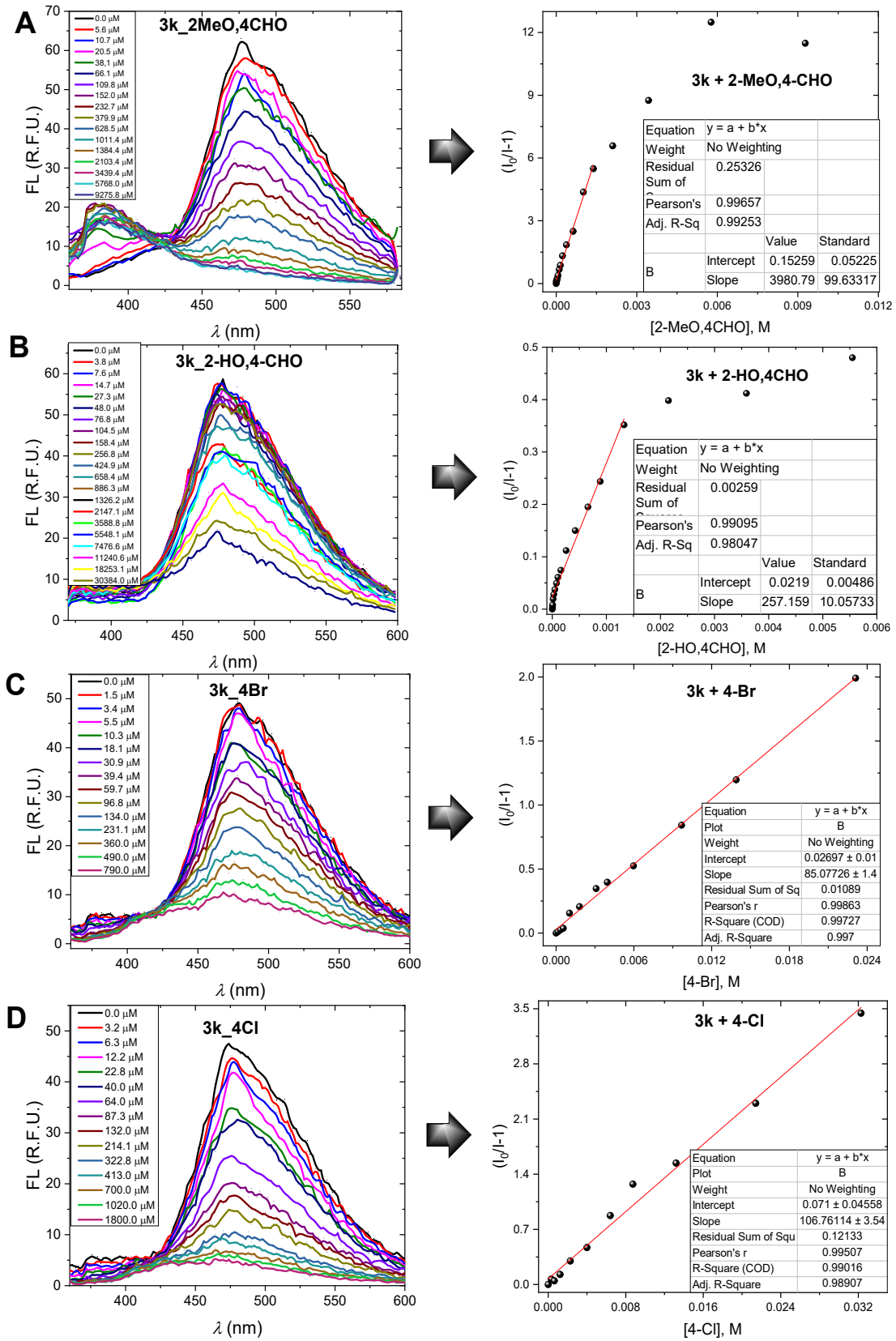


Figure S4. Emission spectra (left) for compounds **3k** in ethanol in presence of different phenols: 3-methoxy-4-hydroxylbenzaldehyde (**A**), 3,4-dihydroxylbenzaldehyde (**B**), 4-bromophenol (**C**) and 4-chlorophenol (**D**) and their corresponding Stern-Volmer plots (right).

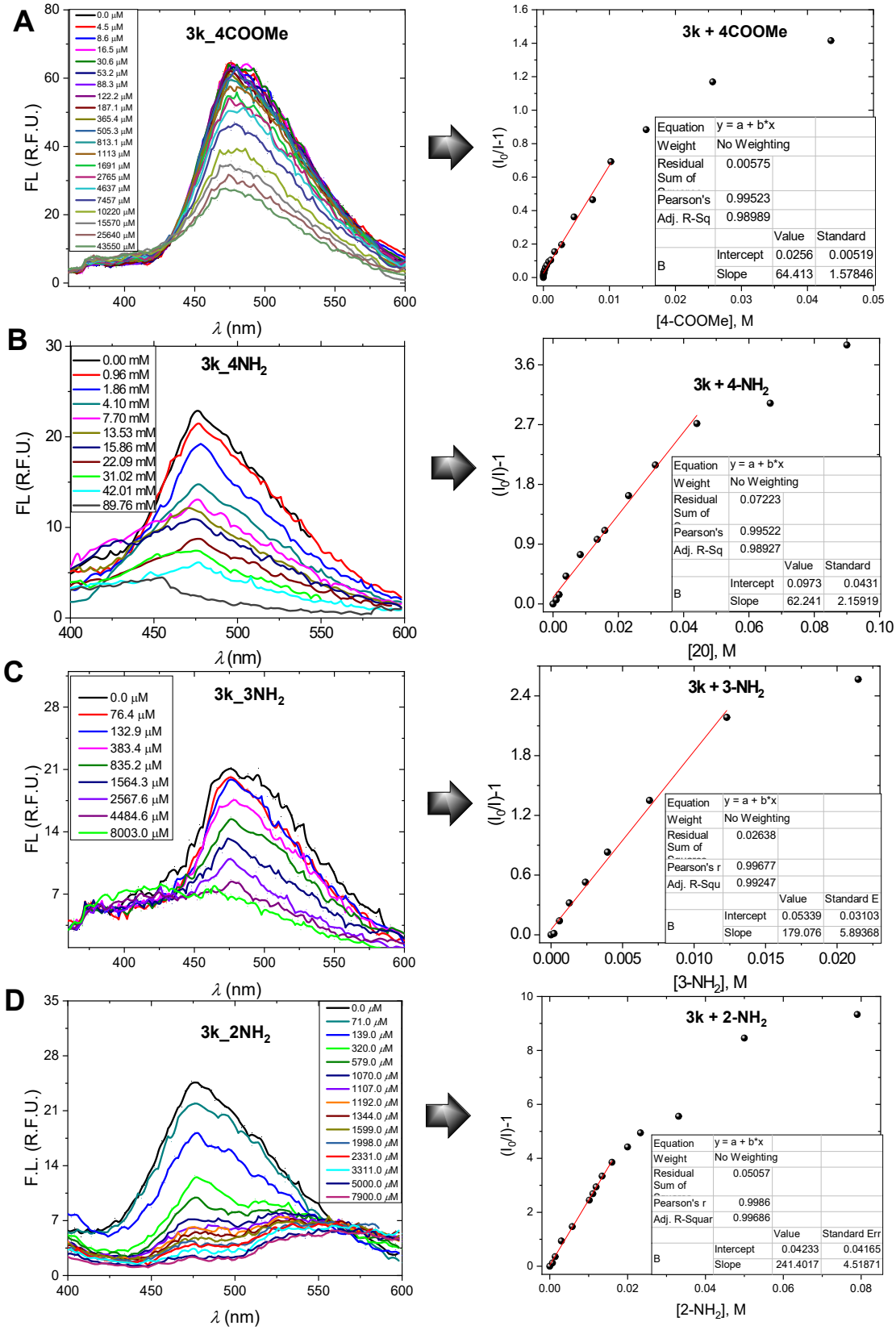


Figure S5. Emission spectra (left) for compounds **3k** in ethanol in presence of different phenols: methyl 4-hydroxylbenzoate (**A**), 4-aminophenol (**B**), 3-aminophenol (**C**) and 2-aminophenol (**D**) and their corresponding Stern-Volmer plots (right).

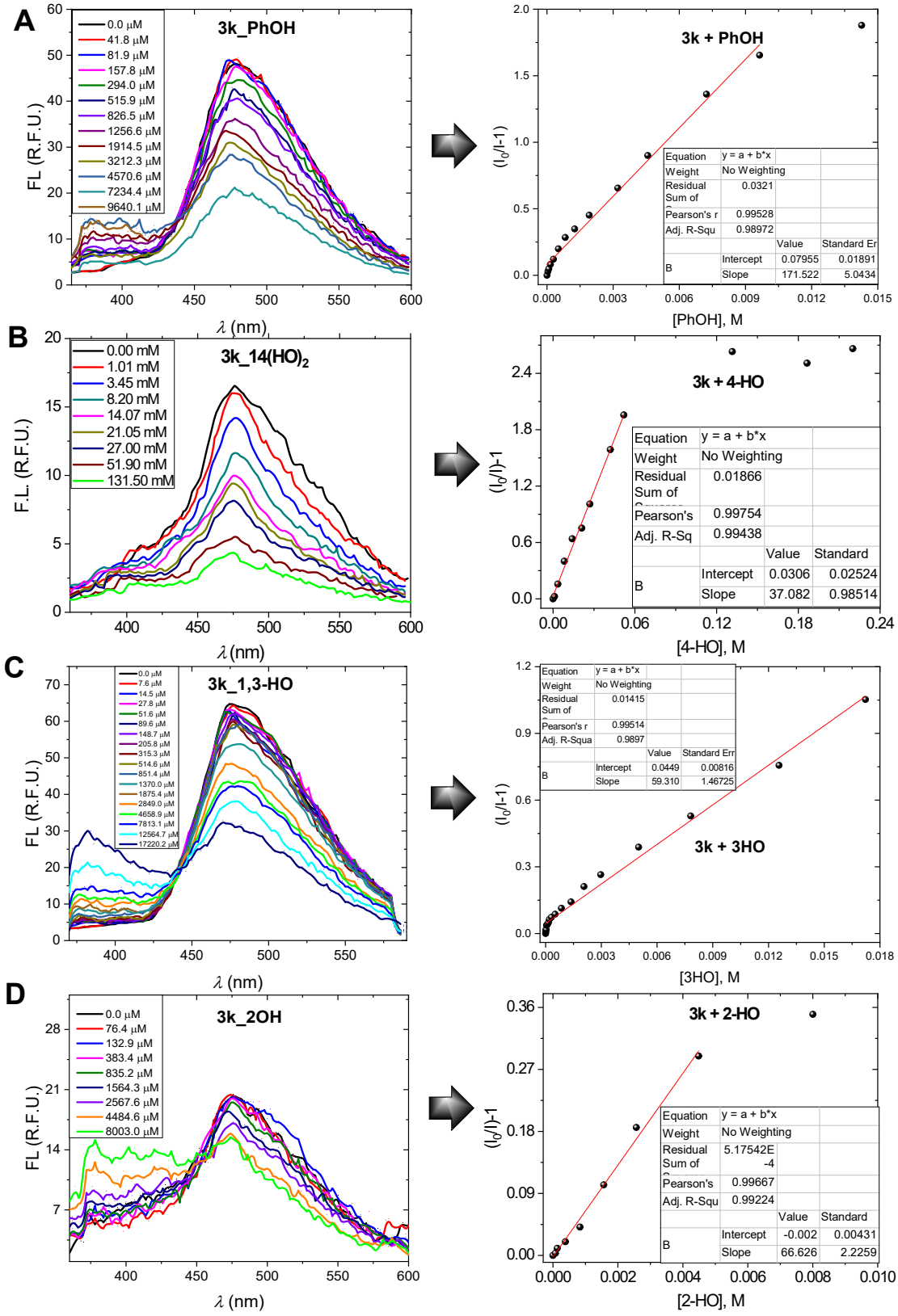


Figure S6. Emission spectra (left) for compounds **3k** in ethanol in presence of different phenols: phenol (**A**), 4-hydroxylphenol (**B**), 3-hydroxylphenol (**C**) and 2-hydroxylphenol (**D**) and their corresponding Stern-Volmer plots (right).

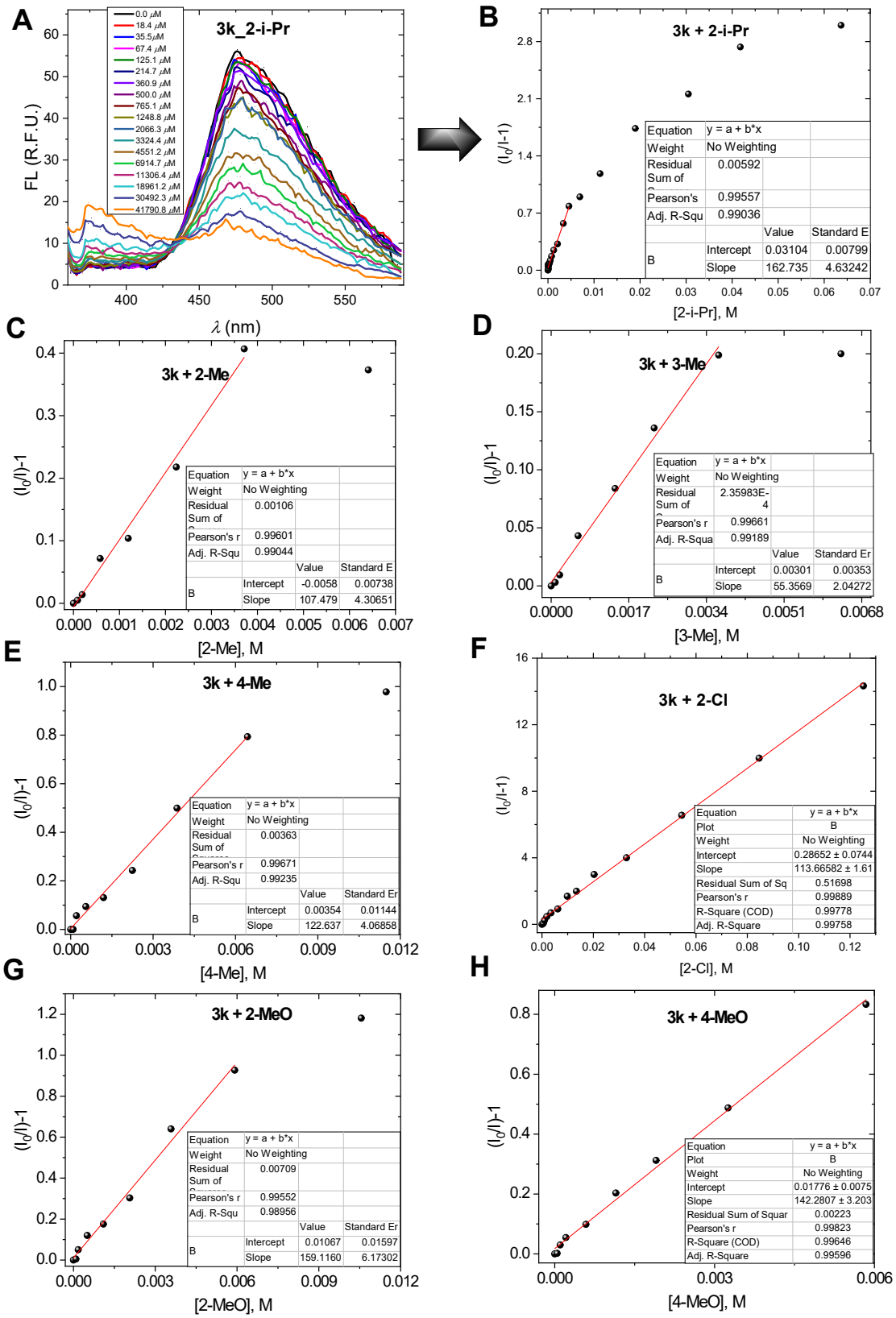


Figure S7. Emission spectra (left) for compounds **3k** in ethanol in presence of different phenols 2-isopropyl-phenol (**A**) and its Stern-Volmer plot (**B**), Stern-Volmer plots for 2-methylphenol (**C**), 3-methylphenol (**D**), 4-methylphenol (**E**), 2-chlorophenol (**F**), 2-methoxyphenol (**G**) and 4-methoxyphenol (**H**).

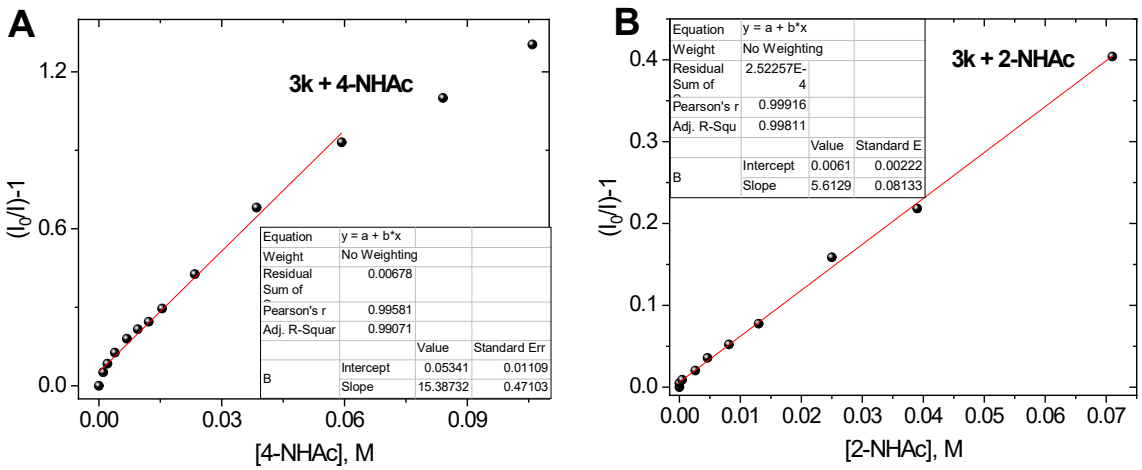


Figure S8. Stern-Volmer plots for the 4-acetamidephenol (**A**) and 2-acetamidephenol (**B**).

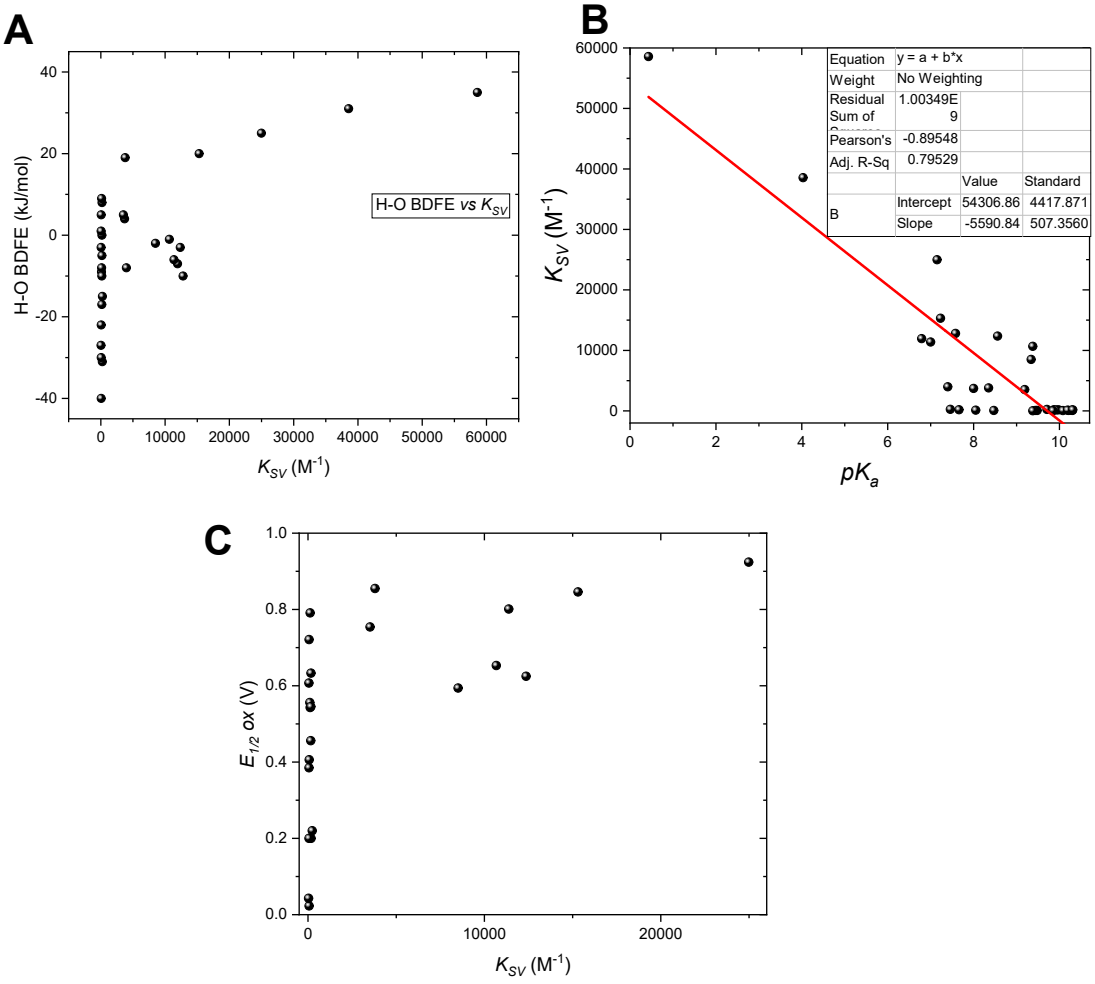


Figure S9. General H-O BDFE free energy vs. K_{SV} plot (**A**); K_{SV} *vs.* pK_a plot **(B)** and $E_{1/2}$ *ox vs.* K_{SV} plots for **3k (C).**

Table S1. Tabulated pK_a`s, H-O BDFE free energies and oxidation potential of the studied phenols.

Entries	Phenol	pK_a[12]	HO BDFE[10]	$E_{1/2\ ox}$[13]
1	2,4,6-Trinitrophenol	0.43	35	
2	2,4-Dinitrophenol	4.03	31	
3	4-Nitrophenol	7.15	25	0.925
4	2-Nitrophenol	7.23	20	0.846
5	3-Nitrophenol	8.35	19	0.800
6	2-Chlorophenol	8.56	-3	0.625
7	4-Chlorophenol	9.38	-1	0.653
8	4-Bromophenol	9.34	-2	0.594
9	2-Hydroxibenzaldehyde	6.79	-7	
10	3-Hydroxibenzaldehyde	8	4	
11	4-Hydroxibenzaldehyde	7.66	8	
12	2,4-Dihydroxibenzaldehyde	7.58	-10	
13	3,4-Dihydroxibenzaldehyde	7.46	-15	
14	3-Methoxy-4-hydroxibenzaldehyde	7.4	-8	
15	2-Hydroxiacetophenone	N.R.	-6	0.801
16	3-Hydroxiacetophenone	9.19	5	0.754
17	4-Hydroxiacetophenone	8.05	9	0.721
18	4-Hydroxibenzoate methyl ester	8.47	5	0.884
19	2-Aminophenol	9.71	-31	0.22
20	3-Aminophenol	9.87	-5	0.20
21	4-Aminophenol	10.3	-40	0.20
22	Phenol	9.98	0	0.633
23	2-Methoxyphenol	9.93	-17	0.456
24	4-Methoxyphenol	10.21	-22	0.406
25	2-Methylphenol	10.28	-9	0.543
26	3-Methylphenol	10.08	-3	0.667
27	4-Methylphenol	10.19	-8	0.556
28	2-Isopropylphenol	10.31	-10	0.500
29	2-Hydroxiphenol	9.48	-30	0.023
30	3-Hydroxiphenol	9.44	1	0.385
31	4-Hydroxiphenol	9.85	-27	0.042
32	4-Acetamidophenol	9.38		
33	2-Acetamidophenol	~9.60		

IV. Ground State Dye-Phenol Complex

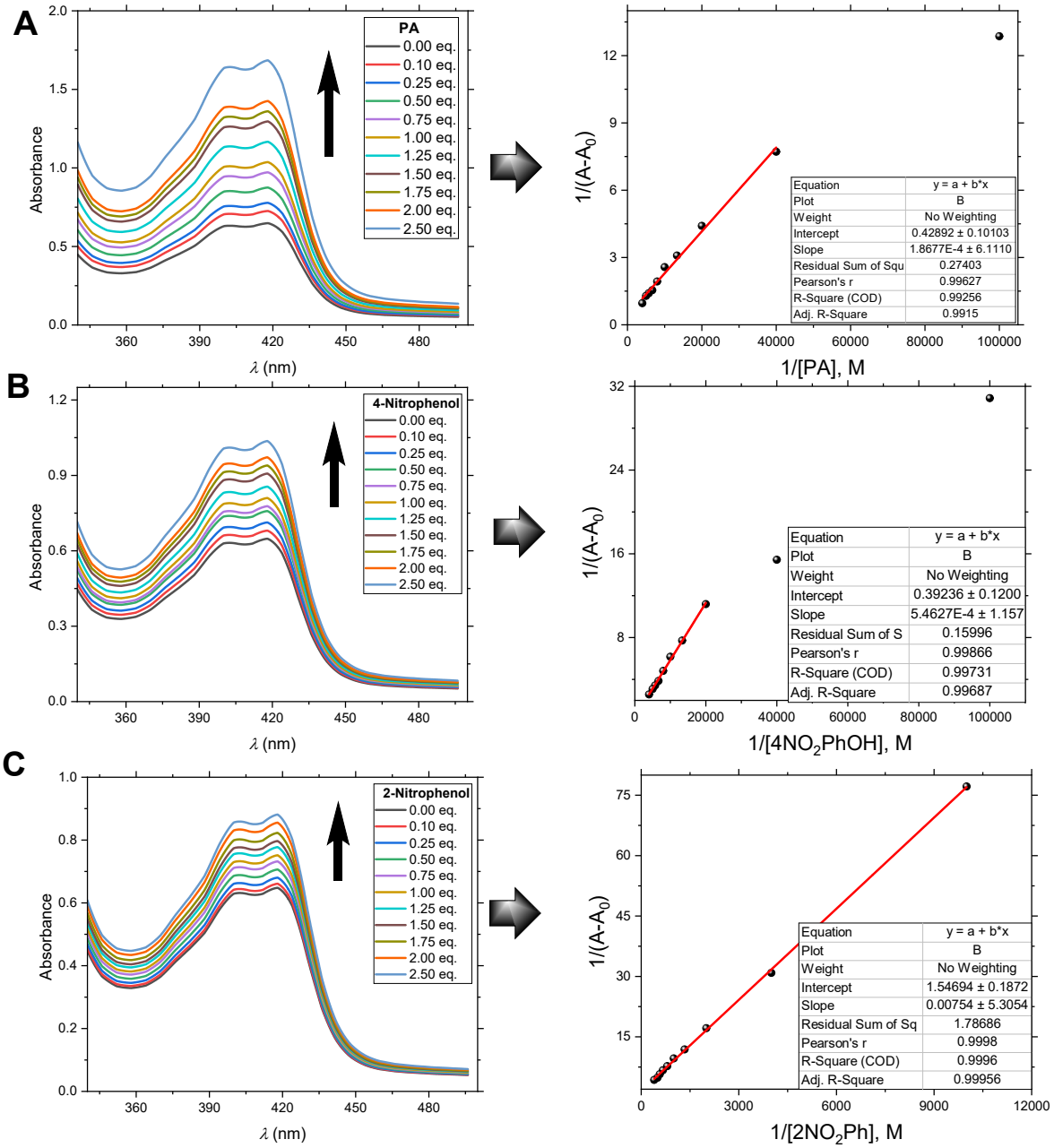


Figure S10. Absorption spectra obtained after sequential addition of phenol aliquotes to an ethanol: H_2O 4:1 v/v solution of dye **3k** and their corresponding absorption change of dye as a function of the phenol concentration: (**A**) PA, (**B**) 4-NO_2PhOH and (**C**) 2NO_2-PhOH. Direction of arrow indicates the spectral response upon phenol addition.

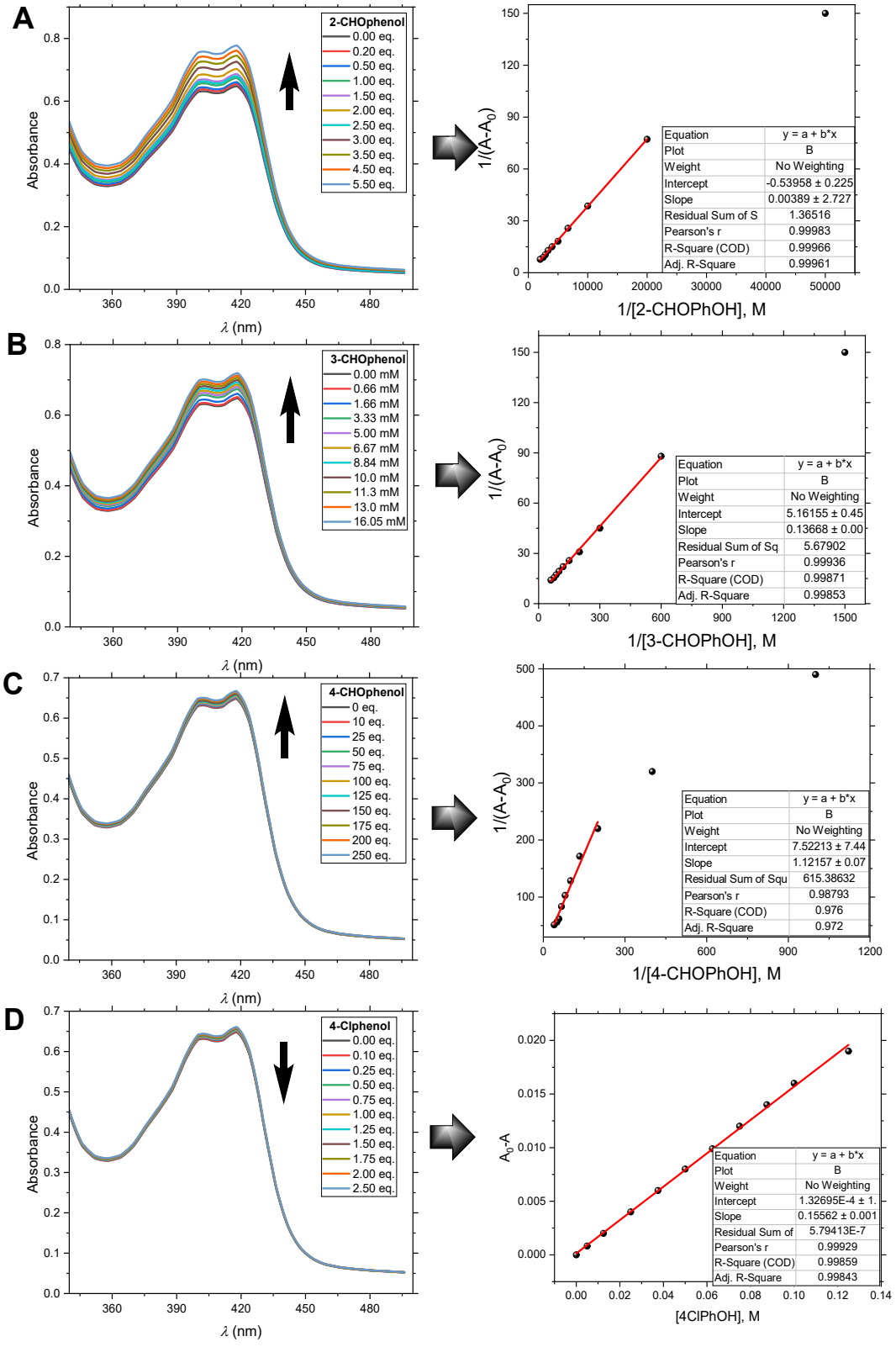


Figure S11. Absorption spectra obtained after sequential addition of phenol aliquotes to an ethanol: H_2O 4:1 v/v solution of dye **3k** and their corresponding absorption change of dye as a function of the phenol concentration: (**A**) 2CHO-PhOH, (**B**) 3-CHO-PhOH, (**C**) 4-

CHO-PhOH and (**D**) 4-Cl-PhOH. Direction of arrow indicates the spectral response upon phenol addition.

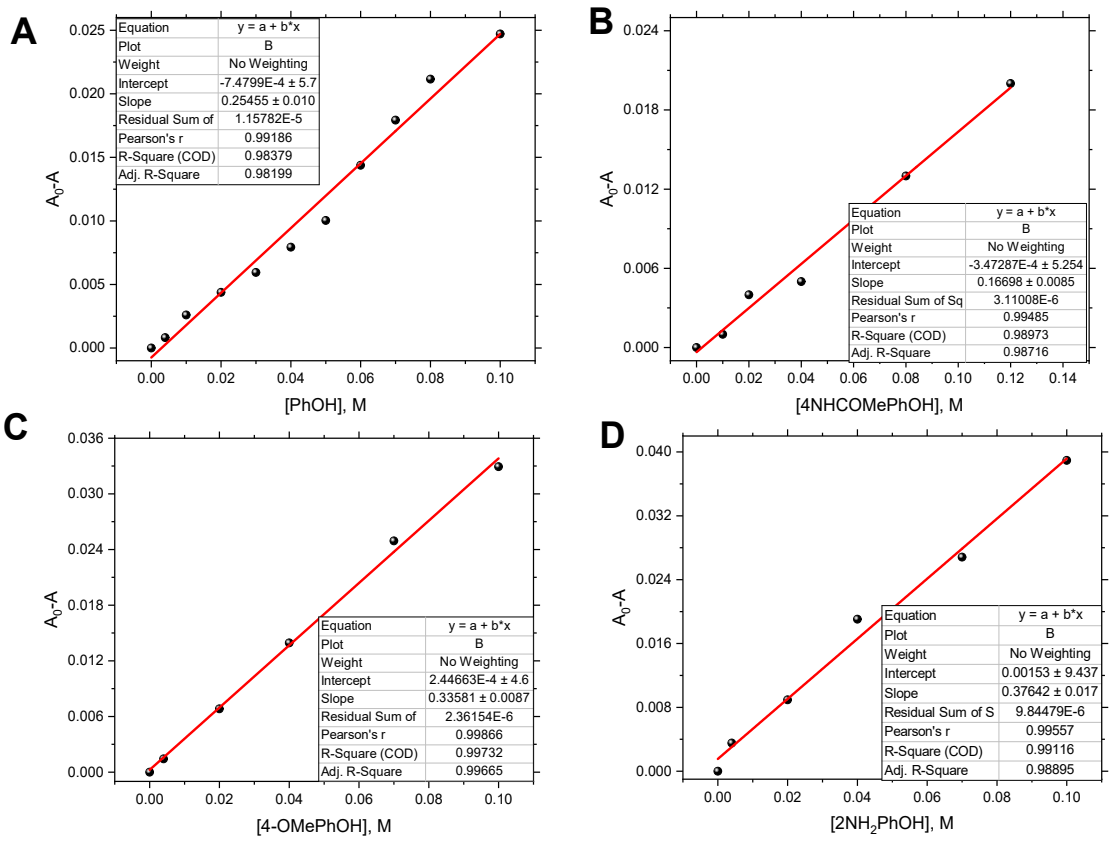
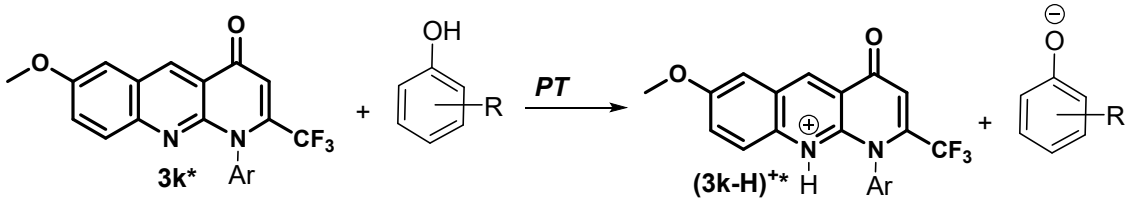


Figure S12. Corresponding absorption change of dye as a function of the phenol concentration from an ethanol: H_2O 4:1 v/v solution of dye **3k**: (**A**) PhOH, (**B**) 4-NHCOMePhOH, (**C**) 4-OMe-PhOH and (**D**) 2-NH_2-PhOH.

V. Theoretical Analysis

Table S2. Thermodynamical feasibility of PT-ET reaction between dye **3k** and phenols

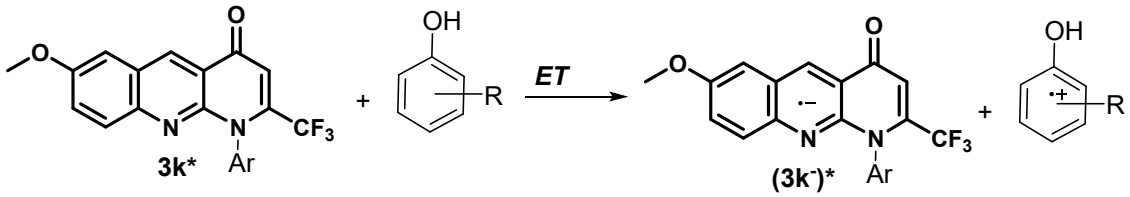


Entries	Phenols	$\Delta E_{(3k\text{-}H^+, 3k)}$[a]	E_{PhO}(in a.u.)[b]	E_{PhOH}(in a.u)[c]	$\Delta E_{(PhO,\ PhOH)}$[d]	ΔE_{CPET} (in a.u.)[e]	ΔE_{CPET} (eV)[f]
1	**PA**	-0.3957159	-920.96338	-920.45238	0.51099674	0.11528082	**3.136952032**
2	**2,4-$(NO_2)_2$-**	-0.3957159	-716.46558	-715.95015	0.51543277	0.11971685	**3.257662629**
3	**4-NO_2-**	-0.3957159	-511.98101	-511.43758	0.5434303	0.14771438	**4.0195144**
4	**3-NO_2-**	-0.3957159	-511.97788	-511.41936	0.55852447	0.16280855	4.430247975
5	**2-NO_2-**	-0.3957159	-511.98825	-511.42095	0.56730722	0.1715913	4.669238864
6	**2-CHO-**	-0.3957159	-420.81727	-420.23518	0.58208303	0.18636711	5.071309202

7	**2-$COCH_3$-**	-0.3957159	-460.14314	-459.55255	0.59059015	0.19487423	5.302799814
8	**3-CHO**	-0.3957159	-420.80224	-420.2327	0.56954689	0.17383097	4.730183466
9	**3-$COCH_3$-**	-0.3957159	-420.80543	-420.25064	0.55479088	0.15907496	4.842548083
10	**4-CHO-**	-0.3957159	-460.13062	-459.57112	0.55949511	0.16377919	4.328651833
11	**4-$COCH_3$-**	-0.3957159	-496.02547	-495.47127	0.55419544	0.15847952	4.456660472
12	**2,4-$(OH)_2$-1CHO**	-0.3957159	-496.01928	-495.46424	0.55504221	0.15932629	4.312448889
13	**3,4-$(OH)_2$-1CHO**	-0.3957159	-535.33384	-534.77127	0.56257588	0.16685996	4.335490683
14	**3-OCH_3,4-OH-1CHO**	-0.3957159	-535.36288	-534.80135	0.56153233	0.16581641	4.540492361
15	**4-$COOCH_3$**	-0.3957159	-2878.575	-2878.01	0.56498823	0.16927231	4.512096018
16	**4-Br**	-0.3957159	-767.06616	-766.49993	0.56623591	0.17051999	4.606135882
17	**4-Cl**	-0.3957159	-767.07474	-766.50087	0.57386767	0.17815175	4.640087105
18	**2-Cl**	-0.3957159	-307.47212	-306.8924	0.57972133	0.18400541	4.847757759
19	**H**	-0.3957159	-346.79971	-346.21547	0.58424594	0.18853002	5.007044156
20	**2-CH_3-**	-0.3957159	-346.7991	-346.21237	0.58673083	0.19101491	5.130165057
21	**3-CH_3-**	-0.3957159	-346.79236	-346.2117	0.58065939	0.18494347	5.197782329
22	**4-CH_3-**	-0.3957159	-422.00496	-421.41151	0.59345185	0.19773593	5.032570079
23	**2-OCH_3-**	-0.3957159	-422.00355	-421.41819	0.58535721	0.18964129	5.380670585
24	**4-OCH_3-**	-0.3957159	-421.99166	-421.41381	0.57784512	0.1821292	4.955989754
25	**2-OH**	-0.3957159	-382.69929	-382.13151	0.56777662	0.1720607	4.682011812
26	**3-OH**	-0.3957159	-382.69893	-382.11409	0.58483567	0.18911975	5.146212406
27	**4-OH**	-0.3957159	-382.68538	-382.10578	0.57960141	0.18388549	5.00378083
28	**2-NH_2-**	-0.3957159	-362.83724	-362.23376	0.60347774	0.20776183	5.653489321
29	**3-NH_2-**	-0.3957159	-362.83738	-362.24827	0.58911512	0.1933992	5.262662352
30	**4-NH_2-**	-0.3957159	-362.83342	-362.24031	0.59311438	0.19739846	5.371487609
31	**2-IPr-**	-0.3957159	-425.42915	-424.85051	0.57863281	0.18291689	4.977423844
32	**2-$NHCOCH_3$-**	-0.3957159	-515.50283	-514.94125	0.56158457	0.16586865	4.513517595
33	**4-$NHCOCH_3$-**	-0.3957159	-515.49492	-514.92726	0.56766038	0.17194446	4.678848895

[a]Energy difference between protonated dye (dye-H+) and excited dye; [b]Energy for deprotonated phenol; [c]Energy for ground-state phenol; [d]Energy difference between deprotonated phenol and phenol; Energy difference between product and starting compounds for limitating PT reaction (in a.u.)[e] and (in eV).[f] **Note:** the lowest energy values for CPET are marked in **bold** text.

Table S3. Thermodynamical feasibility of ET-PT reaction between dye **3k** and phenols

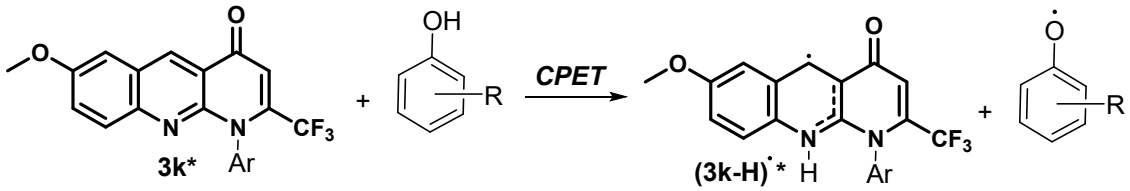


Entries	Phenols	$\Delta E_{(3k^-, 3k)}$	E_{PhO}(in a.u.)[b]	E_{PhOH}(in a.u)[c]	$\Delta E_{(PhO, PhOH)}$[d]	ΔE_{CPET} (in a.u.)[e]	$\Delta E_{ET\text{-}PT}$ (eV)[f]
19	**H**	-0.0471273	-307.47212	-307.18386	0.2882613	0.241134	6.56159274
20	**2-CH_3-**	-0.0471273	-346.79971	-346.51136	0.28835668	0.24122938	6.56418825
21	**3-CH_3-**	-0.0471273	-346.7991	-346.21547	0.58363297	0.53650567	14.5990683
22	**4-CH_3-**	-0.0471273	-346.79236	-346.51666	0.2756964	0.2285691	**6.2196843**
23	**2-OCH_3-**	-0.0471273	-422.00496	-421.73342	0.27153492	0.22440762	**6.10644462**
24	**4-OCH_3-**	-0.0471273	-421.99166	-421.73766	0.25400165	0.20687435	**5.62933991**
25	**2-OH**	-0.0471273	-382.69929	-382.38745	0.31183502	0.26470772	7.20306671
26	**3-OH**	-0.0471273	-382.69893	-382.41674	0.28218763	0.23506033	6.3963197
27	**4-OH**	-0.0471273	-382.68538	-382.42571	0.25967295	0.21254565	**5.7836638**
28	**2-NH_2**	-0.0471273	-362.83724	-362.52334	0.3138949	0.2667676	7.25911881
29	**3-NH_2**	-0.0471273	-362.83738	-362.57712	0.26026595	0.21313865	**5.79980021**
30	**4-NH_2**	-0.0471273	-362.83342	-362.58724	0.24618355	0.19905625	**5.41659853**
31	**2-IPr**	-0.0471273	-425.42915	-425.14668	0.28247039	0.23534309	6.40401391

32	**2-NHCOCH$_3$-**	-0.0471273	-515.50283	-515.21746	0.28537517	0.23824787	6.48305717
33	**4-NHCOCH$_3$-**	-0.0471273	-515.49492	-515.23679	0.25813001	0.21100271	**5.74167825**

[a]Energy difference between anionic dye radical (dye$^-$) and excited dye; [b]Energy for protonated cationic phenol; [c]Energy for ground-state phenol; [d]Energy difference between protonated cationic phenol and phenol; Energy difference between product and starting compounds for limitating PT reaction (in a.u.)[e] and (in eV).[f] **Note:** the lowest energy values for CPET are marked in **bold** text.

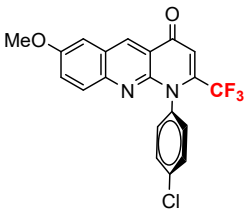
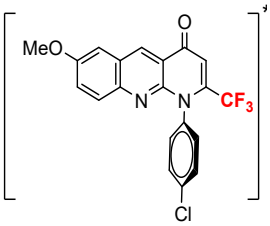
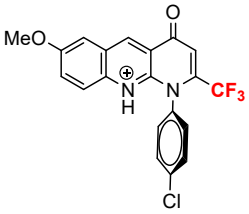
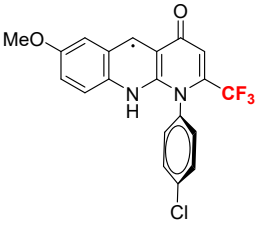
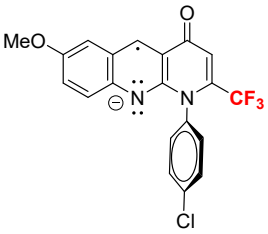
Table S4. Thermodynamical feasibility of CPET reaction between dye **3k** and phenols

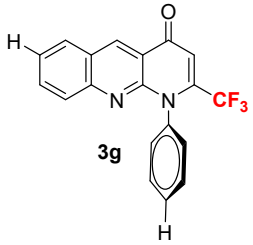
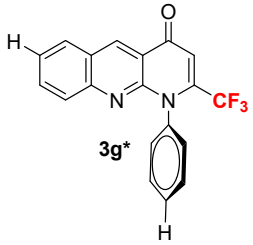


Entries	**Phenols**	$\Delta E_{(3k\text{-}H,\ 3k)}$[a]	E_{PhO}(in a.u.)[b]	E_{PhOH}(in a.u)[c]	$\Delta E_{(PhO,\ PhOH)}$[d]	ΔE_{CPET} *(in a.u.)*[e]	ΔE_{CPET} *(eV)*[f]
1	**PA**	-0.3245	-920.96338	-920.29138	0.67199674	0.34749674	9.45587142
2	**2,4-(NO$_2$)$_2$-**	-0.3245	-716.46558	-715.81204	0.6535381	0.3290381	8.95358616
3	**4-NO$_2$-**	-0.3245	-511.98101	-511.32021	0.66080131	0.33630131	9.15122825
4	**3-NO$_2$-**	-0.3245	-511.97788	-511.33015	0.64773044	0.32323044	8.79555144
5	**2-NO$_2$-**	-0.3245	-511.98825	-511.32009	0.6681635	0.3436635	9.35156372
6	**2-CHO-**	-0.3245	-420.81727	-420.15001	0.66725667	0.34275668	9.32688766
7	**2-COCH$_3$-**	-0.3245	-460.14314	-459.47294	0.67020201	0.34570201	9.40703428
8	**3-CHO**	-0.3245	-420.80224	-420.15544	0.64680382	0.32230382	8.77033689
9	**3-COCH$_3$-**	-0.3245	-460.1277	-459.48171	0.6459993	0.3214993	8.74844486
10	**4-CHO-**	-0.3245	-420.80543	-420.15841	0.64702094	0.32252094	8.77624498
11	**4-COCH$_3$-**	-0.3245	-460.13062	-459.48441	0.64620552	0.32170552	8.75405621
12	**2,4-(OH)$_2$-1CHO**	-0.3245	-496.02547	-495.37865	0.64681332	0.32231332	8.77059535
13	**3,4-(OH)$_2$-1CHO**	-0.3245	-496.01928	-495.38123	0.63805241	0.31355241	**8.53219886**
14	**3-OCH$_3$,4-OH-1CHO**	-0.3245	-535.33384	-534.6884	0.64544176	0.32094176	8.73327345
15	**4-COOCH$_3$**	-0.3245	-535.36288	-534.71652	0.64635646	0.32185646	8.75816369
16	**4-Br**	-0.3245	-2878.575	-2877.9391	0.63589408	0.31139408	**8.47346766**
17	**4-Cl**	-0.3245	-767.06616	-766.43031	0.63585176	0.31135176	**8.47231613**
18	**2-Cl**	-0.3245	-767.07474	-766.42875	0.64598539	0.32148539	8.74806627
19	**H**	-0.3245	-307.47212	-306.83539	0.63673458	0.31223458	**8.49633876**
20	**2-CH$_3$-**	-0.3245	-346.79971	-346.1599	0.63981207	0.31531207	8.58008175
21	**3-CH$_3$-**	-0.3245	-346.7991	-346.15607	0.64303123	0.31853123	8.6676794
22	**4-CH$_3$-**	-0.3245	-346.79236	-346.15817	0.63419507	0.30969507	**8.42723523**
23	**2-OCH$_3$-**	-0.3245	-422.00496	-421.36307	0.64188384	0.31738384	8.63645729
24	**4-OCH$_3$-**	-0.3245	-421.99166	-421.36643	0.62522816	0.30072816	**8.18323304**
25	**2-OH**	-0.3245	-382.69929	-382.07307	0.62621597	0.30171597	**8.21011281**
26	**3-OH**	-0.3245	-382.69893	-382.05429	0.64463202	0.32013202	8.71123927
27	**4-OH**	-0.3245	-382.68538	-382.05121	0.63417244	0.30967244	**8.42661933**
28	**2-NH$_2$-**	-0.3245	-362.83724	-362.21188	0.62535256	0.30085256	**8.18661819**
29	**3-NH$_2$-**	-0.3245	-362.83738	-362.19488	0.64250407	0.31800407	8.65333469
30	**4-NH$_2$-**	-0.3245	-362.83342	-362.20398	0.62944108	0.30494108	**8.29787239**
31	**2-IPr-**	-0.3245	-425.42915	-424.79155	0.63759974	0.31309974	8.51988092
32	**2-NHCOCH$_3$-**	-0.3245	-515.50283	-514.8744	0.62843696	0.30393696	**8.27054894**
33	**4-NHCOCH$_3$-**	-0.3245	-515.49492	-514.85773	0.63719392	0.31269392	8.50883813

[a]Energy difference between radical protonated dye (dye-H) and excited dye; [b]Energy for radical deprotonated phenol; [c]Energy for ground-state phenol; [d]Energy difference between radical deprotonated phenol and phenol; Energy difference between product and starting compounds for CPET reaction (in a.u.)[e] and (in eV).[f] **Note:** the lowest energy values for CPET are marked in **bold** text.

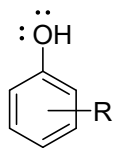
Table S5. HOMO and LUMO energy levels for the ground state of CT-probe **3k** and their corresponding species derived from PCET with phenols. HOMO and LUMO energy levels for the ground state of the low CT-probe **3g**.

Entries	Probes 3k species	E_{HOMO} (eV)	E_{LUMO} (eV)
1	 **3k**	-5.8373	-2.3106
2	 **3k***	-5.8885	-2.5383
3	 **3k-H$^+$**	-9.6348	-6.4707
4	 **3k-H$^\cdot$**	(α-orbital) -3.7276 (β-orbital) -5.7152	(α-orbital) -1.4681 (β-orbital) -1.9957
5	 **3k$^{\cdot-}$**	(α-orbital) 0.3600 (β-orbital)-1.9138	(α-orbital) 1.9946 (β-orbital) 1.8605

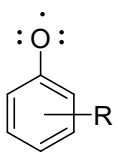
6		-6.1316	-2.2711
7		-6.0426	-2.4705

[a]*HOMO* values calculated for the phenol species. [b]*LUMO* values calculated for the phenol species. HOMO and LUMO are expressed in eV unit. Note: HOMO-LUMO energies calculated from B3LYP/6-31G(d,p) approach.

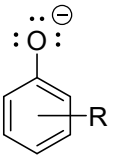
Table S6. HOMO and LUMO energy levels for the tested phenols and their species derived from PCET including deprotonated neutral phenol radical and pheonolate anion.



Phenol



Deprotonated neutral phenol radical



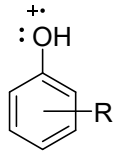
Phenolate anion

Entries	Phenol	Phenol		Phenol radical		Phenolate ion	
		$E_{HOMO}{}^{a}$	$E_{LUMO}{}^{b}$	$E_{HOMO}{}^{a}$	$E_{LUMO}{}^{b}$	$E_{HOMO}{}^{a}$	$E_{LUMO}{}^{b}$
1	2,4,6-Trinitrophenol	-8.2886	-3.9508	-8.3768	-4.0167	-2.9350	0.6585
2	2,4-Dinitrophenol	-7.6625	-2.8197	-7.8363	-3.1848	-2.0613	1.4164
3	4-Nitrophenol	-6.9226	-2.2237	-7.2094	-2.6784	-1.0626	2.4199
4	2-Nitrophenol	-6.7980	-2.7244	-7.1010	-2.4961	-0.8702	2.6430
5	3-Nitrophenol	-6.7838	-2.3995	-7.0659	-2.9777	-0.4536	1.7968
6	2-Chlorophenol	-6.2559	-0.3701	-6.3781	-0.9056	-0.0027	4.7269
7	4-Chlorophenol	-6.5218	-0.4463	-6.3152	-0.9491	0.0778	4.6836
8	4-Bromophenol	-6.4273	-0.4430	-6.2654	-0.9257	0.0084	4.2433
9	2-Hydroxibenzaldehyde	-6.3794	-1.9209	-6.6844	-1.8468	-0.4199	3.4539
10	3-Hydroxibenzaldehyde	-6.4567	-1.7113	-6.7389	-2.3217	-0.1434	2.7497
11	4-Hydroxibenzaldehyde	-6.4956	-1.4607	-6.7903	-1.8770	-0.6340	3.4153
12	2,4-Dihydroxibenzaldehyde	-6.3076	-1.3217	-6.7367	-1.7440	-0.6814	3.4858
13	3,4-Dihydroxibenzaldehyde	-6.0545	-1.4675	-6.2219	-1.8063	-0.4604	3.3475
14	3-Methoxy-4-hydroxibenzaldehyde	-6.0739	-1.4060	-6.0823	-1.6966	-0.5110	3.3745
15	2-Hydroxiacetophenone	-6.1846	-1.7132	-6.3663	-1.6553	-0.3162	3.4779
16	3-Hydroxiacetophenone	-6.3038	-1.4561	-6.5745	-2.0297	-0.0359	2.8569
17	4-Hydroxiacetophenone	-6.3457	-1.2340	-6.6178	-1.6428	-0.5352	3.4243
18	4-Hydroxibenzoate methyl ester	-6.3182	-0.9293	-6.5609	-1.2604	-0.5271	3.6964

19	2-Aminophenol	-5.7381	0.0033	-5.0727	0.1059	0.5499	5.1247
20	3-Aminophenol	-5.3405	0.3916	-6.0058	-0.1282	0.5290	5.4249
21	4-Aminophenol	-4.9884	0.1083	-4.9914	-0.3282	0.8631	5.1114
22	Phenol	-6.4793	-0.0188	-6.2703	-0.6014	0.5426	5.2820
23	2-Methoxyphenol	-5.5370	0.2985	-5.5707	-0.1605	0.6022	5.4055
24	4-Methoxyphenol	-6.2491	-0.1097	-5.4758	-0.5203	0.4332	4.9761
25	2-Methylphenol	-5.8279	0.1649	-6.0306	-0.4133	0.4895	5.2660
26	3-Methylphenol	-5.8834	0.0411	-6.1732	-0.5290	0.4923	5.0934
27	4-Methylphenol	-6.2064	0.0272	-5.9620	-0.5184	0.5336	5.1522
28	2-Isopropylphenol	-5.8137	0.1339	-6.0096	-0.4191	0.2977	5.0548
29	2-Hydroxiphenol	-5.6290	0.2046	-5.8379	-0.3532	0.3856	5.4439
30	3-Hydroxiphenol	-5.8354	0.1720	-6.2924	-0.3978	0.4169	5.3906
31	4-Hydroxiphenol	-6.2709	-0.1108	-6.0197	-0.6593	0.5478	5.0888
32	4-Acetamidophenol	-5.8515	-0.4400	-5.6885	-0.8076	-0.1954	4.2953
33	2-Acetamidophenol	-5.6679	-0.2422	-5.7438	-0.7720	-0.0473	4.0847
34	3-Bromophenol	-6.2886	-0.3976	-6.6249	-0.9704	-0.1148	4.1119
35	3-Chlorophenol	-6.3130	-0.3801	-6.6440	-0.9619	-0.0479	4.7200
36	3-Methoxyphenol	-5.7892	0.1916			0.3755	5.2543

[a]*HOMO* values calculated for the phenol species. [b]*LUMO* values calculated for the phenol species. HOMO and LUMO are expressed in eV unit. Note: HOMO-LUMO energies calculated from B3LYP/6-31G(d,p) approach.

Table S7. HOMO and LUMO energy levels for the cationic phenol radical of the phenol featuring electron-donor groups.



Phenol cationic radical

Entries	**Phenol specie**	***α*-orbital**		***β*-orbital**	
		E_{HOMO}[a]	E_{LUMO}[b]	E_{HOMO}[a]	E_{LUMO}[b]
19	2-Aminophenol	-11.4457	-7.3827	-12.1036	-9.1955
20	3-Aminophenol	-11.3014	-5.2235	-11.3676	-8.9346
21	4-Aminophenol	-10.6037	-5.2907	-12.1270	-8.5460
22	Phenol	-12.3972	-6.2175	-12.7311	-10.0535
23	2-Methoxyphenol	-11.3784	-5.5753	-11.8340	-9.2282
24	4-Methoxyphenol	-11.0152	-5.4845	-12.3053	-8.9678
25	2-Methylphenol				
26	3-Methylphenol	-12.1014	-5.9269	-12.2117	-9.7648
27	4-Methylphenol	-11.7317	-5.8643	-12.4522	-9.5705
28	2-Isopropylphenol	-11.7986	-5.7827	-12.0391	-9.5430
29	2-Hydroxiphenol	-12.1251	-7.7827	-12.0059	-9.7482
30	3-Hydroxiphenol	-11.9521	-5.8251	-12.0810	-9.5683

31	4-Hydroxiphenol	-11.3722	-5.7386	-12.5913	-9.2777
32	4-Acetamidophenol	-10.7204	-5.3783	-11.5945	-8.7994
33	2-Acetamidophenol	-11.2457	-5.7549	-11.5847	-9.2081
36	3-Methoxyphenol	-11.5989	-5.5568	-11.7730	-9.2628

[a]*HOMO* values calculated for the phenol species. [b]*LUMO* values calculated for the phenol species. HOMO and LUMO are expressed in eV unit. Note: HOMO-LUMO energies calculated from B3LYP/6-31G(d,p) approach.

VI. References

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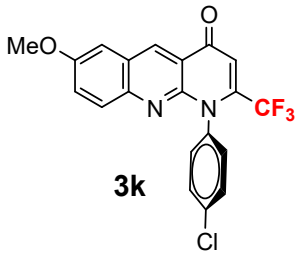
VII. Theoretical Calculation Output

VII.1. Output derived from the probes 3k

VII.1.1. Ground state of the *N*^{1}-(4-chlorophenyl)-2-(trifluoromethyl)-7-methoxybenzo[*b*][1,8]naphthyridin-4(1*H*)-one **3k**



3k

N-N= 2.678840456819D+03 E-N=-9.555963944615D+03 KE= 1.776115191847D+03

Orbital energies and kinetic energies (alpha):

		1	2
1	O	-101.556694	136.907089
2	O	-24.743223	37.081335
3	O	-24.739424	37.082858
4	O	-24.739410	37.082570
5	O	-19.191448	29.024013
6	O	-19.119237	29.025232

7	O	-14.415684	21.956712
8	O	-14.340324	21.959738
9	O	-10.455342	15.901744
10	O	-10.283427	15.884425
11	O	-10.278058	15.882061
12	O	-10.268842	15.886740
13	O	-10.266407	15.883698
14	O	-10.264878	15.885022
15	O	-10.253816	15.885262
16	O	-10.250976	15.885471
17	O	-10.239150	15.882959
18	O	-10.217859	15.878197
19	O	-10.217483	15.876547
20	O	-10.217473	15.876978
21	O	-10.216640	15.884413
22	O	-10.216638	15.884083
23	O	-10.216145	15.881830
24	O	-10.212771	15.880022
25	O	-10.212309	15.879861
26	O	-10.205702	15.880956
27	O	-10.202636	15.878924
28	O	-10.199600	15.879874
29	O	-9.472961	21.547652
30	O	-7.236946	20.528948
31	O	-7.227245	20.555121
32	O	-7.226881	20.550268
33	O	-1.320392	3.269457
34	O	-1.232870	3.828799
35	O	-1.230232	3.826108
36	O	-1.077292	2.522209
37	O	-1.024235	2.155934
38	O	-1.013794	2.298343
39	O	-0.949530	1.853861
40	O	-0.901737	1.921133
41	O	-0.860905	1.636852
42	O	-0.854926	2.079823
43	O	-0.825823	1.770080
44	O	-0.813106	1.897070
45	O	-0.779670	1.768168
46	O	-0.774517	1.614742
47	O	-0.766901	1.702341
48	O	-0.740112	2.022541
49	O	-0.729351	2.175427
50	O	-0.710479	1.757880
51	O	-0.674468	2.132541
52	O	-0.653682	1.737943
53	O	-0.640335	1.460761
54	O	-0.640024	1.902454
55	O	-0.623064	1.684035
56	O	-0.609021	1.640083
57	O	-0.600436	2.550294
58	O	-0.597847	2.800072
59	O	-0.578276	1.509640
60	O	-0.574151	1.944901
61	O	-0.550171	1.472384
62	O	-0.545179	1.550359
63	O	-0.521359	1.748936
64	O	-0.512531	1.683316
65	O	-0.501460	1.428904
66	O	-0.498463	1.674543

67	O	-0.489301	1.640181
68	O	-0.480335	1.244346
69	O	-0.473082	2.355731
70	O	-0.472362	3.051283
71	O	-0.469950	2.069822
72	O	-0.455498	1.451085
73	O	-0.452809	1.411484
74	O	-0.447421	1.605677
75	O	-0.444854	1.227003
76	O	-0.440966	2.329904
77	O	-0.435352	2.997914
78	O	-0.433358	1.898744
79	O	-0.427595	1.986894
80	O	-0.418325	1.974091
81	O	-0.413538	3.525201
82	O	-0.410728	2.051994
83	O	-0.406789	1.375895
84	O	-0.404461	1.244978
85	O	-0.400575	2.084381
86	O	-0.395670	1.688005
87	O	-0.388337	1.459053
88	O	-0.386627	2.045969
89	O	-0.376296	1.753920
90	O	-0.375520	1.394826
91	O	-0.361591	1.523572
92	O	-0.342238	1.839440
93	O	-0.340693	1.971834
94	O	-0.320624	2.348300
95	O	-0.317817	1.421216
96	O	-0.311995	1.363912
97	O	-0.281890	1.915017
98	O	-0.275214	1.152897
99	O	-0.262221	1.430820
100	O	-0.256429	1.710294
101	O	-0.246253	1.580176
102	O	-0.243004	2.310269
103	O	-0.214518	1.638931
104	V	-0.084913	1.619907
105	V	-0.035727	1.544208
106	V	-0.030146	1.548480
107	V	-0.023258	1.622374
108	V	-0.020529	1.597141
109	V	0.014025	1.531820
110	V	0.020590	2.085433
111	V	0.051753	1.841819
112	V	0.083602	1.211554
113	V	0.093911	1.709774
114	V	0.099694	1.441105
115	V	0.111225	2.404323
116	V	0.120901	1.583647
117	V	0.125133	1.164528
118	V	0.128252	1.382486
119	V	0.130413	1.417500
120	V	0.133147	1.880100
121	V	0.140213	1.754903
122	V	0.144965	1.139650
123	V	0.154534	1.222375
124	V	0.155734	1.077439
125	V	0.164109	1.294733
126	V	0.176300	1.296144

127	V	0.184168	1.397463
128	V	0.188804	2.508636
129	V	0.193785	1.994140
130	V	0.203094	2.954134
131	V	0.205455	3.607242
132	V	0.206003	2.517463
133	V	0.222104	2.057202
134	V	0.235631	2.060323
135	V	0.243626	2.074164
136	V	0.252205	1.945085
137	V	0.256257	1.761055
138	V	0.271235	2.477291
139	V	0.273399	1.525863
140	V	0.285135	2.290619
141	V	0.295655	2.261869
142	V	0.297571	1.787674
143	V	0.317762	1.912512
144	V	0.326113	2.090338
145	V	0.330371	2.505942
146	V	0.340197	2.220022
147	V	0.378299	2.142429
148	V	0.390061	2.255944
149	V	0.397762	2.095605
150	V	0.402278	2.679791
151	V	0.411823	1.890973
152	V	0.421759	2.232702
153	V	0.425440	2.272283
154	V	0.434592	2.195976
155	V	0.437272	2.574349
156	V	0.445417	2.239109
157	V	0.458021	2.297096
158	V	0.462555	2.251125
159	V	0.480193	2.201722
160	V	0.484485	2.090839
161	V	0.494489	2.094331
162	V	0.494654	2.255963
163	V	0.503639	2.207941
164	V	0.508171	1.937409
165	V	0.508400	2.380463
166	V	0.516354	2.259154
167	V	0.519231	2.152157
168	V	0.526951	1.953907
169	V	0.535930	1.849134
170	V	0.538994	2.407122
171	V	0.549624	2.125250
172	V	0.553838	2.384136
173	V	0.558311	2.448416
174	V	0.558840	2.540161
175	V	0.563961	2.124033
176	V	0.568009	2.154915
177	V	0.569609	2.174113
178	V	0.576369	2.383580
179	V	0.583198	2.197968
180	V	0.591823	2.170826
181	V	0.592216	2.143417
182	V	0.595906	2.139839
183	V	0.603495	2.480786
184	V	0.607525	2.128479
185	V	0.613414	2.489798
186	V	0.620905	2.221572

187	V	0.624930	2.451463
188	V	0.637221	2.256313
189	V	0.638465	2.471515
190	V	0.649615	2.695590
191	V	0.659559	3.002783
192	V	0.670050	2.187318
193	V	0.681786	2.428241
194	V	0.689102	2.252815
195	V	0.701549	3.116619
196	V	0.719867	2.297517
197	V	0.722207	2.254095
198	V	0.725683	2.280499
199	V	0.733227	2.425725
200	V	0.736463	2.249682
201	V	0.742693	2.377918
202	V	0.773152	2.523185
203	V	0.775569	2.318281
204	V	0.787208	2.797180
205	V	0.795097	2.595250
206	V	0.799819	2.583148
207	V	0.802481	2.664242
208	V	0.816999	2.303718
209	V	0.818174	2.652195
210	V	0.820916	2.557050
211	V	0.825192	2.595277
212	V	0.825574	2.436467
213	V	0.831425	2.635909
214	V	0.835803	2.415432
215	V	0.845207	2.503968
216	V	0.853228	2.432395
217	V	0.865284	2.619065
218	V	0.865774	2.504362
219	V	0.874651	2.564616
220	V	0.881564	2.503280
221	V	0.885092	2.800496
222	V	0.887440	2.517985
223	V	0.897930	2.489443
224	V	0.911901	2.485449
225	V	0.916039	2.709047
226	V	0.921753	2.552170
227	V	0.939122	2.476891
228	V	0.947679	2.614819
229	V	0.960883	2.784853
230	V	0.964041	2.414458
231	V	0.972243	2.539847
232	V	0.990509	2.496771
233	V	0.997549	2.436681
234	V	1.004343	2.953184
235	V	1.006673	2.537339
236	V	1.013053	2.483722
237	V	1.015171	2.572469
238	V	1.021641	3.339399
239	V	1.036511	2.530931
240	V	1.048496	3.246169
241	V	1.053310	2.547524
242	V	1.084566	3.001177
243	V	1.091002	2.857070
244	V	1.092255	3.099835
245	V	1.112233	2.932397
246	V	1.124522	2.797666

247	V	1.127455	2.523540
248	V	1.128165	3.038797
249	V	1.145437	2.850271
250	V	1.164878	2.622673
251	V	1.168787	2.834857
252	V	1.170313	2.820242
253	V	1.189641	2.736654
254	V	1.190865	2.516811
255	V	1.207073	2.632848
256	V	1.219702	2.432246
257	V	1.224918	2.701020
258	V	1.227445	2.472367
259	V	1.240008	2.728343
260	V	1.256856	2.508160
261	V	1.257885	2.985173
262	V	1.291630	3.076744
263	V	1.303095	2.801595
264	V	1.303164	2.563479
265	V	1.312573	3.608067
266	V	1.329480	2.652144
267	V	1.333538	2.557848
268	V	1.334478	2.932051
269	V	1.340122	2.738258
270	V	1.347792	3.078302
271	V	1.356226	2.879725
272	V	1.360531	2.954673
273	V	1.360690	2.794268
274	V	1.372561	2.604351
275	V	1.376920	2.955968
276	V	1.382620	2.598838
277	V	1.386526	2.580680
278	V	1.390234	2.640657
279	V	1.391835	3.053108
280	V	1.395035	2.922575
281	V	1.407095	2.782386
282	V	1.432039	2.579753
283	V	1.432975	2.895838
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287	V	1.464398	2.708648
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290	V	1.497517	2.838901
291	V	1.534802	2.853223
292	V	1.572780	3.120431
293	V	1.583894	2.949415
294	V	1.590271	3.361928
295	V	1.614695	3.030366
296	V	1.617969	2.875781
297	V	1.634684	2.918092
298	V	1.665024	3.092829
299	V	1.677113	2.996239
300	V	1.682910	3.046475
301	V	1.719491	3.205126
302	V	1.721703	2.906206
303	V	1.728448	3.251799
304	V	1.739743	3.209547
305	V	1.742161	2.888678
306	V	1.767533	3.160767

307	V	1.770302	3.121099
308	V	1.781111	3.219186
309	V	1.782240	3.223947
310	V	1.795851	2.918463
311	V	1.803051	3.229356
312	V	1.812344	3.247387
313	V	1.821546	3.182005
314	V	1.822957	3.210690
315	V	1.831978	3.206484
316	V	1.832941	3.009430
317	V	1.839074	2.928026
318	V	1.841015	3.283935
319	V	1.841812	2.906216
320	V	1.863349	2.962095
321	V	1.867447	3.132176
322	V	1.878705	3.293773
323	V	1.886709	3.027097
324	V	1.892120	3.302765
325	V	1.903580	3.318507
326	V	1.907795	3.261574
327	V	1.913656	3.286960
328	V	1.917821	3.117803
329	V	1.929526	3.366200
330	V	1.936284	3.506652
331	V	1.944089	3.107426
332	V	1.950740	3.132081
333	V	1.954754	3.536867
334	V	1.960048	3.518478
335	V	1.974397	3.212003
336	V	1.978083	3.629258
337	V	1.983973	3.628363
338	V	1.991896	3.419675
339	V	1.997467	3.570681
340	V	2.001549	3.496195
341	V	2.005614	3.421676
342	V	2.009143	2.940304
343	V	2.020331	3.128420
344	V	2.023416	3.504435
345	V	2.032405	4.106056
346	V	2.052851	3.501020
347	V	2.053939	3.314483
348	V	2.061508	3.418183
349	V	2.061982	3.356924
350	V	2.063062	3.333159
351	V	2.071812	3.315349
352	V	2.074767	3.579858
353	V	2.091563	3.518044
354	V	2.102389	3.510278
355	V	2.110054	3.560322
356	V	2.120385	3.370322
357	V	2.152589	3.510873
358	V	2.172730	3.740399
359	V	2.185032	3.562537
360	V	2.198998	3.451301
361	V	2.214311	3.858984
362	V	2.227715	3.506857
363	V	2.232371	3.453553
364	V	2.258893	3.475821
365	V	2.266647	3.705636
366	V	2.278193	3.890570

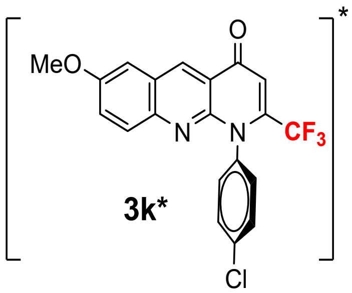
367	V	2.280593	3.543189
368	V	2.298765	3.523487
369	V	2.299703	3.640413
370	V	2.318550	3.497339
371	V	2.336307	3.868986
372	V	2.347360	3.879559
373	V	2.356942	3.550004
374	V	2.367106	3.915604
375	V	2.382438	3.874617
376	V	2.391956	3.345869
377	V	2.397721	3.915765
378	V	2.400076	3.860752
379	V	2.405810	3.885792
380	V	2.418132	3.951622
381	V	2.419505	3.568979
382	V	2.440462	3.668790
383	V	2.443783	3.790824
384	V	2.452589	3.737450
385	V	2.460477	3.575640
386	V	2.474488	4.037553
387	V	2.486850	3.805462
388	V	2.488413	3.918354
389	V	2.500764	3.600486
390	V	2.504134	4.080895
391	V	2.509206	3.950979
392	V	2.527515	3.964255
393	V	2.539078	3.857342
394	V	2.551023	4.022819
395	V	2.561202	3.674119
396	V	2.561303	4.168540
397	V	2.576352	3.673493
398	V	2.581360	3.615976
399	V	2.598383	3.956777
400	V	2.617453	3.855954
401	V	2.618844	3.857147
402	V	2.639778	3.930189
403	V	2.644640	3.985257
404	V	2.656331	3.910237
405	V	2.660299	3.959531
406	V	2.668812	3.978388
407	V	2.682003	4.004827
408	V	2.694774	4.289583
409	V	2.707508	4.010635
410	V	2.714518	4.227283
411	V	2.731292	4.315323
412	V	2.731490	4.359536
413	V	2.744510	4.259215
414	V	2.750464	4.010099
415	V	2.756541	4.252744
416	V	2.768131	4.440718
417	V	2.777646	4.218758
418	V	2.778326	4.431648
419	V	2.794847	4.342251
420	V	2.820641	4.463914
421	V	2.825740	3.889393
422	V	2.829703	4.416870
423	V	2.853837	4.527071
424	V	2.885893	4.496847
425	V	2.892964	4.543945
426	V	2.939978	4.629050

427	V	2.950656	4.611312
428	V	2.991131	4.755447
429	V	3.012460	4.859915
430	V	3.019492	5.584402
431	V	3.023547	5.473194
432	V	3.040258	4.948567
433	V	3.057758	4.895122
434	V	3.063622	4.736564
435	V	3.086142	4.764726
436	V	3.131777	4.836781
437	V	3.151592	5.073565
438	V	3.163855	5.146356
439	V	3.178749	5.013780
440	V	3.204154	5.065670
441	V	3.226455	4.884423
442	V	3.227769	5.616565
443	V	3.261884	5.332473
444	V	3.269396	4.970244
445	V	3.292045	5.002422
446	V	3.315840	5.107026
447	V	3.325451	5.110238
448	V	3.338650	5.136155
449	V	3.387437	5.056681
450	V	3.434881	5.128614
451	V	3.459015	5.300819
452	V	3.493149	5.418912
453	V	3.575370	5.538467
454	V	3.634611	5.616983
455	V	3.771921	5.849434
456	V	3.777427	6.019275
457	V	3.977481	10.099742
458	V	4.063774	10.331870
459	V	4.069482	10.446967
460	V	4.084054	10.159178
461	V	4.127495	10.242777
462	V	4.129841	10.120968
463	V	4.150995	10.159956
464	V	4.172978	10.176293
465	V	4.211263	10.644608
466	V	4.279683	10.440571
467	V	4.280842	12.187946
468	V	4.309143	10.953944
469	V	4.315795	11.084833
470	V	4.321891	10.993223
471	V	4.354437	10.665625
472	V	4.430493	10.767596
473	V	4.437221	10.218434
474	V	4.453587	10.159887
475	V	4.502701	11.028300
476	V	4.511822	10.639685
477	V	4.578432	11.201145
478	V	4.601492	10.502447
479	V	4.610053	10.809858
480	V	4.738049	10.665148
481	V	4.818028	10.823631
482	V	4.928690	10.665477
483	V	5.191191	13.238502
484	V	5.871258	15.386029

Total kinetic energy from orbitals= 1.776115191847D+03

1\1\GINC-COPERNICO\FOpt\RB3LYP\6-31G(d,p)\C20H12Cl1F3N2O2\IVAN\22-Nov-
2019\0\\# opt b3lyp/6-31g(d,p) geom=connectivity pop=full\\A15MOD\\0,1
\C,-4.5353277952,1.2360444082,0.0218598078\C,-3.1600441389,1.271471816
6,0.0493208764\C,-2.3982904152,0.0753429103,0.0116264348\C,-3.10067905
42,-1.1764852625,-0.0561588426\C,-4.5150458612,-1.1904187475,-0.083431
9773\C,-5.2272992192,-0.0068673674,-0.0452972858\C,-2.3113574492,-2.34
45520799,-0.092173207\C,-0.9332883044,-2.2592697413,-0.0624394066\C,-0
.3465092893,-0.9561989092,0.0054343957\C,1.8422633641,-1.9705210758,0.
0028849029\C,1.3317128365,-3.228862449,-0.0616413694\C,-0.1001880644,-
3.483661958,-0.1001120368\H,-2.6248771926,2.2135619713,0.1004293641\H,
-5.052924491,-2.1314471792,-0.1345639286\H,-2.7594759675,-3.3325842667
,-0.1437226349\H,1.9967588042,-4.0800408259,-0.0858716831\C,1.60779604
92,0.5094446702,0.1054663686\C,1.8751996171,1.2085389521,-1.0705409923
\C,1.8294434115,1.104821366,1.3462657839\C,2.3775188515,2.5064903432,-
1.0110144421\H,1.6917946916,0.7375946682,-2.0299509646\C,2.3315487067,
2.4022996069,1.4171265124\H,1.6106901629,0.5537578765,2.2542080201\C,2
.6001638199,3.0913525552,0.235044068\H,2.5926010429,3.0584934544,-1.91
85859184\H,2.5112761247,2.8741955006,2.376117931\C,3.3532470938,-1.795
6010661,0.0397459451\N,1.057838989,-0.82931684,0.0375698383\F,3.978787
7018,-2.9840068995,0.0003375384\F,3.7994215587,-1.0758898963,-1.011468
9838\F,3.7570808923,-1.1703296211,1.1657912923\N,-1.0444809424,0.16114
4219,0.0409054942\O,-0.5861379837,-4.6135724,-0.1586944294\H,-5.089362
9511,2.1666886403,0.0519409887\C,-7.3707124364,1.0703312515,-0.0387748
221\H,-7.2065081146,1.6396206903,0.8847024881\H,-7.1728303909,1.717448
903,-0.9024534644\H,-8.4092336885,0.7389966679,-0.0727683722\O,-6.5860
698498,-0.1132953277,-0.0755327994\Cl,3.2313545913,4.7287008518,0.3172
531902\\Version=AM64L-G09RevD.01\State=1-A\HF=-1789.0510556\RMSD=3.708
e-09\RMSF=4.271e-06\Dipole=-1.2500513,1.5481728,0.0439387\Quadrupole=1
3.346948,-15.9797448,2.6327968,-11.0835453,-0.2831478,-1.0164525\PG=C0
1 [X(C20H12Cl1F3N2O2)]\\@

VII.1.2. Excited state of the *N*^{1}-(4-chlorophenyl)-2-(trifluoromethyl)-7-methoxybenzo[*b*][1,8]naphthyridin-4(1*H*)-one **3k***



Orbital symmetries:
Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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The electronic state is 1-A.
Alpha occ. eigenvalues -- -101.55796 -24.74422 -24.74047 -24.74047 -19.19301

Alpha occ. eigenvalues -- -19.10421 -14.42051 -14.34210 -10.45768 -10.28543
Alpha occ. eigenvalues -- -10.28176 -10.26797 -10.26716 -10.25877 -10.25460
Alpha occ. eigenvalues -- -10.25292 -10.24177 -10.22336 -10.21938 -10.21937
Alpha occ. eigenvalues -- -10.21896 -10.21835 -10.21835 -10.21690 -10.21514
Alpha occ. eigenvalues -- -10.20831 -10.20515 -10.20256 -9.47423 -7.23822
Alpha occ. eigenvalues -- -7.22851 -7.22814 -1.32041 -1.23334 -1.23015
Alpha occ. eigenvalues -- -1.07866 -1.02565 -0.97211 -0.94991 -0.90347
Alpha occ. eigenvalues -- -0.86399 -0.85679 -0.82568 -0.81460 -0.78481
Alpha occ. eigenvalues -- -0.77647 -0.76818 -0.74229 -0.73404 -0.71245
Alpha occ. eigenvalues -- -0.67942 -0.65743 -0.64237 -0.64148 -0.62595
Alpha occ. eigenvalues -- -0.61127 -0.60142 -0.59833 -0.58034 -0.57758
Alpha occ. eigenvalues -- -0.55245 -0.54598 -0.52259 -0.51313 -0.50382
Alpha occ. eigenvalues -- -0.50115 -0.49168 -0.48148 -0.47435 -0.47287
Alpha occ. eigenvalues -- -0.47169 -0.45722 -0.45476 -0.44854 -0.44659
Alpha occ. eigenvalues -- -0.44315 -0.43579 -0.43368 -0.42747 -0.41953
Alpha occ. eigenvalues -- -0.41426 -0.41336 -0.40806 -0.40601 -0.39737
Alpha occ. eigenvalues -- -0.39540 -0.38444 -0.37962 -0.37482 -0.37161
Alpha occ. eigenvalues -- -0.36005 -0.34411 -0.34323 -0.32189 -0.31937
Alpha occ. eigenvalues -- -0.30844 -0.28114 -0.27705 -0.26253 -0.25705
Alpha occ. eigenvalues -- -0.23926 -0.23103 -0.21640
Alpha virt. eigenvalues -- -0.09328 -0.04156 -0.03166 -0.02583 -0.02228
Alpha virt. eigenvalues -- 0.01132 0.01930 0.04776 0.08197 0.09314
Alpha virt. eigenvalues -- 0.09824 0.10761 0.11988 0.12389 0.12771
Alpha virt. eigenvalues -- 0.12896 0.13260 0.13773 0.14393 0.15303
Alpha virt. eigenvalues -- 0.15456 0.16541 0.17475 0.18239 0.18538
Alpha virt. eigenvalues -- 0.19176 0.19892 0.20278 0.20405 0.22158
Alpha virt. eigenvalues -- 0.23002 0.24609 0.24886 0.25542 0.27031
Alpha virt. eigenvalues -- 0.27164 0.28978 0.29561 0.29778 0.31626
Alpha virt. eigenvalues -- 0.32555 0.33033 0.33857 0.37851 0.39165
Alpha virt. eigenvalues -- 0.39706 0.40137 0.40996 0.41610 0.42652
Alpha virt. eigenvalues -- 0.43600 0.44039 0.44307 0.45373 0.46094
Alpha virt. eigenvalues -- 0.47963 0.48337 0.49311 0.49410 0.49734
Alpha virt. eigenvalues -- 0.50583 0.50777 0.51495 0.51787 0.52688
Alpha virt. eigenvalues -- 0.53465 0.53582 0.54966 0.55244 0.55381
Alpha virt. eigenvalues -- 0.55909 0.56265 0.56676 0.56848 0.57320
Alpha virt. eigenvalues -- 0.58170 0.58660 0.59081 0.59278 0.59537
Alpha virt. eigenvalues -- 0.60724 0.61129 0.62186 0.62280 0.63237
Alpha virt. eigenvalues -- 0.63468 0.64258 0.65980 0.67118 0.68063
Alpha virt. eigenvalues -- 0.68313 0.68957 0.71900 0.72004 0.72561
Alpha virt. eigenvalues -- 0.73121 0.73805 0.74112 0.77484 0.78454
Alpha virt. eigenvalues -- 0.78762 0.79621 0.79823 0.80184 0.81649
Alpha virt. eigenvalues -- 0.81668 0.82045 0.82410 0.82541 0.83331
Alpha virt. eigenvalues -- 0.83418 0.84402 0.85186 0.86395 0.86403
Alpha virt. eigenvalues -- 0.87292 0.88046 0.88275 0.89049 0.89615
Alpha virt. eigenvalues -- 0.91006 0.91443 0.91938 0.93720 0.94624
Alpha virt. eigenvalues -- 0.96000 0.96316 0.97181 0.98789 0.99947
Alpha virt. eigenvalues -- 1.00521 1.00949 1.01082 1.01867 1.01967
Alpha virt. eigenvalues -- 1.03608 1.04927 1.05223 1.08393 1.08679
Alpha virt. eigenvalues -- 1.09031 1.11618 1.12484 1.12488 1.12722
Alpha virt. eigenvalues -- 1.14989 1.16578 1.16730 1.16789 1.18764
Alpha virt. eigenvalues -- 1.18809 1.20536 1.21713 1.21774 1.22589
Alpha virt. eigenvalues -- 1.23653 1.25221 1.26086 1.28454 1.30045
Alpha virt. eigenvalues -- 1.30192 1.31161 1.32495 1.32821 1.33298
Alpha virt. eigenvalues -- 1.33622 1.34470 1.35533 1.35807 1.35841
Alpha virt. eigenvalues -- 1.37011 1.37447 1.37916 1.38414 1.38740

Alpha virt. eigenvalues -- 1.39168 1.39784 1.40344 1.43007 1.43390
Alpha virt. eigenvalues -- 1.44051 1.44681 1.44756 1.46389 1.46792
Alpha virt. eigenvalues -- 1.48668 1.49780 1.53331 1.57432 1.57783
Alpha virt. eigenvalues -- 1.58808 1.61412 1.61683 1.63120 1.66254
Alpha virt. eigenvalues -- 1.67649 1.67991 1.71741 1.72337 1.72378
Alpha virt. eigenvalues -- 1.75725 1.75831 1.76819 1.77243 1.78092
Alpha virt. eigenvalues -- 1.78744 1.79793 1.80331 1.80919 1.82113
Alpha virt. eigenvalues -- 1.82545 1.82963 1.83575 1.84165 1.84755
Alpha virt. eigenvalues -- 1.85257 1.86328 1.86490 1.87233 1.88529
Alpha virt. eigenvalues -- 1.88539 1.90118 1.90179 1.91438 1.91554
Alpha virt. eigenvalues -- 1.92107 1.93523 1.94266 1.94687 1.94971
Alpha virt. eigenvalues -- 1.96288 1.97077 1.97245 1.97848 1.98904
Alpha virt. eigenvalues -- 1.99317 2.00160 2.00214 2.00763 2.02074
Alpha virt. eigenvalues -- 2.02342 2.03608 2.05054 2.05067 2.05644
Alpha virt. eigenvalues -- 2.05755 2.06085 2.06770 2.07635 2.09233
Alpha virt. eigenvalues -- 2.09889 2.11232 2.11774 2.15120 2.16708
Alpha virt. eigenvalues -- 2.18189 2.20865 2.20886 2.21654 2.22823
Alpha virt. eigenvalues -- 2.25467 2.26542 2.28002 2.28189 2.28744
Alpha virt. eigenvalues -- 2.29450 2.31554 2.33890 2.34023 2.35615
Alpha virt. eigenvalues -- 2.35695 2.38097 2.39075 2.39427 2.39897
Alpha virt. eigenvalues -- 2.40052 2.41109 2.42094 2.43946 2.44069
Alpha virt. eigenvalues -- 2.44778 2.44924 2.45720 2.47976 2.48073
Alpha virt. eigenvalues -- 2.49594 2.50120 2.50647 2.52657 2.54519
Alpha virt. eigenvalues -- 2.54586 2.54994 2.55755 2.57217 2.57952
Alpha virt. eigenvalues -- 2.59759 2.61480 2.61740 2.63461 2.63558
Alpha virt. eigenvalues -- 2.64778 2.65006 2.67268 2.67523 2.68993
Alpha virt. eigenvalues -- 2.70090 2.70894 2.72857 2.73215 2.74088
Alpha virt. eigenvalues -- 2.74445 2.75160 2.76970 2.77214 2.77568
Alpha virt. eigenvalues -- 2.80061 2.80693 2.82435 2.82578 2.84169
Alpha virt. eigenvalues -- 2.88494 2.88980 2.92561 2.95608 2.99189
Alpha virt. eigenvalues -- 2.99930 3.01355 3.02421 3.03727 3.04988
Alpha virt. eigenvalues -- 3.05867 3.08759 3.12632 3.15248 3.16412
Alpha virt. eigenvalues -- 3.18769 3.19819 3.22475 3.22887 3.25200
Alpha virt. eigenvalues -- 3.26778 3.28831 3.31352 3.33221 3.34378
Alpha virt. eigenvalues -- 3.38654 3.43349 3.45399 3.49161 3.57697
Alpha virt. eigenvalues -- 3.64497 3.76943 3.77695 3.97412 4.06252
Alpha virt. eigenvalues -- 4.06822 4.07895 4.12484 4.12594 4.14749
Alpha virt. eigenvalues -- 4.16700 4.20785 4.27715 4.28190 4.30350
Alpha virt. eigenvalues -- 4.31234 4.32089 4.33761 4.42646 4.43471
Alpha virt. eigenvalues -- 4.45260 4.49799 4.50699 4.54644 4.58320
Alpha virt. eigenvalues -- 4.60259 4.73125 4.81057 4.92464 5.16983
Alpha virt. eigenvalues -- 5.87932

N-N= 2.678143328929D+03 E-N=-9.554336238669D+03 KE= 1.775994548912D+03

1\1\GINC-COPERNICO\FOpt\RB3LYP TD-FC\6-31G(d,p)\C20H12Cl1F3N2O2\IVAN\0

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ctivity guess=read\\A15MODTDOPTIMIZACION\\0,1\C,-4.2877767562,1.857437

944,0.0002473594\C,-2.9060847238,1.7236940232,0.0002489288\C,-2.295161

0536,0.4575250563,0.0001229093\C,-3.131780098,-0.7124377096,-0.0000111

352\C,-4.5341881554,-0.5585446142,-0.000012478\C,-5.1081957248,0.70661

55629,0.0001156302\C,-2.4885022452,-1.9709893183,-0.0001395025\C,-1.08

67962804,-2.0383991686,-0.0001252445\C,-0.3546341742,-0.8009823946,0.0
000182002\C,1.7270686864,-2.0309908819,-0.00009519\C,1.0505122771,-3.2
341381352,-0.0002511735\C,-0.3545718829,-3.2634321962,-0.0002610287\H,
-2.2644381312,2.5984465158,0.0003487205\H,-5.1823554092,-1.428948806,-
0.0001137357\H,-3.0773567227,-2.8799719337,-0.0002497179\H,1.604738422
7,-4.1603034299,-0.0003600773\C,1.7410632755,0.4468248348,0.000032712\
C,2.0552184931,1.0608363158,-1.2105539059\C,2.0549916947,1.0609655081,
1.2106139292\C,2.6995986956,2.2957821304,-1.2155254196\H,1.7966946797,
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003479143\C,-7.1188760588,2.0072899188,0.0002133398\H,-6.8683281876,2.
5926926294,0.8941225873\H,-6.868293404,2.5928648013,-0.8935732796\H,-8
.18932249,1.7968509561,0.0001726891\O,-6.473737465,0.7436294415,0.0001
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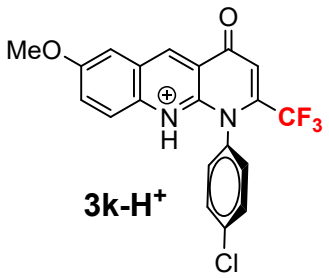
VII.1.3. Protonated *N*^{1}-(4-chlorophenyl)-2-(trifluoromethyl)-7-methoxybenzo[*b*][1,8]naphthyridin-4(1*H*)-one **3k-H**$^{+}$



3k-H^{+}

Orbital energies and kinetic energies (alpha):

		1	2
1	O	-101.658875	136.907088
2	O	-24.849319	37.081387
3	O	-24.846717	37.083661

4	O	-24.846714	37.081884
5	O	-19.307796	29.023605
6	O	-19.255412	29.025056
7	O	-14.576602	21.955141
8	O	-14.568561	21.956979
9	O	-10.566550	15.901737
10	O	-10.463141	15.884354
11	O	-10.406601	15.882007
12	O	-10.405622	15.882622
13	O	-10.405299	15.886405
14	O	-10.396509	15.885157
15	O	-10.382821	15.883879
16	O	-10.381251	15.885230
17	O	-10.374277	15.880287
18	O	-10.365331	15.880586
19	O	-10.363342	15.879417
20	O	-10.352639	15.879244
21	O	-10.352360	15.885108
22	O	-10.349249	15.881733
23	O	-10.343497	15.880128
24	O	-10.343493	15.881252
25	O	-10.336286	15.878976
26	O	-10.335540	15.879839
27	O	-10.334122	15.880315
28	O	-10.334118	15.881265
29	O	-9.575102	21.547705
30	O	-7.339364	20.528087
31	O	-7.329351	20.555134
32	O	-7.328701	20.550387
33	O	-1.428695	3.265963
34	O	-1.341232	3.819571
35	O	-1.338366	3.821893
36	O	-1.196419	2.516934
37	O	-1.192782	1.865903
38	O	-1.156897	2.609133
39	O	-1.128813	1.950082
40	O	-1.020228	1.740930
41	O	-1.012996	1.616155
42	O	-0.987913	1.786598
43	O	-0.969142	1.973942
44	O	-0.948443	1.940784
45	O	-0.921319	1.781957
46	O	-0.905502	1.735015
47	O	-0.895877	1.617905
48	O	-0.868528	2.007684
49	O	-0.855955	2.045138
50	O	-0.840126	1.680398
51	O	-0.815505	1.943139
52	O	-0.797866	1.796029
53	O	-0.791815	1.790153
54	O	-0.766060	1.976905
55	O	-0.761352	1.460449
56	O	-0.751473	1.856084
57	O	-0.724772	1.957032
58	O	-0.713613	1.615182

59	O	-0.705772	2.795622
60	O	-0.703518	1.604648
61	O	-0.696951	2.334797
62	O	-0.686400	1.773387
63	O	-0.661788	1.546249
64	O	-0.657304	1.830172
65	O	-0.641595	1.587753
66	O	-0.636294	1.304077
67	O	-0.634422	1.543845
68	O	-0.615668	1.668605
69	O	-0.603961	1.334113
70	O	-0.599145	1.485154
71	O	-0.590335	1.380558
72	O	-0.587634	1.311123
73	O	-0.580150	2.738484
74	O	-0.578263	2.992855
75	O	-0.574000	1.514595
76	O	-0.571015	1.757926
77	O	-0.567388	1.333069
78	O	-0.558258	2.128922
79	O	-0.553531	1.881423
80	O	-0.547284	1.680737
81	O	-0.541542	2.683380
82	O	-0.538666	2.651528
83	O	-0.532963	1.758765
84	O	-0.530769	1.907439
85	O	-0.524714	1.407908
86	O	-0.522137	1.678557
87	O	-0.519363	3.512191
88	O	-0.513811	2.173844
89	O	-0.506375	1.917740
90	O	-0.505322	1.333236
91	O	-0.502234	1.941580
92	O	-0.488580	1.497895
93	O	-0.464733	1.335908
94	O	-0.457489	1.787953
95	O	-0.455205	2.021427
96	O	-0.454459	1.512304
97	O	-0.420838	2.382892
98	O	-0.407256	1.368686
99	O	-0.397819	1.154713
100	O	-0.383238	1.648562
101	O	-0.378949	2.349122
102	O	-0.375437	1.807940
103	O	-0.354072	1.721284
104	V	-0.237794	1.561051
105	V	-0.171008	1.602132
106	V	-0.166512	1.914062
107	V	-0.156979	1.558931
108	V	-0.146634	1.391411
109	V	-0.136262	1.537154
110	V	-0.089371	1.797170
111	V	-0.080639	2.031864
112	V	-0.065729	1.233759
113	V	-0.035394	1.848325

114	V	-0.029252	1.762505
115	V	-0.013546	2.145706
116	V	-0.008319	1.519952
117	V	-0.004352	2.036165
118	V	-0.002084	1.562226
119	V	0.003354	1.280108
120	V	0.016219	1.032202
121	V	0.017098	1.746338
122	V	0.020526	1.741253
123	V	0.044674	2.059771
124	V	0.045440	1.309359
125	V	0.048740	1.372339
126	V	0.053427	1.186395
127	V	0.056515	1.608291
128	V	0.061819	1.058051
129	V	0.062582	2.599836
130	V	0.068830	1.346440
131	V	0.071743	1.598550
132	V	0.082903	1.867148
133	V	0.090064	3.008401
134	V	0.093608	3.114133
135	V	0.100556	2.650007
136	V	0.110639	2.775235
137	V	0.118734	2.042511
138	V	0.129130	1.834210
139	V	0.131288	2.318589
140	V	0.151780	2.289108
141	V	0.158209	1.548864
142	V	0.162958	2.051745
143	V	0.179796	2.146243
144	V	0.185190	1.934028
145	V	0.189298	2.410214
146	V	0.197690	1.914824
147	V	0.198131	2.046747
148	V	0.234538	2.175228
149	V	0.259958	2.340440
150	V	0.277975	2.172333
151	V	0.288795	2.098316
152	V	0.289438	2.332589
153	V	0.294667	1.726173
154	V	0.301022	2.183267
155	V	0.310656	2.580321
156	V	0.319739	1.930728
157	V	0.325340	2.315310
158	V	0.334110	2.190730
159	V	0.340840	2.441890
160	V	0.348043	2.219708
161	V	0.348912	2.039053
162	V	0.351673	2.342157
163	V	0.367915	2.423645
164	V	0.374664	2.143333
165	V	0.376256	2.160295
166	V	0.378099	1.975872
167	V	0.385578	2.279124
168	V	0.392161	2.166915

169	V	0.408051	2.441937
170	V	0.408900	2.259604
171	V	0.409109	2.120529
172	V	0.415190	2.365792
173	V	0.419238	2.006154
174	V	0.423148	2.365813
175	V	0.435772	2.552290
176	V	0.438908	1.963886
177	V	0.440225	2.359795
178	V	0.445608	2.220412
179	V	0.449105	2.188874
180	V	0.451308	2.271561
181	V	0.456197	2.139269
182	V	0.460039	2.290817
183	V	0.466807	2.284225
184	V	0.472898	2.068266
185	V	0.480227	2.193503
186	V	0.487166	2.421515
187	V	0.487551	2.501256
188	V	0.493679	2.233451
189	V	0.498211	2.714587
190	V	0.508755	2.634270
191	V	0.509267	2.299640
192	V	0.523485	2.447465
193	V	0.540298	2.173716
194	V	0.559028	2.245731
195	V	0.564691	2.505082
196	V	0.568009	3.225702
197	V	0.585970	2.255477
198	V	0.600910	2.377279
199	V	0.604303	2.266619
200	V	0.608981	2.337542
201	V	0.623531	2.450341
202	V	0.631423	2.306071
203	V	0.642208	2.474670
204	V	0.651545	2.455714
205	V	0.661252	2.662385
206	V	0.665719	2.522761
207	V	0.673800	2.669265
208	V	0.678112	2.287355
209	V	0.685588	2.553013
210	V	0.694820	2.681700
211	V	0.698493	2.519688
212	V	0.703789	2.553489
213	V	0.705843	2.493314
214	V	0.711942	2.546902
215	V	0.718836	2.558559
216	V	0.723267	2.520317
217	V	0.726320	2.542533
218	V	0.730867	2.407736
219	V	0.736244	2.417906
220	V	0.744682	2.485738
221	V	0.757115	2.500831
222	V	0.764859	2.622346
223	V	0.765653	2.489343

224	V	0.780914	2.560037
225	V	0.787719	2.649440
226	V	0.799268	2.426139
227	V	0.803558	2.608110
228	V	0.805463	2.467561
229	V	0.815681	2.380134
230	V	0.816933	2.904377
231	V	0.823601	2.529929
232	V	0.832143	2.394029
233	V	0.853509	2.466343
234	V	0.862608	2.563824
235	V	0.875299	2.446004
236	V	0.875415	2.897898
237	V	0.891737	2.528533
238	V	0.892765	2.386127
239	V	0.910526	2.532865
240	V	0.910596	3.313492
241	V	0.917388	2.566167
242	V	0.921942	3.213885
243	V	0.955951	2.627782
244	V	0.971849	2.774975
245	V	0.977766	2.713044
246	V	0.985926	2.795656
247	V	0.993910	2.961938
248	V	0.999518	2.799238
249	V	1.009686	3.255629
250	V	1.020824	2.859922
251	V	1.029715	2.692234
252	V	1.035141	2.468291
253	V	1.036466	2.785462
254	V	1.049671	2.571356
255	V	1.054489	2.746863
256	V	1.065814	2.937262
257	V	1.077249	2.519155
258	V	1.097709	2.576844
259	V	1.100741	2.802703
260	V	1.107157	2.496458
261	V	1.111816	2.648980
262	V	1.125064	2.645992
263	V	1.140221	2.954201
264	V	1.160036	2.495790
265	V	1.162553	2.959430
266	V	1.178552	2.479521
267	V	1.190554	2.969300
268	V	1.194663	2.538258
269	V	1.198009	2.638302
270	V	1.210792	3.570071
271	V	1.215646	2.664137
272	V	1.226872	2.716920
273	V	1.231182	2.985799
274	V	1.237863	2.908654
275	V	1.245232	2.565158
276	V	1.250637	3.248742
277	V	1.251576	2.794353
278	V	1.255286	2.581715

279	V	1.256090	2.974812
280	V	1.265278	2.604090
281	V	1.271910	3.102742
282	V	1.272343	2.629154
283	V	1.281083	3.026061
284	V	1.296401	2.992683
285	V	1.313136	3.270985
286	V	1.321412	2.874822
287	V	1.324589	2.553600
288	V	1.333074	3.044258
289	V	1.341235	3.128966
290	V	1.349060	3.183006
291	V	1.356885	3.021752
292	V	1.410723	3.020496
293	V	1.423782	2.897489
294	V	1.444454	2.930975
295	V	1.448567	2.914273
296	V	1.472679	3.035093
297	V	1.477542	3.228603
298	V	1.489750	3.018432
299	V	1.505150	2.950277
300	V	1.515866	3.034842
301	V	1.542412	2.991998
302	V	1.551265	3.093199
303	V	1.575409	2.887790
304	V	1.579067	3.187342
305	V	1.599880	3.242653
306	V	1.604786	2.905717
307	V	1.616274	3.248984
308	V	1.633486	3.273080
309	V	1.644278	3.238703
310	V	1.645663	2.929460
311	V	1.650325	3.161896
312	V	1.654410	3.301415
313	V	1.673952	3.245255
314	V	1.687750	3.242826
315	V	1.691968	2.978257
316	V	1.694379	3.183695
317	V	1.699469	3.278331
318	V	1.701130	3.279339
319	V	1.703455	2.919392
320	V	1.729898	3.005095
321	V	1.730847	3.345001
322	V	1.735609	2.909468
323	V	1.742316	3.069496
324	V	1.749274	2.944891
325	V	1.758478	3.366829
326	V	1.770214	3.322711
327	V	1.771966	3.324833
328	V	1.773078	3.102509
329	V	1.784671	3.303559
330	V	1.789641	3.317955
331	V	1.804348	3.501474
332	V	1.812672	3.078813
333	V	1.821736	3.503322

334	V	1.824392	3.433211
335	V	1.830765	3.177561
336	V	1.843301	3.514081
337	V	1.857939	3.559432
338	V	1.862362	3.262321
339	V	1.862677	3.713866
340	V	1.869751	3.471368
341	V	1.873963	3.691953
342	V	1.874200	3.202196
343	V	1.885452	3.392344
344	V	1.888109	3.525265
345	V	1.912068	2.886732
346	V	1.916522	3.494842
347	V	1.919099	3.621733
348	V	1.921351	3.600215
349	V	1.928775	3.456648
350	V	1.930303	3.398572
351	V	1.936311	3.494640
352	V	1.936905	3.459932
353	V	1.946392	3.209584
354	V	1.948910	3.428115
355	V	1.951433	3.664953
356	V	1.965022	3.495833
357	V	1.995122	3.544021
358	V	2.007586	3.441650
359	V	2.008898	3.313231
360	V	2.048628	3.539641
361	V	2.059710	3.468402
362	V	2.063210	3.456865
363	V	2.064513	3.704015
364	V	2.082347	3.444781
365	V	2.098943	3.889327
366	V	2.112459	3.542720
367	V	2.127138	3.461481
368	V	2.139315	3.786424
369	V	2.147434	3.585205
370	V	2.158710	3.841132
371	V	2.168286	3.568440
372	V	2.174239	3.764140
373	V	2.191333	3.764563
374	V	2.197817	3.426897
375	V	2.213028	3.790906
376	V	2.241058	3.941607
377	V	2.241919	3.963758
378	V	2.263368	3.980443
379	V	2.273545	3.398775
380	V	2.279026	3.411806
381	V	2.284723	3.761777
382	V	2.287334	3.854908
383	V	2.292006	3.649199
384	V	2.293581	3.977575
385	V	2.322560	3.778767
386	V	2.328756	3.774638
387	V	2.329596	3.835631
388	V	2.335433	3.699563

389	V	2.353162	4.051384
390	V	2.359973	3.629612
391	V	2.361134	4.044150
392	V	2.366368	3.709424
393	V	2.381058	3.957473
394	V	2.394708	3.996996
395	V	2.398456	3.766825
396	V	2.399647	3.822411
397	V	2.407068	3.904320
398	V	2.416843	4.123038
399	V	2.432795	4.043213
400	V	2.434955	3.704821
401	V	2.450551	3.989632
402	V	2.458343	3.676428
403	V	2.464402	3.634233
404	V	2.483524	3.923484
405	V	2.495528	3.872201
406	V	2.515874	3.901708
407	V	2.515921	3.788572
408	V	2.529284	4.074687
409	V	2.533137	3.939850
410	V	2.545263	4.309154
411	V	2.547258	3.996922
412	V	2.557342	3.903428
413	V	2.568796	4.265604
414	V	2.579769	4.022228
415	V	2.593641	4.403646
416	V	2.605667	4.286315
417	V	2.613877	4.094913
418	V	2.616389	4.009597
419	V	2.629603	4.378800
420	V	2.640313	4.411997
421	V	2.660974	4.251636
422	V	2.674648	4.272720
423	V	2.679234	4.314439
424	V	2.691244	4.544145
425	V	2.727651	4.550243
426	V	2.731173	3.883196
427	V	2.735124	4.318281
428	V	2.759333	4.482652
429	V	2.760948	4.528978
430	V	2.797553	4.566538
431	V	2.808020	4.596033
432	V	2.871468	4.705137
433	V	2.887921	4.649798
434	V	2.896080	4.802429
435	V	2.911804	4.909501
436	V	2.917667	5.450774
437	V	2.932332	5.830163
438	V	2.938197	4.692210
439	V	2.976190	4.756237
440	V	2.989920	4.899508
441	V	3.001452	4.913749
442	V	3.039487	5.074305
443	V	3.063829	5.464602

444	V	3.079170	5.049817
445	V	3.095845	5.318093
446	V	3.110135	4.877411
447	V	3.138013	5.489240
448	V	3.143561	4.954080
449	V	3.144822	5.071241
450	V	3.159643	5.000205
451	V	3.201809	5.089017
452	V	3.239378	5.139363
453	V	3.288773	5.064967
454	V	3.310101	5.484248
455	V	3.318771	5.320222
456	V	3.343208	5.167227
457	V	3.373068	5.414528
458	V	3.442483	5.531054
459	V	3.525212	5.750706
460	V	3.652958	5.967869
461	V	3.661688	5.836467
462	V	3.840678	10.088172
463	V	3.935905	10.276999
464	V	3.942492	10.196401
465	V	3.955167	10.437264
466	V	3.998212	10.134777
467	V	4.008069	10.222326
468	V	4.019075	10.156131
469	V	4.038646	10.152066
470	V	4.114272	10.589409
471	V	4.132715	10.604062
472	V	4.166823	11.326058
473	V	4.177483	10.703978
474	V	4.199606	11.883637
475	V	4.215339	10.858148
476	V	4.223281	10.502746
477	V	4.313552	10.231380
478	V	4.316597	10.760675
479	V	4.350231	10.205980
480	V	4.382298	10.763472
481	V	4.393342	11.223688
482	V	4.436489	10.921455
483	V	4.472720	10.568191
484	V	4.495939	11.170159
485	V	4.620389	10.738384
486	V	4.689301	10.800562
487	V	4.796912	10.615933
488	V	5.100959	13.359368
489	V	5.763719	15.345632

Total kinetic energy from orbitals= 1.776419166598D+03

1\1\GINC-COPERNICO\FOpt\RB3LYP\6-31G(d,p)\C20H13Cl1F3N2O2(1+)\IVAN\12-May-2021\0\\# opt b3lyp/6-31g(d,p) geom=connectivity pop=full\\A15MOCATION\\1,1\C,4.3214923868,1.8733393662,-0.0026684796\C,2.9411829994,1.7793376825,-0.0027087368\C,2.3352122338,0.5163057016,-0.0022442142\C,3.1359252519,-0.6646870409,-0.0017103814\C,4.5384944569,-0.5447379429,-0

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97,4.4468234183,-0.0049493579\H,0.390548265,1.2259965218,-0.0027771105
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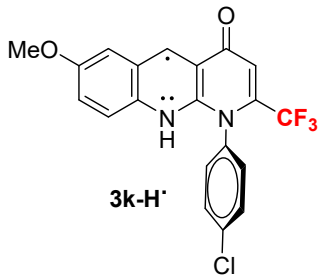
923,-11.5613838,-16.6550085,13.9147014,-0.0037037,-0.0020256\PG=C01 [X
(C20H13Cl1F3N2O2)]\\@

VII.1.4. Protonated *N*^{1}-(4-chlorophenyl)-2-(trifluoromethyl)-7-methoxybenzo[*b*][1,8]naphthyridin-4(1*H*)-one radical **3k-H**·



Orbital energies and kinetic energies (alpha):

		1	2
1	O	-101.573544	136.907087
2	O	-24.740799	37.081395
3	O	-24.736058	37.083488
4	O	-24.736056	37.081922

5	O	-19.178952	29.024244
6	O	-19.095103	29.024091
7	O	-14.428703	21.957298
8	O	-14.403748	21.953756
9	O	-10.451688	15.901976
10	O	-10.300457	15.883091
11	O	-10.287383	15.883762
12	O	-10.272385	15.885349
13	O	-10.264828	15.880288
14	O	-10.249159	15.885688
15	O	-10.247995	15.886191
16	O	-10.243970	15.885251
17	O	-10.243385	15.881522
18	O	-10.239747	15.878776
19	O	-10.239742	15.880104
20	O	-10.237604	15.881255
21	O	-10.237602	15.882593
22	O	-10.206894	15.882131
23	O	-10.201163	15.880422
24	O	-10.199028	15.880238
25	O	-10.197466	15.879205
26	O	-10.195145	15.879000
27	O	-10.187346	15.875619
28	O	-10.184931	15.878187
29	O	-9.489811	21.547655
30	O	-7.253875	20.528705
31	O	-7.244081	20.555121
32	O	-7.243643	20.550296
33	O	-1.316213	3.271027
34	O	-1.230154	3.826752
35	O	-1.225251	3.832243
36	O	-1.064555	2.519718
37	O	-1.038803	1.832272
38	O	-0.995055	2.585961
39	O	-0.974871	1.916761
40	O	-0.921607	1.902507
41	O	-0.871711	2.146879
42	O	-0.858406	1.598358
43	O	-0.823846	1.738852
44	O	-0.816958	1.861296
45	O	-0.795737	1.616420
46	O	-0.779908	1.783137
47	O	-0.760415	1.712618
48	O	-0.751156	1.985023
49	O	-0.725124	2.212044
50	O	-0.705667	1.653438
51	O	-0.676770	2.071641
52	O	-0.660783	1.463290
53	O	-0.655983	1.887674
54	O	-0.650019	1.675517
55	O	-0.635592	1.543730
56	O	-0.623084	1.847447
57	O	-0.597728	2.565094
58	O	-0.594307	2.782632
59	O	-0.589114	1.408634

60	O	-0.571290	1.640578
61	O	-0.569268	1.951862
62	O	-0.540209	1.515410
63	O	-0.527600	1.773466
64	O	-0.520221	1.404448
65	O	-0.518823	1.805038
66	O	-0.505073	1.632698
67	O	-0.499759	1.560781
68	O	-0.486782	1.459089
69	O	-0.479945	1.534067
70	O	-0.472027	1.996575
71	O	-0.469988	2.970027
72	O	-0.469683	1.394359
73	O	-0.467656	2.142657
74	O	-0.460003	1.302509
75	O	-0.453320	1.533690
76	O	-0.443447	1.586142
77	O	-0.434918	2.575871
78	O	-0.434004	3.103613
79	O	-0.428277	1.380100
80	O	-0.420544	2.054974
81	O	-0.418310	1.607648
82	O	-0.413135	1.752431
83	O	-0.411103	3.413913
84	O	-0.410446	1.536810
85	O	-0.408901	2.202053
86	O	-0.399262	1.921282
87	O	-0.394150	1.365847
88	O	-0.383227	1.930358
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90	O	-0.373205	1.867663
91	O	-0.361739	1.826344
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93	O	-0.357271	1.756521
94	O	-0.336916	2.358135
95	O	-0.330636	1.967369
96	O	-0.317882	1.580764
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101	O	-0.238659	1.605980
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103	O	-0.219416	1.651551
104	O	-0.136987	1.554874
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108	V	-0.019545	1.640130
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110	V	0.004639	1.489241
111	V	0.048274	1.781296
112	V	0.069323	1.203269
113	V	0.081631	1.619076
114	V	0.090459	1.423351

115	V	0.101020	1.719816
116	V	0.104130	2.119498
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118	V	0.110574	0.994576
119	V	0.128601	1.593436
120	V	0.135897	1.492484
121	V	0.139332	2.098355
122	V	0.141968	1.248303
123	V	0.143979	1.562068
124	V	0.153466	1.143820
125	V	0.161285	1.270646
126	V	0.163862	1.086350
127	V	0.175189	1.677201
128	V	0.185180	1.618112
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131	V	0.194630	1.552700
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133	V	0.206022	3.614256
134	V	0.229352	2.041633
135	V	0.229960	1.731182
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137	V	0.239166	2.135923
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139	V	0.254554	2.293407
140	V	0.269662	2.360622
141	V	0.288217	2.409062
142	V	0.290615	2.299488
143	V	0.297814	1.926949
144	V	0.315604	1.934416
145	V	0.322878	2.284441
146	V	0.326916	2.058915
147	V	0.345977	2.031884
148	V	0.376272	2.119756
149	V	0.377494	2.188647
150	V	0.388653	2.685297
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152	V	0.401619	2.334747
153	V	0.420596	2.383381
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156	V	0.430831	2.214225
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160	V	0.481592	2.149444
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164	V	0.492741	2.048762
165	V	0.508053	2.325040
166	V	0.511828	2.195056
167	V	0.515033	1.975415
168	V	0.521360	2.704600
169	V	0.529202	2.269612

170	V	0.535652	2.083234
171	V	0.540127	2.263435
172	V	0.542400	1.889729
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177	V	0.561617	2.236836
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213	V	0.829184	2.526957
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223	V	0.894840	2.651657
224	V	0.898038	2.705708

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228	V	0.926181	2.509232
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233	V	0.988199	2.639807
234	V	0.991634	2.449180
235	V	0.995777	2.471768
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238	V	1.016329	2.583426
239	V	1.032354	3.343868
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261	V	1.247945	2.708384
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266	V	1.307642	2.767611
267	V	1.312428	2.461890
268	V	1.321903	2.843153
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271	V	1.345093	2.498207
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307	V	1.750832	3.105406
308	V	1.756866	2.941855
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312	V	1.795518	3.219796
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327	V	1.899656	3.295241
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339	V	1.982244	3.402192
340	V	1.990844	3.461592
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343	V	2.008030	3.477097
344	V	2.008848	3.071818
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346	V	2.035395	3.347288
347	V	2.036730	3.980984
348	V	2.038721	3.239616
349	V	2.043529	3.430791
350	V	2.048934	3.405047
351	V	2.058621	3.482005
352	V	2.058797	3.436509
353	V	2.066692	3.492727
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355	V	2.079859	3.562314
356	V	2.108584	3.506173
357	V	2.119207	3.536914
358	V	2.127696	3.382492
359	V	2.129948	3.468479
360	V	2.173828	3.610643
361	V	2.189003	3.776715
362	V	2.193229	3.467301
363	V	2.212522	3.415056
364	V	2.223041	3.831016
365	V	2.235494	3.469778
366	V	2.254537	3.520614
367	V	2.261271	3.733635
368	V	2.268259	3.573536
369	V	2.274486	3.448312
370	V	2.277756	3.884228
371	V	2.294374	3.550228
372	V	2.306469	3.743640
373	V	2.312116	3.798583
374	V	2.326227	3.466953
375	V	2.342869	3.842534
376	V	2.367222	3.812670
377	V	2.372929	3.346958
378	V	2.375937	3.917462
379	V	2.388069	3.926476
380	V	2.389265	3.775412
381	V	2.398714	3.882886
382	V	2.408061	3.941670
383	V	2.410748	3.753730
384	V	2.420115	3.493972
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388	V	2.462457	3.881819
389	V	2.476340	4.014739

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392	V	2.499979	3.599964
393	V	2.505406	3.999198
394	V	2.522283	4.033422
395	V	2.533827	3.756944
396	V	2.534154	3.993359
397	V	2.540069	3.656570
398	V	2.545395	3.886636
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402	V	2.581315	3.937376
403	V	2.600552	3.726410
404	V	2.607929	3.870889
405	V	2.621234	3.879729
406	V	2.631560	3.948646
407	V	2.641761	3.792995
408	V	2.657891	3.914928
409	V	2.660894	4.016667
410	V	2.667561	4.036344
411	V	2.679606	3.945867
412	V	2.691059	4.223364
413	V	2.693072	4.328814
414	V	2.707156	4.258713
415	V	2.719998	4.087708
416	V	2.735526	4.393680
417	V	2.746330	4.103252
418	V	2.752675	3.975407
419	V	2.762833	4.328442
420	V	2.772400	4.385357
421	V	2.781930	4.185728
422	V	2.784383	4.288350
423	V	2.806016	4.375334
424	V	2.827781	4.555078
425	V	2.835184	3.893261
426	V	2.848215	4.366843
427	V	2.864732	4.576628
428	V	2.866345	4.478038
429	V	2.897775	4.430276
430	V	2.934300	4.559048
431	V	2.956816	4.612037
432	V	3.000051	4.659704
433	V	3.014786	4.772992
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435	V	3.029080	5.476239
436	V	3.030224	4.749878
437	V	3.051078	5.056974
438	V	3.060988	4.778439
439	V	3.108758	4.754278
440	V	3.119075	5.007643
441	V	3.136589	4.901147
442	V	3.167565	5.048746
443	V	3.173695	5.250437
444	V	3.199196	5.097742

445	V	3.207875	4.881732
446	V	3.222941	5.497482
447	V	3.247364	4.963177
448	V	3.265742	5.278422
449	V	3.280658	5.094416
450	V	3.296292	4.998249
451	V	3.302154	5.094153
452	V	3.375415	5.127328
453	V	3.396501	5.053498
454	V	3.439679	5.152689
455	V	3.465966	5.288686
456	V	3.469251	5.544948
457	V	3.472707	5.417769
458	V	3.582979	5.537021
459	V	3.672537	5.742195
460	V	3.756922	6.028486
461	V	3.805468	5.777055
462	V	3.991129	10.129841
463	V	4.051187	10.448877
464	V	4.080493	10.335711
465	V	4.100871	10.179159
466	V	4.105787	10.230432
467	V	4.141557	10.104725
468	V	4.155664	10.137498
469	V	4.188676	10.216278
470	V	4.216944	10.936413
471	V	4.270163	12.244913
472	V	4.281775	11.151236
473	V	4.305234	10.914868
474	V	4.318015	10.350439
475	V	4.321656	10.678962
476	V	4.355308	10.385106
477	V	4.418505	10.804180
478	V	4.451356	10.208304
479	V	4.469457	10.108081
480	V	4.484862	11.079583
481	V	4.516246	10.537143
482	V	4.567259	11.001720
483	V	4.606753	10.481341
484	V	4.631753	11.077014
485	V	4.735554	10.637673
486	V	4.825234	10.850097
487	V	4.942823	10.587056
488	V	5.192861	13.265356
489	V	5.872954	15.380727

Orbital energies and kinetic energies (beta):

		1	2
1	O	-101.573544	136.907087
2	O	-24.740796	37.081400
3	O	-24.735926	37.083608
4	O	-24.735923	37.082051
5	O	-19.179200	29.023948
6	O	-19.092885	29.026948
7	O	-14.429355	21.956452

8	O	-14.401250	21.957270
9	O	-10.451739	15.901963
10	O	-10.298696	15.885958
11	O	-10.287389	15.883752
12	O	-10.272360	15.885380
13	O	-10.263513	15.882387
14	O	-10.249999	15.884478
15	O	-10.247505	15.887024
16	O	-10.243951	15.885284
17	O	-10.241917	15.883882
18	O	-10.239767	15.878766
19	O	-10.239762	15.880096
20	O	-10.237603	15.881244
21	O	-10.237601	15.882580
22	O	-10.208400	15.880036
23	O	-10.201569	15.880029
24	O	-10.200125	15.878811
25	O	-10.197327	15.879487
26	O	-10.192697	15.882779
27	O	-10.182713	15.881697
28	O	-10.180626	15.886255
29	O	-9.489812	21.547654
30	O	-7.253875	20.528705
31	O	-7.244083	20.555121
32	O	-7.243644	20.550296
33	O	-1.316039	3.270871
34	O	-1.230044	3.826380
35	O	-1.224944	3.831740
36	O	-1.065047	2.521501
37	O	-1.037096	1.833659
38	O	-0.991122	2.573892
39	O	-0.971682	1.908424
40	O	-0.921537	1.904895
41	O	-0.871366	2.152111
42	O	-0.855534	1.596438
43	O	-0.820712	1.782826
44	O	-0.814018	1.821439
45	O	-0.795765	1.616453
46	O	-0.776701	1.787547
47	O	-0.758718	1.717501
48	O	-0.750389	1.972787
49	O	-0.723170	2.249600
50	O	-0.704435	1.652063
51	O	-0.671399	2.070551
52	O	-0.660827	1.463529
53	O	-0.654240	1.873492
54	O	-0.648250	1.664092
55	O	-0.632588	1.515350
56	O	-0.621477	1.840027
57	O	-0.597426	2.582218
58	O	-0.593796	2.785445
59	O	-0.588703	1.407050
60	O	-0.570052	1.633105
61	O	-0.567488	1.943670
62	O	-0.538639	1.517448

63	O	-0.526616	1.765245
64	O	-0.519852	1.409465
65	O	-0.518097	1.811478
66	O	-0.503738	1.621167
67	O	-0.498554	1.552613
68	O	-0.485591	1.463225
69	O	-0.479465	1.551634
70	O	-0.471335	2.137843
71	O	-0.469776	2.966787
72	O	-0.469714	1.294351
73	O	-0.467426	2.111346
74	O	-0.453696	1.337341
75	O	-0.452166	1.537456
76	O	-0.442606	1.607594
77	O	-0.434442	2.534009
78	O	-0.432881	3.135696
79	O	-0.427710	1.400854
80	O	-0.419996	2.037005
81	O	-0.416807	1.640698
82	O	-0.412220	1.708473
83	O	-0.410943	3.508111
84	O	-0.407992	2.237515
85	O	-0.407164	1.379697
86	O	-0.397700	1.887161
87	O	-0.390842	1.334831
88	O	-0.381826	1.934061
89	O	-0.371500	1.856454
90	O	-0.367428	1.344766
91	O	-0.361086	1.848918
92	O	-0.356027	1.753286
93	O	-0.355254	1.551256
94	O	-0.336904	2.358197
95	O	-0.330074	1.956478
96	O	-0.313395	1.525442
97	O	-0.297902	1.151546
98	O	-0.293139	1.252965
99	O	-0.279921	1.672240
100	O	-0.258268	1.419670
101	O	-0.229412	1.635073
102	O	-0.224463	2.366754
103	O	-0.210031	1.627365
104	V	-0.073340	1.510173
105	V	-0.053803	1.546129
106	V	-0.048585	1.380193
107	V	-0.023128	1.779308
108	V	-0.014468	1.668519
109	V	0.004578	2.095613
110	V	0.017751	1.524566
111	V	0.062688	1.762132
112	V	0.069971	1.202007
113	V	0.081668	1.610525
114	V	0.091711	1.409401
115	V	0.101321	1.704132
116	V	0.104554	2.140076
117	V	0.110501	1.593214

118	V	0.110686	0.991173
119	V	0.129768	1.601441
120	V	0.136178	1.470077
121	V	0.143122	1.194264
122	V	0.144315	1.601981
123	V	0.145429	2.089483
124	V	0.153923	1.155503
125	V	0.161353	1.267726
126	V	0.164008	1.088281
127	V	0.175687	1.706056
128	V	0.187420	2.026317
129	V	0.188403	2.099494
130	V	0.192211	2.600699
131	V	0.196562	1.599068
132	V	0.206259	3.538264
133	V	0.211266	2.315151
134	V	0.230531	1.819563
135	V	0.230785	1.922515
136	V	0.239409	1.960348
137	V	0.241577	2.158888
138	V	0.254215	1.536737
139	V	0.256137	2.328565
140	V	0.270988	2.347971
141	V	0.289265	2.419308
142	V	0.291910	2.274738
143	V	0.297863	1.927494
144	V	0.317724	1.913170
145	V	0.325092	2.262459
146	V	0.328248	2.125312
147	V	0.346965	2.037584
148	V	0.377594	2.183933
149	V	0.377749	2.131707
150	V	0.388746	2.688988
151	V	0.395579	1.897718
152	V	0.402999	2.314910
153	V	0.420854	2.470363
154	V	0.422408	2.307052
155	V	0.431405	2.206705
156	V	0.432095	2.396566
157	V	0.441855	2.030255
158	V	0.456332	2.295610
159	V	0.460478	1.858481
160	V	0.483426	2.150371
161	V	0.486361	2.184590
162	V	0.490459	2.352869
163	V	0.493936	2.199795
164	V	0.496491	2.038106
165	V	0.509044	2.314453
166	V	0.512265	2.201758
167	V	0.517915	1.971806
168	V	0.522088	2.725680
169	V	0.530358	2.260193
170	V	0.539181	2.100434
171	V	0.540462	2.270740
172	V	0.543808	2.129422

173	V	0.544145	1.865079
174	V	0.549111	2.300049
175	V	0.550892	2.459349
176	V	0.553373	2.247940
177	V	0.563035	2.294702
178	V	0.566355	2.468152
179	V	0.571395	2.103834
180	V	0.572209	2.321335
181	V	0.582555	2.144315
182	V	0.590662	2.345200
183	V	0.596970	2.445187
184	V	0.604116	2.303677
185	V	0.606640	2.139898
186	V	0.607072	2.287897
187	V	0.619793	2.310496
188	V	0.627292	2.140261
189	V	0.639237	2.648293
190	V	0.645385	2.524727
191	V	0.645740	2.229033
192	V	0.649484	2.770343
193	V	0.679972	2.207306
194	V	0.680098	2.422689
195	V	0.693894	2.255671
196	V	0.705962	2.482372
197	V	0.709338	3.096324
198	V	0.716731	2.567240
199	V	0.723302	2.268972
200	V	0.729241	2.303227
201	V	0.750546	2.287500
202	V	0.764805	2.742822
203	V	0.774816	2.370650
204	V	0.782515	2.575146
205	V	0.785055	2.321484
206	V	0.790815	2.683420
207	V	0.798419	2.596632
208	V	0.808881	2.423741
209	V	0.809905	2.633911
210	V	0.815036	2.598494
211	V	0.821204	2.314602
212	V	0.826253	2.655720
213	V	0.829894	2.515000
214	V	0.830610	2.612111
215	V	0.840308	2.568973
216	V	0.841581	2.472970
217	V	0.844661	2.507034
218	V	0.848845	2.607838
219	V	0.850113	2.491982
220	V	0.860682	2.613483
221	V	0.863367	2.520474
222	V	0.879432	2.502188
223	V	0.895408	2.643774
224	V	0.898108	2.707225
225	V	0.908831	2.488980
226	V	0.911590	2.522729
227	V	0.921215	2.521696

228	V	0.927015	2.510340
229	V	0.937549	2.744921
230	V	0.943595	2.422636
231	V	0.952338	2.568254
232	V	0.964491	2.374254
233	V	0.988715	2.628457
234	V	0.992546	2.436439
235	V	0.996433	2.484414
236	V	0.998307	2.683796
237	V	1.010232	2.568335
238	V	1.019229	2.592948
239	V	1.032113	3.340881
240	V	1.042884	2.465665
241	V	1.049577	2.655825
242	V	1.064191	3.367094
243	V	1.072040	2.885494
244	V	1.082329	3.029917
245	V	1.086811	2.799617
246	V	1.104829	2.584410
247	V	1.114380	2.692330
248	V	1.124732	3.020120
249	V	1.126160	3.114878
250	V	1.145589	2.873278
251	V	1.158075	2.563838
252	V	1.162672	2.983192
253	V	1.167354	2.852072
254	V	1.184412	2.417273
255	V	1.188235	2.695719
256	V	1.193509	2.731776
257	V	1.210941	2.460404
258	V	1.228219	2.435806
259	V	1.233716	2.748052
260	V	1.242122	2.812679
261	V	1.248438	2.702256
262	V	1.254342	2.517468
263	V	1.272575	2.951690
264	V	1.291587	3.026193
265	V	1.300455	3.084212
266	V	1.308104	2.755245
267	V	1.314083	2.465144
268	V	1.322255	3.205160
269	V	1.324789	2.729118
270	V	1.325496	2.830756
271	V	1.349083	2.728917
272	V	1.351900	2.919100
273	V	1.353756	2.518593
274	V	1.355113	2.947676
275	V	1.359677	2.938160
276	V	1.365905	2.739386
277	V	1.374036	2.877534
278	V	1.376179	2.769635
279	V	1.382949	2.835534
280	V	1.384017	3.215837
281	V	1.399829	2.578857
282	V	1.403432	2.628789

283	V	1.418492	2.571580
284	V	1.425547	3.260432
285	V	1.433940	3.225331
286	V	1.443417	3.092480
287	V	1.451043	2.957199
288	V	1.452559	2.596817
289	V	1.465246	3.019197
290	V	1.480328	2.947093
291	V	1.491855	2.828276
292	V	1.514754	2.866668
293	V	1.553339	3.113192
294	V	1.577431	2.903510
295	V	1.584238	3.348560
296	V	1.594548	2.894939
297	V	1.598921	3.021220
298	V	1.618429	2.887532
299	V	1.640995	2.924016
300	V	1.662269	3.031345
301	V	1.681667	3.074071
302	V	1.688172	2.959144
303	V	1.711489	2.903132
304	V	1.714911	3.172499
305	V	1.723330	3.230352
306	V	1.743768	3.202860
307	V	1.752133	3.165775
308	V	1.762717	2.877767
309	V	1.781140	3.270847
310	V	1.781653	3.309815
311	V	1.791523	3.227101
312	V	1.796928	3.226147
313	V	1.798528	3.327951
314	V	1.810878	2.918019
315	V	1.817417	3.235759
316	V	1.821385	2.953673
317	V	1.832536	3.148205
318	V	1.843927	2.909969
319	V	1.844738	3.234544
320	V	1.855082	2.924543
321	V	1.858253	3.012357
322	V	1.870234	3.347689
323	V	1.873494	3.108646
324	V	1.879514	2.953697
325	V	1.885522	3.301795
326	V	1.888879	3.292617
327	V	1.902008	3.287019
328	V	1.907777	3.373490
329	V	1.910200	3.090705
330	V	1.916214	3.318627
331	V	1.937477	3.152366
332	V	1.939533	3.434628
333	V	1.948003	3.083443
334	V	1.950586	3.516736
335	V	1.956158	3.529485
336	V	1.966783	3.204882
337	V	1.969418	3.556446

338	V	1.981063	3.456098
339	V	1.983759	3.433831
340	V	1.991502	3.468370
341	V	1.993997	3.706354
342	V	1.998654	3.632137
343	V	2.008766	3.477886
344	V	2.010420	3.036035
345	V	2.024820	3.015988
346	V	2.035714	3.423060
347	V	2.036956	3.923522
348	V	2.038903	3.227283
349	V	2.044208	3.450023
350	V	2.049916	3.385536
351	V	2.058879	3.435329
352	V	2.060115	3.482249
353	V	2.068424	3.499682
354	V	2.079077	3.440964
355	V	2.081945	3.590307
356	V	2.111936	3.514397
357	V	2.120205	3.511216
358	V	2.128627	3.399208
359	V	2.130977	3.469968
360	V	2.175561	3.637440
361	V	2.190391	3.758262
362	V	2.194806	3.466563
363	V	2.215652	3.412996
364	V	2.225040	3.825036
365	V	2.237802	3.471683
366	V	2.259727	3.526928
367	V	2.261464	3.737501
368	V	2.272484	3.541253
369	V	2.276751	3.469156
370	V	2.280961	3.894395
371	V	2.299703	3.544062
372	V	2.306864	3.752424
373	V	2.315739	3.811613
374	V	2.328191	3.478196
375	V	2.347685	3.815256
376	V	2.368576	3.810313
377	V	2.372955	3.347195
378	V	2.378910	3.912830
379	V	2.389166	3.919741
380	V	2.389586	3.773033
381	V	2.399740	3.878353
382	V	2.409144	3.937041
383	V	2.411791	3.761214
384	V	2.422625	3.492210
385	V	2.427684	3.582589
386	V	2.442372	3.583224
387	V	2.458656	3.955039
388	V	2.464945	3.878129
389	V	2.477015	4.015119
390	V	2.492052	3.792791
391	V	2.497384	4.058932
392	V	2.504071	3.615811

393	V	2.506469	3.998695
394	V	2.522782	4.031157
395	V	2.534430	3.999162
396	V	2.539370	3.750456
397	V	2.543679	3.658700
398	V	2.545936	3.887567
399	V	2.557676	4.083017
400	V	2.557850	3.625920
401	V	2.567200	3.701582
402	V	2.581757	3.937617
403	V	2.603753	3.780441
404	V	2.610854	3.828766
405	V	2.621912	3.873514
406	V	2.632444	3.943371
407	V	2.641957	3.795089
408	V	2.660552	3.912689
409	V	2.661182	4.012096
410	V	2.667758	4.040213
411	V	2.682312	3.947362
412	V	2.691315	4.223778
413	V	2.694216	4.326291
414	V	2.708059	4.281622
415	V	2.724312	4.063178
416	V	2.737560	4.379699
417	V	2.746822	4.109059
418	V	2.756852	3.981727
419	V	2.764135	4.329486
420	V	2.773880	4.389133
421	V	2.783757	4.176854
422	V	2.785838	4.283941
423	V	2.806730	4.381040
424	V	2.829001	4.551047
425	V	2.835266	3.893958
426	V	2.848666	4.369020
427	V	2.866633	4.476407
428	V	2.867949	4.584378
429	V	2.899627	4.422454
430	V	2.935618	4.558668
431	V	2.959524	4.609072
432	V	3.000392	4.656453
433	V	3.015537	4.786063
434	V	3.023784	5.620393
435	V	3.029288	5.475710
436	V	3.030963	4.755546
437	V	3.051787	5.051602
438	V	3.061946	4.774452
439	V	3.109355	4.756729
440	V	3.120626	5.008459
441	V	3.137399	4.902298
442	V	3.167875	5.045043
443	V	3.174010	5.248674
444	V	3.200071	5.104532
445	V	3.207870	4.881733
446	V	3.223746	5.494236
447	V	3.247340	4.963128

448	V	3.266144	5.274817
449	V	3.281563	5.096309
450	V	3.296597	4.998210
451	V	3.302290	5.094170
452	V	3.376088	5.127465
453	V	3.396465	5.053536
454	V	3.440041	5.151089
455	V	3.466744	5.266737
456	V	3.471082	5.566619
457	V	3.472698	5.417768
458	V	3.583534	5.536496
459	V	3.674103	5.741265
460	V	3.756966	6.028388
461	V	3.806656	5.776880
462	V	3.992685	10.129783
463	V	4.051206	10.448560
464	V	4.081545	10.338222
465	V	4.104277	10.179656
466	V	4.105780	10.230303
467	V	4.143808	10.107522
468	V	4.157347	10.139208
469	V	4.191105	10.212993
470	V	4.217131	10.942362
471	V	4.270609	12.354154
472	V	4.283741	11.084967
473	V	4.305301	10.914120
474	V	4.322107	10.648192
475	V	4.324974	10.351236
476	V	4.357405	10.382343
477	V	4.418713	10.800115
478	V	4.452212	10.227914
479	V	4.472665	10.089750
480	V	4.484901	11.080458
481	V	4.517459	10.534176
482	V	4.569898	11.018319
483	V	4.608625	10.468156
484	V	4.634253	11.071725
485	V	4.735984	10.638162
486	V	4.826453	10.853753
487	V	4.945453	10.583462
488	V	5.192976	13.265254
489	V	5.873052	15.380537

Total kinetic energy from orbitals= 1.776672203881D+03

1\1\GINC-COPERNICO\FOpt\UB3LYP\6-31G(d,p)\C20H13Cl1F3N2O2(2)\IVAN\12-May-2021\0\\# opt b3lyp/6-31g(d,p) geom=connectivity pop=full\\A15MODRADICAL\\0,2\C,4.3444382089,1.8899392293,-0.0031706124\C,2.948567212,1.7644995504,-0.003460495\C,2.3523857968,0.5116883449,-0.0026854051\C,3.1432248518,-0.6770800076,-0.0015414397\C,4.5433864924,-0.5287489595,-0.0012485754\C,5.1394574688,0.7336881908,-0.0020642836\C,2.4778272417,-1.9311188234,-0.0007277045\C,1.0676958565,-2.0097219504,-0.0009669346\C,0.3132879002,-0.8327086658,-0.0021338905\C,-1.7438999212,-2.061912065

3,-0.0017816797\C,-1.0645512517,-3.238744218,-0.0006433679\C,0.3889226
264,-3.312785381,0.0000133329\H,2.3314730336,2.65977054,-0.0043195092\
H,5.1800154265,-1.4068955183,-0.0003787383\H,3.0297670696,-2.863073304
,0.0001656718\H,-1.611768744,-4.171425872,-0.0002536353\C,-1.771436634
8,0.4345127588,-0.0027329306\C,-2.0862005076,1.0550468518,1.2092315495
\C,-2.0868976053,1.0542163321,-1.2149265627\C,-2.7244150886,2.29386114
93,1.2130196586\H,-1.8401761021,0.5624947241,2.1436665867\C,-2.7251228
405,2.2930380512,-1.2191893566\H,-1.8414255654,0.5610164759,-2.1491591
268\C,-3.0379554277,2.902042406,-0.0032058048\H,-2.9786261725,2.781115
7481,2.1471325705\H,-2.9798676115,2.7796529371,-2.1534899539\C,-3.2521
586951,-2.0467412874,-0.0027313122\N,-1.0738747621,-0.8318843058,-0.00
24816484\F,-3.7471360135,-3.2942896401,-0.002098297\F,-3.7591681711,-1
.4146256505,1.0842842557\F,-3.757697253,-1.416295757,-1.0914274361\N,0
.9546757642,0.3786935723,-0.0030611956\O,1.007410022,-4.3846265972,0.0
011822592\H,4.7860812064,2.8779791028,-0.0038124494\C,7.1725327509,1.9
92257988,-0.0023695425\H,6.9310767345,2.5812882927,-0.8967304189\H,6.9
304570545,2.582557366,0.890985687\H,8.2394725468,1.7648326074,-0.00184
15202\O,6.5059883556,0.7407686464,-0.0017099605\Cl,-3.8371164483,4.461
4123029,-0.0034982804\H,0.4009110858,1.2223150148,-0.0039733243\\Versi
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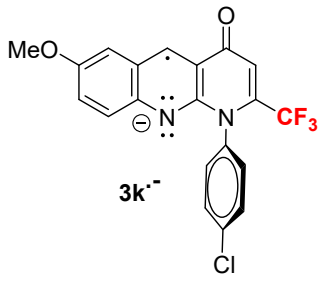
=0.75027\RMSD=4.316e-09\RMSF=4.018e-06\Dipole=-0.15731,2.951776,-0.002
0596\Quadrupole=5.7466547,-11.5102852,5.7636306,11.6778834,-0.006797,0
.0114328\PG=C01 [X(C20H13Cl1F3N2O2)]\\@

VII.1.5. *N*^{1}-(4-chlorophenyl)-2-(trifluoromethyl)-7-methoxybenzo[*b*][1,8]naphthyridin-4(1*H*)-one radical anion **3k**$^{\cdot-}$



Orbital energies and kinetic energies (alpha):

		1	2
1	O	-101.471533	136.907099
2	O	-24.626134	37.081387
3	O	-24.617135	37.082879
4	O	-24.617132	37.082303
5	O	-19.070392	29.024552
6	O	-18.950537	29.023352
7	O	-14.272769	21.956847
8	O	-14.179924	21.958227
9	O	-10.329806	15.902084

10	O	-10.170351	15.883661
11	O	-10.150620	15.885463
12	O	-10.141681	15.885885
13	O	-10.135112	15.885247
14	O	-10.124667	15.885236
15	O	-10.123463	15.878938
16	O	-10.119455	15.879483
17	O	-10.119450	15.880517
18	O	-10.112671	15.880521
19	O	-10.112665	15.881578
20	O	-10.101189	15.885716
21	O	-10.088017	15.883013
22	O	-10.068154	15.881757
23	O	-10.067817	15.879057
24	O	-10.061213	15.879994
25	O	-10.059301	15.880465
26	O	-10.057053	15.878884
27	O	-10.056594	15.880097
28	O	-10.048453	15.877483
29	O	-9.387761	21.547686
30	O	-7.151513	20.529701
31	O	-7.142122	20.555113
32	O	-7.141913	20.550255
33	O	-1.195568	3.277629
34	O	-1.111538	3.834430
35	O	-1.103687	3.842483
36	O	-0.953485	2.515565
37	O	-0.877439	1.834819
38	O	-0.845106	2.556646
39	O	-0.806507	2.027501
40	O	-0.793289	1.889067
41	O	-0.749642	2.111838
42	O	-0.717296	1.624865
43	O	-0.687905	1.867557
44	O	-0.673542	1.611229
45	O	-0.668090	1.771482
46	O	-0.647426	1.832297
47	O	-0.632965	1.724343
48	O	-0.620298	1.880785
49	O	-0.595017	2.241089
50	O	-0.582114	1.715587
51	O	-0.540388	2.045490
52	O	-0.538509	1.460517
53	O	-0.522615	1.780517
54	O	-0.510170	1.722201
55	O	-0.489576	1.888260
56	O	-0.475485	2.560804
57	O	-0.474780	2.763286
58	O	-0.471909	1.391455
59	O	-0.456841	1.521796
60	O	-0.440850	1.854382
61	O	-0.415291	1.751444
62	O	-0.409817	1.416201
63	O	-0.397065	1.630791
64	O	-0.394123	1.429253
65	O	-0.378074	1.638235
66	O	-0.371717	1.642733
67	O	-0.369648	1.193683
68	O	-0.359596	1.584585
69	O	-0.358236	1.762140

70	O	-0.354579	2.944970
71	O	-0.352157	2.777459
72	O	-0.348805	1.378758
73	O	-0.326261	1.705441
74	O	-0.317390	2.543842
75	O	-0.316742	2.843029
76	O	-0.309950	1.614420
77	O	-0.306384	1.494764
78	O	-0.304524	1.683399
79	O	-0.303350	2.035491
80	O	-0.294902	3.500195
81	O	-0.294353	1.672989
82	O	-0.286414	2.209835
83	O	-0.281699	1.722509
84	O	-0.279626	1.314197
85	O	-0.271670	1.647116
86	O	-0.263581	1.249040
87	O	-0.255731	1.670106
88	O	-0.247608	1.953978
89	O	-0.238250	2.033218
90	O	-0.236179	2.234734
91	O	-0.235616	1.512993
92	O	-0.234384	1.855059
93	O	-0.225105	1.566429
94	O	-0.215024	1.780602
95	O	-0.183660	1.467809
96	O	-0.174412	1.161464
97	O	-0.165273	1.267561
98	O	-0.161199	1.562917
99	O	-0.127718	1.905301
100	O	-0.126115	1.463216
101	O	-0.103738	1.536965
102	O	-0.086942	2.329217
103	O	-0.080674	1.612433
104	O	0.013230	1.637970
105	V	0.073301	1.538816
106	V	0.075132	1.391660
107	V	0.094604	1.676642
108	V	0.104925	2.102928
109	V	0.121802	1.635759
110	V	0.150603	1.523795
111	V	0.185477	1.818696
112	V	0.187308	1.035170
113	V	0.198703	1.395394
114	V	0.212737	1.579791
115	V	0.220134	0.983040
116	V	0.222751	2.456071
117	V	0.227824	1.976778
118	V	0.235052	1.021410
119	V	0.246071	1.153413
120	V	0.248220	1.578113
121	V	0.253295	1.094052
122	V	0.258035	1.031164
123	V	0.263059	1.647691
124	V	0.267761	2.082352
125	V	0.272627	1.351433
126	V	0.296340	1.422434
127	V	0.301994	1.231755
128	V	0.308467	2.677914
129	V	0.311370	2.185678

130	V	0.318772	3.599419
131	V	0.337257	2.520868
132	V	0.342833	2.103904
133	V	0.355702	2.274274
134	V	0.359153	1.908411
135	V	0.369275	1.515237
136	V	0.369449	1.823000
137	V	0.375706	2.005405
138	V	0.387429	2.020214
139	V	0.408016	2.436591
140	V	0.415617	2.440502
141	V	0.417345	1.921757
142	V	0.430217	1.863943
143	V	0.434403	2.016533
144	V	0.459261	2.185547
145	V	0.469228	2.371492
146	V	0.479006	2.396296
147	V	0.481586	2.426880
148	V	0.492608	2.353851
149	V	0.504275	2.099785
150	V	0.515201	2.147237
151	V	0.519275	2.616600
152	V	0.535008	2.200313
153	V	0.545963	2.207719
154	V	0.555102	2.070734
155	V	0.555761	2.134912
156	V	0.572224	2.231500
157	V	0.584373	2.326866
158	V	0.596076	2.333469
159	V	0.604166	2.354816
160	V	0.606823	2.190897
161	V	0.618339	1.976336
162	V	0.623842	1.909774
163	V	0.631839	1.926052
164	V	0.632569	2.390841
165	V	0.635324	2.518192
166	V	0.637009	2.223498
167	V	0.646004	2.253880
168	V	0.653148	2.039337
169	V	0.655033	2.516572
170	V	0.665551	2.251890
171	V	0.668739	1.926242
172	V	0.671850	2.225882
173	V	0.673023	2.139512
174	V	0.673047	2.103825
175	V	0.688225	2.243475
176	V	0.688779	2.114216
177	V	0.691075	2.537594
178	V	0.697209	2.139613
179	V	0.700022	2.486383
180	V	0.701584	2.290785
181	V	0.723981	2.325958
182	V	0.725413	2.322754
183	V	0.731449	2.286353
184	V	0.733377	2.251008
185	V	0.737966	2.363866
186	V	0.745683	2.268165
187	V	0.753902	2.134220
188	V	0.764244	2.249418
189	V	0.768919	2.353511

190	V	0.776429	2.768817
191	V	0.796683	2.819769
192	V	0.805776	2.204299
193	V	0.809012	2.549345
194	V	0.821147	2.252749
195	V	0.825338	2.540955
196	V	0.830915	2.332357
197	V	0.837490	2.502031
198	V	0.840963	2.868286
199	V	0.855584	2.266694
200	V	0.866156	2.431931
201	V	0.874346	2.250809
202	V	0.886403	2.783799
203	V	0.894535	2.585811
204	V	0.905523	2.381377
205	V	0.915241	2.538955
206	V	0.917077	2.665029
207	V	0.924176	2.461388
208	V	0.927060	2.582671
209	V	0.930780	2.585873
210	V	0.938285	2.676262
211	V	0.942116	2.372990
212	V	0.949774	2.600083
213	V	0.949973	2.573918
214	V	0.953045	2.477803
215	V	0.960270	2.377874
216	V	0.967382	2.695443
217	V	0.975797	2.594369
218	V	0.978944	2.561823
219	V	0.991026	2.534871
220	V	1.006506	2.838381
221	V	1.007180	2.540043
222	V	1.009096	2.480458
223	V	1.010219	2.652422
224	V	1.019335	2.504285
225	V	1.039832	2.432097
226	V	1.042412	2.616373
227	V	1.066989	2.531172
228	V	1.079149	2.553717
229	V	1.083771	2.714905
230	V	1.086670	2.404823
231	V	1.091614	2.566872
232	V	1.111667	2.545245
233	V	1.117414	2.490777
234	V	1.123569	2.876364
235	V	1.132900	2.529844
236	V	1.136890	3.348277
237	V	1.142822	2.577494
238	V	1.154931	2.599132
239	V	1.166245	2.821356
240	V	1.172899	2.732375
241	V	1.185091	3.330124
242	V	1.186209	2.550359
243	V	1.204099	3.295042
244	V	1.214873	2.965033
245	V	1.229922	2.450907
246	V	1.239718	3.061909
247	V	1.252496	2.884381
248	V	1.255688	2.755839
249	V	1.276185	2.808881

250	V	1.284227	2.604838
251	V	1.288802	3.006392
252	V	1.297564	2.770701
253	V	1.311736	2.708312
254	V	1.317908	2.412157
255	V	1.342468	2.722149
256	V	1.347498	2.446677
257	V	1.349450	2.625315
258	V	1.362494	2.413616
259	V	1.364257	2.840699
260	V	1.383385	3.058104
261	V	1.397936	2.537460
262	V	1.410628	3.133824
263	V	1.417708	3.113797
264	V	1.428927	2.762117
265	V	1.430398	2.545289
266	V	1.431426	3.471199
267	V	1.437155	2.545271
268	V	1.462801	2.777301
269	V	1.469699	3.477078
270	V	1.472223	2.645428
271	V	1.477300	2.513858
272	V	1.481137	2.767786
273	V	1.482481	2.923583
274	V	1.495210	2.570438
275	V	1.500301	2.914556
276	V	1.502764	3.162445
277	V	1.511152	2.709207
278	V	1.516231	2.546284
279	V	1.526032	2.553094
280	V	1.527798	3.050251
281	V	1.537292	2.665591
282	V	1.556094	2.563566
283	V	1.557698	3.430506
284	V	1.561104	3.059543
285	V	1.565193	2.841055
286	V	1.577321	2.982333
287	V	1.605296	3.060832
288	V	1.606031	2.625410
289	V	1.612615	2.904933
290	V	1.620742	2.769370
291	V	1.644762	2.917644
292	V	1.693383	3.169140
293	V	1.699271	3.394567
294	V	1.709725	2.891683
295	V	1.748826	2.976036
296	V	1.749057	2.835676
297	V	1.764135	2.939127
298	V	1.806908	3.086628
299	V	1.818726	2.958027
300	V	1.822220	2.993563
301	V	1.835391	3.230857
302	V	1.852570	3.187826
303	V	1.853601	2.965295
304	V	1.877308	3.096861
305	V	1.884267	3.204741
306	V	1.896319	2.868002
307	V	1.903477	3.289930
308	V	1.909914	3.207851
309	V	1.917033	3.180584

310	V	1.921232	3.239606
311	V	1.926204	3.261834
312	V	1.943062	2.927301
313	V	1.946313	2.967354
314	V	1.951084	3.159899
315	V	1.959272	3.185870
316	V	1.960643	2.911237
317	V	1.964655	3.174059
318	V	1.977249	3.254853
319	V	1.983152	2.957132
320	V	1.987663	2.913018
321	V	1.993952	3.172168
322	V	2.005744	3.319326
323	V	2.008622	3.269012
324	V	2.019529	3.251569
325	V	2.020672	3.037625
326	V	2.026417	3.272541
327	V	2.038996	3.310439
328	V	2.051989	3.115646
329	V	2.054724	3.175283
330	V	2.058290	3.320906
331	V	2.067133	3.541575
332	V	2.071362	3.554314
333	V	2.075672	3.060263
334	V	2.080443	3.122032
335	V	2.088610	3.493313
336	V	2.092994	3.511946
337	V	2.103999	3.604236
338	V	2.107880	3.477028
339	V	2.109514	2.903158
340	V	2.113326	3.504731
341	V	2.122402	3.546222
342	V	2.125518	3.402109
343	V	2.133556	3.099039
344	V	2.139507	3.470931
345	V	2.155912	3.182688
346	V	2.157335	3.885173
347	V	2.170113	3.636357
348	V	2.176724	3.507808
349	V	2.178667	3.542987
350	V	2.187168	3.438367
351	V	2.202604	3.535075
352	V	2.206858	3.220999
353	V	2.221976	3.492023
354	V	2.231914	3.457311
355	V	2.240949	3.448301
356	V	2.251221	3.595245
357	V	2.271668	3.520174
358	V	2.294884	3.824110
359	V	2.308425	3.608131
360	V	2.324906	3.457963
361	V	2.334931	3.729105
362	V	2.365616	3.434320
363	V	2.374547	3.486941
364	V	2.378287	3.827298
365	V	2.388565	3.502398
366	V	2.400935	3.473542
367	V	2.408717	3.702535
368	V	2.418819	3.660557
369	V	2.431382	3.509087

370	V	2.450495	3.951833
371	V	2.450690	3.539481
372	V	2.479272	3.825755
373	V	2.485289	3.843990
374	V	2.488142	3.496015
375	V	2.490548	3.416656
376	V	2.506399	3.876639
377	V	2.509453	3.776559
378	V	2.519047	3.848813
379	V	2.521380	3.862368
380	V	2.535264	3.887600
381	V	2.538360	3.772881
382	V	2.552629	3.704158
383	V	2.554139	3.587325
384	V	2.574610	3.884381
385	V	2.585753	3.549173
386	V	2.594245	3.993960
387	V	2.607212	3.751682
388	V	2.608550	3.944930
389	V	2.625880	3.971842
390	V	2.630806	4.061038
391	V	2.630931	3.564322
392	V	2.651077	3.997340
393	V	2.667732	3.764669
394	V	2.668533	3.949958
395	V	2.680143	3.695045
396	V	2.682165	3.632865
397	V	2.690702	4.141755
398	V	2.701247	3.689237
399	V	2.729382	3.932325
400	V	2.737779	3.862079
401	V	2.739627	3.813155
402	V	2.752627	3.992113
403	V	2.767130	3.961069
404	V	2.785118	3.892464
405	V	2.785308	3.925269
406	V	2.792935	4.148343
407	V	2.794430	3.913189
408	V	2.809000	4.197570
409	V	2.826751	4.233639
410	V	2.844571	4.140029
411	V	2.845633	4.138392
412	V	2.862185	4.366837
413	V	2.877502	4.294721
414	V	2.881734	4.007690
415	V	2.887439	4.294899
416	V	2.890590	4.106589
417	V	2.895835	4.409696
418	V	2.908720	4.373490
419	V	2.924920	3.899682
420	V	2.928555	4.361647
421	V	2.947342	4.389364
422	V	2.965315	4.542079
423	V	2.975820	4.558713
424	V	2.991372	4.488008
425	V	3.016174	4.552240
426	V	3.067436	4.693464
427	V	3.094534	4.674289
428	V	3.114799	4.768585
429	V	3.121913	5.627779

430	V	3.140488	4.714074
431	V	3.149477	5.487921
432	V	3.166755	4.817022
433	V	3.172501	4.820985
434	V	3.197943	4.865704
435	V	3.213682	4.790011
436	V	3.259856	5.037406
437	V	3.261640	5.153593
438	V	3.281095	4.849829
439	V	3.306888	4.862349
440	V	3.324482	4.887385
441	V	3.327686	5.221439
442	V	3.342939	5.564688
443	V	3.372628	4.974206
444	V	3.389575	5.233553
445	V	3.415933	5.074957
446	V	3.425004	5.034067
447	V	3.462415	5.063394
448	V	3.476825	5.175741
449	V	3.489334	5.042381
450	V	3.539770	5.104295
451	V	3.585923	5.291462
452	V	3.593422	5.420133
453	V	3.708272	5.506193
454	V	3.772500	5.587085
455	V	3.876160	6.061448
456	V	3.905077	5.798303
457	V	4.133373	10.152941
458	V	4.165906	10.460423
459	V	4.200451	10.395175
460	V	4.225175	10.257109
461	V	4.230453	10.142541
462	V	4.268106	10.121021
463	V	4.285284	10.156843
464	V	4.311727	10.756122
465	V	4.321938	10.353393
466	V	4.376555	13.053158
467	V	4.408313	11.020224
468	V	4.427412	10.084434
469	V	4.435421	10.609085
470	V	4.446638	10.830693
471	V	4.480472	10.610598
472	V	4.533359	10.684896
473	V	4.546541	10.230463
474	V	4.584856	10.121734
475	V	4.595566	10.867163
476	V	4.644924	10.502352
477	V	4.705044	11.202757
478	V	4.742111	10.461539
479	V	4.745732	10.698559
480	V	4.849236	10.574371
481	V	4.952985	10.828192
482	V	5.072278	10.656536
483	V	5.281112	13.094507
484	V	5.977484	15.403289

Orbital energies and kinetic energies (beta):

		1	2
1	O	-101.471533	136.907098
2	O	-24.626089	37.081440
3	O	-24.616758	37.083252

4	O	-24.616755	37.082605
5	O	-19.070481	29.024448
6	O	-18.946181	29.028929
7	O	-14.272916	21.956694
8	O	-14.177357	21.961852
9	O	-10.329784	15.902286
10	O	-10.170355	15.883653
11	O	-10.150598	15.885501
12	O	-10.141671	15.885900
13	O	-10.135366	15.884881
14	O	-10.124992	15.884820
15	O	-10.120488	15.883675
16	O	-10.119456	15.879481
17	O	-10.119451	15.880514
18	O	-10.112687	15.880509
19	O	-10.112682	15.881566
20	O	-10.099890	15.887899
21	O	-10.087653	15.883650
22	O	-10.069133	15.880426
23	O	-10.066305	15.881473
24	O	-10.061576	15.879547
25	O	-10.058569	15.881749
26	O	-10.057162	15.879481
27	O	-10.055351	15.881550
28	O	-10.044269	15.884038
29	O	-9.387761	21.547686
30	O	-7.151513	20.529701
31	O	-7.142123	20.555113
32	O	-7.141913	20.550255
33	O	-1.195023	3.277450
34	O	-1.111161	3.833169
35	O	-1.102781	3.841359
36	O	-0.953614	2.516691
37	O	-0.876210	1.832186
38	O	-0.837401	2.531822
39	O	-0.806264	2.040807
40	O	-0.790238	1.870591
41	O	-0.749212	2.112835
42	O	-0.714761	1.624807
43	O	-0.685310	1.868013
44	O	-0.673559	1.611267
45	O	-0.663753	1.777924
46	O	-0.645883	1.826392
47	O	-0.631461	1.743303
48	O	-0.618559	1.866033
49	O	-0.593537	2.273782
50	O	-0.580201	1.710199
51	O	-0.538523	1.460717
52	O	-0.536647	2.016221
53	O	-0.521684	1.777313
54	O	-0.508686	1.712624
55	O	-0.487900	1.885327
56	O	-0.475148	2.565220
57	O	-0.473144	2.768690
58	O	-0.469963	1.382446
59	O	-0.455173	1.522873
60	O	-0.438975	1.845544
61	O	-0.413952	1.755088
62	O	-0.408731	1.429714
63	O	-0.396523	1.623002

64	O	-0.393921	1.429593
65	O	-0.376890	1.619922
66	O	-0.370614	1.638014
67	O	-0.369545	1.195699
68	O	-0.359106	1.570371
69	O	-0.357192	1.831147
70	O	-0.353867	2.922092
71	O	-0.351423	2.735105
72	O	-0.348736	1.405527
73	O	-0.325478	1.729624
74	O	-0.316938	2.528585
75	O	-0.315276	3.027801
76	O	-0.309510	1.609170
77	O	-0.305824	1.501182
78	O	-0.302636	1.993925
79	O	-0.301197	1.535482
80	O	-0.294421	3.492055
81	O	-0.293131	1.636711
82	O	-0.284854	2.269875
83	O	-0.280289	1.725130
84	O	-0.277556	1.307694
85	O	-0.270067	1.626343
86	O	-0.259613	1.259024
87	O	-0.254878	1.675473
88	O	-0.246270	1.901128
89	O	-0.236132	2.299663
90	O	-0.235291	2.104258
91	O	-0.233165	1.857053
92	O	-0.228817	1.447111
93	O	-0.213969	1.769069
94	O	-0.213360	1.483009
95	O	-0.178035	1.349241
96	O	-0.173025	1.244772
97	O	-0.160986	1.560569
98	O	-0.151285	1.226140
99	O	-0.125088	1.903862
100	O	-0.118654	1.427384
101	O	-0.088725	1.580334
102	O	-0.082932	2.322890
103	O	-0.070331	1.581905
104	V	0.068372	1.598954
105	V	0.073393	1.538990
106	V	0.075612	1.381632
107	V	0.104919	2.102963
108	V	0.110457	1.622251
109	V	0.124808	1.692910
110	V	0.164913	1.526424
111	V	0.187584	1.034629
112	V	0.198746	1.485430
113	V	0.198750	1.727285
114	V	0.212918	1.590340
115	V	0.220220	0.983937
116	V	0.223121	2.396753
117	V	0.228319	2.040730
118	V	0.235093	1.021618
119	V	0.246138	1.148013
120	V	0.248781	1.569268
121	V	0.253815	1.084222
122	V	0.259257	1.028179
123	V	0.263306	1.639220

124	V	0.271308	1.357674
125	V	0.276737	2.103056
126	V	0.298044	1.481165
127	V	0.303529	1.221493
128	V	0.312176	2.130494
129	V	0.315017	2.640574
130	V	0.319584	3.606261
131	V	0.339886	2.465804
132	V	0.350666	2.076869
133	V	0.356412	2.269715
134	V	0.360146	1.920262
135	V	0.369318	1.519292
136	V	0.370168	1.862543
137	V	0.376663	1.990690
138	V	0.389323	2.007857
139	V	0.410924	2.446848
140	V	0.417463	2.425670
141	V	0.417696	1.925954
142	V	0.431373	1.832661
143	V	0.435961	2.054669
144	V	0.460694	2.191584
145	V	0.470240	2.360512
146	V	0.479624	2.507536
147	V	0.482382	2.315358
148	V	0.492899	2.351949
149	V	0.504444	2.103484
150	V	0.516533	2.176747
151	V	0.519370	2.594721
152	V	0.536865	2.191507
153	V	0.546963	2.212347
154	V	0.555853	2.065871
155	V	0.557433	2.139026
156	V	0.573297	2.215616
157	V	0.585419	2.326744
158	V	0.597395	2.340834
159	V	0.605045	2.371111
160	V	0.608644	2.192768
161	V	0.618591	1.974017
162	V	0.625843	1.871809
163	V	0.633169	2.389446
164	V	0.633559	1.976421
165	V	0.636732	2.552558
166	V	0.637958	2.203821
167	V	0.647416	2.248071
168	V	0.655474	2.515207
169	V	0.655948	2.053397
170	V	0.665684	2.246651
171	V	0.669524	1.933034
172	V	0.673009	2.192981
173	V	0.673924	2.142979
174	V	0.675403	2.141915
175	V	0.688862	2.115708
176	V	0.689365	2.243951
177	V	0.693508	2.578521
178	V	0.700856	2.270816
179	V	0.701082	2.481167
180	V	0.707358	2.183980
181	V	0.725481	2.345298
182	V	0.726920	2.321989
183	V	0.733162	2.272240

184	V	0.736344	2.248013
185	V	0.739129	2.374363
186	V	0.746433	2.265123
187	V	0.759815	2.152052
188	V	0.769869	2.257803
189	V	0.771953	2.375526
190	V	0.777835	2.741780
191	V	0.798112	2.805072
192	V	0.809049	2.214129
193	V	0.809762	2.578707
194	V	0.825404	2.263410
195	V	0.825709	2.538586
196	V	0.831341	2.322472
197	V	0.838096	2.472842
198	V	0.842917	2.918566
199	V	0.859223	2.276999
200	V	0.867009	2.444536
201	V	0.880079	2.262671
202	V	0.886517	2.779985
203	V	0.894528	2.585664
204	V	0.907018	2.379417
205	V	0.916456	2.618555
206	V	0.917857	2.587037
207	V	0.924286	2.462640
208	V	0.928223	2.591885
209	V	0.931534	2.586809
210	V	0.939779	2.673538
211	V	0.943840	2.372058
212	V	0.949876	2.597744
213	V	0.950857	2.566849
214	V	0.953341	2.492115
215	V	0.961449	2.374553
216	V	0.968571	2.704418
217	V	0.976913	2.591268
218	V	0.979914	2.566045
219	V	0.991275	2.535431
220	V	1.006736	2.791800
221	V	1.007374	2.538160
222	V	1.010451	2.494752
223	V	1.012578	2.711994
224	V	1.021076	2.488382
225	V	1.040853	2.459580
226	V	1.043106	2.586968
227	V	1.067855	2.536025
228	V	1.080258	2.548790
229	V	1.086790	2.719349
230	V	1.087852	2.411009
231	V	1.092260	2.571712
232	V	1.112509	2.545482
233	V	1.118496	2.498738
234	V	1.126740	2.857586
235	V	1.134159	2.527642
236	V	1.137038	3.345734
237	V	1.145534	2.590123
238	V	1.156254	2.596387
239	V	1.166789	2.840349
240	V	1.173822	2.729434
241	V	1.188402	2.517459
242	V	1.198320	3.358881
243	V	1.204661	3.341961

244	V	1.215847	2.972754
245	V	1.230336	2.454898
246	V	1.240792	3.048928
247	V	1.254260	2.882771
248	V	1.256464	2.745689
249	V	1.277564	2.807434
250	V	1.284733	2.606620
251	V	1.290090	3.024723
252	V	1.298821	2.774310
253	V	1.312542	2.711092
254	V	1.318536	2.411380
255	V	1.343623	2.731529
256	V	1.349926	2.445690
257	V	1.350575	2.624636
258	V	1.364999	2.411296
259	V	1.365247	2.839674
260	V	1.384484	3.060138
261	V	1.401382	2.560922
262	V	1.411366	3.128482
263	V	1.418265	3.083001
264	V	1.429799	2.754341
265	V	1.431722	3.423210
266	V	1.432692	2.607036
267	V	1.437499	2.552988
268	V	1.463531	2.778774
269	V	1.470267	3.484722
270	V	1.472342	2.622095
271	V	1.482111	2.516637
272	V	1.482835	2.773581
273	V	1.483264	2.919127
274	V	1.497453	2.618326
275	V	1.500622	2.941288
276	V	1.503390	3.137601
277	V	1.514564	2.671373
278	V	1.520396	2.545329
279	V	1.528599	3.061394
280	V	1.529926	2.545198
281	V	1.540665	2.682694
282	V	1.558261	3.438894
283	V	1.558450	2.557004
284	V	1.561851	3.042407
285	V	1.566322	2.830957
286	V	1.578314	2.978366
287	V	1.606708	3.060120
288	V	1.609050	2.625760
289	V	1.613833	2.894175
290	V	1.621599	2.774326
291	V	1.646067	2.915081
292	V	1.693956	3.169060
293	V	1.700452	3.390047
294	V	1.711701	2.889764
295	V	1.749486	2.977620
296	V	1.752022	2.839378
297	V	1.764640	2.938846
298	V	1.808708	3.081519
299	V	1.819959	2.961335
300	V	1.824108	2.996981
301	V	1.835867	3.231564
302	V	1.853433	3.183872
303	V	1.855731	2.976535

304	V	1.877858	3.086824
305	V	1.885918	3.204597
306	V	1.903297	2.872131
307	V	1.904218	3.290265
308	V	1.910686	3.218933
309	V	1.918482	3.207232
310	V	1.921995	3.198773
311	V	1.927439	3.268654
312	V	1.945980	2.976343
313	V	1.950736	2.918317
314	V	1.952686	3.162108
315	V	1.960790	3.176964
316	V	1.960956	2.911192
317	V	1.966470	3.181141
318	V	1.980290	3.254593
319	V	1.984401	2.958162
320	V	1.994734	2.917065
321	V	1.994881	3.179234
322	V	2.005968	3.315540
323	V	2.009808	3.268499
324	V	2.020530	3.256564
325	V	2.023729	3.037973
326	V	2.027588	3.268106
327	V	2.041807	3.322034
328	V	2.054107	3.114305
329	V	2.055291	3.180560
330	V	2.061510	3.306819
331	V	2.068404	3.537258
332	V	2.072916	3.566657
333	V	2.077690	3.068322
334	V	2.082718	3.106935
335	V	2.090307	3.510357
336	V	2.093690	3.504020
337	V	2.105535	3.610364
338	V	2.109641	3.453411
339	V	2.109954	2.895926
340	V	2.114586	3.516762
341	V	2.123745	3.524467
342	V	2.128344	3.407729
343	V	2.133758	3.099073
344	V	2.141024	3.475102
345	V	2.156074	3.182650
346	V	2.157684	3.882549
347	V	2.170666	3.635064
348	V	2.178445	3.520622
349	V	2.178819	3.547277
350	V	2.188602	3.437631
351	V	2.204413	3.530968
352	V	2.210212	3.218053
353	V	2.224640	3.491285
354	V	2.233106	3.468514
355	V	2.243654	3.434954
356	V	2.251570	3.597573
357	V	2.272657	3.521942
358	V	2.295696	3.840318
359	V	2.310363	3.602934
360	V	2.327107	3.458603
361	V	2.338024	3.714329
362	V	2.367507	3.436672
363	V	2.375650	3.484677

364	V	2.378709	3.834300
365	V	2.391004	3.494444
366	V	2.402230	3.477045
367	V	2.409248	3.688532
368	V	2.423621	3.676573
369	V	2.436203	3.507300
370	V	2.450957	3.954652
371	V	2.457312	3.544644
372	V	2.481966	3.815535
373	V	2.486390	3.853919
374	V	2.489653	3.390611
375	V	2.491483	3.527129
376	V	2.507471	3.871044
377	V	2.511210	3.758072
378	V	2.520810	3.820929
379	V	2.522802	3.881224
380	V	2.536507	3.878099
381	V	2.540059	3.780183
382	V	2.553018	3.704233
383	V	2.554905	3.582501
384	V	2.575709	3.886376
385	V	2.587556	3.551194
386	V	2.595406	3.991675
387	V	2.611322	3.951670
388	V	2.611556	3.758050
389	V	2.627126	3.976846
390	V	2.631495	4.055870
391	V	2.634782	3.566729
392	V	2.651399	3.995921
393	V	2.668952	3.944654
394	V	2.669808	3.745519
395	V	2.682330	3.669523
396	V	2.683951	3.681010
397	V	2.692541	4.145158
398	V	2.703767	3.696792
399	V	2.730501	3.935370
400	V	2.739775	3.813202
401	V	2.739913	3.862253
402	V	2.753188	3.991408
403	V	2.767613	3.960147
404	V	2.785536	3.924782
405	V	2.789023	3.897203
406	V	2.793585	4.149055
407	V	2.797392	3.906239
408	V	2.809707	4.197489
409	V	2.827916	4.269327
410	V	2.845195	4.137974
411	V	2.848868	4.107129
412	V	2.862555	4.363143
413	V	2.878438	4.296707
414	V	2.885926	4.010495
415	V	2.888045	4.292749
416	V	2.893800	4.098383
417	V	2.898196	4.412993
418	V	2.910056	4.374897
419	V	2.925113	3.900893
420	V	2.929299	4.356578
421	V	2.948324	4.387946
422	V	2.967061	4.541686
423	V	2.977042	4.564554

424	V	2.991870	4.486199
425	V	3.018500	4.557306
426	V	3.068962	4.695484
427	V	3.096576	4.683711
428	V	3.115900	4.745933
429	V	3.122541	5.627149
430	V	3.141657	4.712809
431	V	3.150438	5.485821
432	V	3.168326	4.807416
433	V	3.173615	4.843242
434	V	3.199713	4.861112
435	V	3.214321	4.790638
436	V	3.260321	4.979448
437	V	3.262066	5.213645
438	V	3.281917	4.844992
439	V	3.307520	4.860630
440	V	3.324479	4.887388
441	V	3.328887	5.239726
442	V	3.343800	5.550981
443	V	3.372675	4.974137
444	V	3.390023	5.232250
445	V	3.416032	5.075351
446	V	3.425401	5.034413
447	V	3.462937	5.063661
448	V	3.478064	5.175346
449	V	3.489359	5.042394
450	V	3.539976	5.104228
451	V	3.586706	5.290819
452	V	3.593416	5.420123
453	V	3.708931	5.506019
454	V	3.773840	5.585821
455	V	3.876192	6.061362
456	V	3.906075	5.797699
457	V	4.136860	10.156602
458	V	4.166013	10.457629
459	V	4.201332	10.397581
460	V	4.225208	10.256572
461	V	4.232610	10.142555
462	V	4.271077	10.124025
463	V	4.287962	10.158621
464	V	4.312186	10.782863
465	V	4.323636	10.327954
466	V	4.376653	13.050537
467	V	4.408574	11.018465
468	V	4.431163	10.140955
469	V	4.437032	10.597723
470	V	4.448799	10.785593
471	V	4.481546	10.610691
472	V	4.533658	10.680651
473	V	4.546768	10.231845
474	V	4.587464	10.122814
475	V	4.595696	10.869472
476	V	4.645401	10.501072
477	V	4.707160	11.198903
478	V	4.746168	10.411933
479	V	4.748118	10.749778
480	V	4.849930	10.577507
481	V	4.954879	10.833006
482	V	5.074398	10.657213
483	V	5.281332	13.094650

484 V 5.977762 15.402918
Total kinetic energy from orbitals= 1.776249909581D+03
1\1\GINC-COPERNICO\FOpt\UB3LYP\6-31G(d,p)\C20H12Cl1F3N2O2(1-,2)\IVAN\2
0-Oct-2021\0\\# opt b3lyp/6-31g(d,p) geom=connectivity pop=full\\A15MO
D_RADICALNEGATIVO\\-1,2\C,4.3095117351,1.8675087827,-0.0004531002\C,2.
9169840384,1.7281346246,-0.0004770801\C,2.29712271,0.4690972338,-0.000
2150156\C,3.1290914314,-0.7077406935,0.0000938239\C,4.5336604977,-0.54
8775785,0.000118525\C,5.1131471213,0.716882474,-0.0001532911\C,2.47590
19997,-1.9636974743,0.0003659003\C,1.0783825213,-2.0405398163,0.000311
6259\C,0.3631632928,-0.8025276538,-0.0000330682\C,-1.7349558298,-2.050
636587,0.0001153253\C,-1.0523205092,-3.2391479542,0.0004472322\C,0.389
0236996,-3.3299424957,0.00062445\H,2.276888153,2.605578359,-0.00070663
54\H,5.1800136625,-1.4218056138,0.0003504856\H,3.0330262614,-2.8945771
613,0.00063628\H,-1.6081264094,-4.1675890262,0.0005316811\C,-1.7255809
418,0.4410351359,-0.0000050376\C,-2.0521113777,1.0627563041,1.20602577
09\C,-2.0517572706,1.0631355468,-1.2059357824\C,-2.7067752766,2.293132
1475,1.2151077318\H,-1.787850915,0.5766886536,2.1384191178\C,-2.706410
6838,2.293515455,-1.2148219203\H,-1.7872214487,0.5773557208,-2.1383990
072\C,-3.0265434763,2.8941263024,0.0001908065\H,-2.963382613,2.7793290
957,2.1496401047\H,-2.9627371069,2.780009567,-2.1492765095\C,-3.226009
1132,-2.0334440911,-0.0003126564\N,-1.0470583109,-0.8258336567,-0.0001
034371\F,-3.7423211795,-3.2825697746,-0.0003706425\F,-3.7649840247,-1.
4012320041,1.0854224772\F,-3.7643020822,-1.4013705623,-1.0864614146\N,
0.9224497224,0.3971576866,-0.0002682563\O,1.0009017392,-4.4276430071,0
.0010138017\H,4.7460185395,2.8597706906,-0.0006680621\C,7.1286373308,2
.0018301998,-0.0003457067\H,6.8734699858,2.5944139326,-0.8914517218\H,
6.8733801513,2.5947985264,0.8904784619\H,8.2051231971,1.8099915343,-0.
0002509942\O,6.4994668932,0.7423619416,-0.0001042065\Cl,-3.8609641142,
4.455198442,0.0003109443\\Version=AM64L-G09RevD.01\State=2-A\HF=-1789.
0867273\S2=0.764916\S2-1=0.\S2A=0.75018\RMSD=7.764e-09\RMSF=3.247e-05\
Dipole=-1.2550216,2.8457604,-0.0005203\Quadrupole=-10.3695872,-14.9513
885,25.3209758,11.3731281,-0.0032628,0.004184\PG=C01 [X(C20H12Cl1F3N2O 2)]\\@

VII.2. Output for the phenol species

VII.2.1. PICRIC ACID

VII.2.1.1. *Neutral form of Picric acid*

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C6H3N3O7|PCUSER|11-Aug-2020|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||2,4,6-trinitrofenol||0,1| C, 0.4340992585,-0.8154406911,1.1765504282| C,0.1016228185,0.5342240419,1.1953195932| C,-0.3059289323, 1.2472201768, 0.0238616241| C,-0.3525318778, 0.4858611069, -1.1793703066| C, -0.0217375206, -0.8590758162,-1.2006630178| C,0.3676481917,-1.4966285056,-0.0261299571| H, 0.7375425009, -1.3169582301, 2.0860063048| H, -0.069692823, -1.4029295306, 2.1348885462| O, -0.619174114, 2.5233080808,0.0469890544|H,-0.5090414454,2.8245279354, 0.9895696035| N, 0.1837033728, 1.2178671718, 2.4810609819| O, 0.533976223, 0.586363212, 3.4640682808| O, -0.1114794152, 2.4335527694, 2.5204189869| N, -0.7555028526,1.08511502, -2.4717863715| N,0.7160123723, -2.9243169256, -0.0629146476| O, -1.0554246516, 2.2712676356, -2.4947965839| O, 1.0542405099, -3.4473646241, 0.9964147322| O,-0.7597129204, 0.3336831935, -3.4464652967| O, 0.6441581047, -3.4923426326, -1.1494563346|| Version=x86-Win32-G03RevB.03| State=1-A| HF=-920.9633765| RMSD=7.718e-009| RMSF=3.850e-005| Dipole= 0.0491597, 0.336219, 0.676167| PG=C01 [X(C6H3N3O7)]||@

VII.2.1.2. *Neutral radical of deprotonated picric acid*

1\1\GINC-COPERNICO\FOpt\UB3LYP\6-31G(d,p)\C6H2N3O7(2)\IVAN\20-May-2021 \0\\# opt b3lyp/6-31g(d,p) geom=connectivity\\2,4,6-trinitrofenolradical\\ 0,2\ C, 0.753680533,-1.3020491708, -0.000011651\ C, -0.6191489554, -1.1314968216, -0.0000083881\ C,-1.2405420529, 0.1499490372, -0.0000009607\ C, -0.3441534066, 1.2566138807, 0.0000114011\ C, 1.0314629244, 1.1103346763, 0.000008567\ C, 1.5688548198, -0.1737529421, -0.0000039393\ H, 1.1773193597, -2.299097242, -0.0000186521\ H, 1.6707023467, 1.9849492464, 0.0000149817\ O, -2.5207940444, 0.2972838549, 0.000029274\ N, -1.5018540576, -2.2831832484, -0.000015181\ O, -1.0087656702, -3.405544741, 0.0000100196\ O, -2.7180054138, -2.0410169078, -0.0000159877\ N, -0.9415045543, 2.5792371005, 0.0000267505\ N, 3.027062534, -0.3416766687, -0.0000066866\ O, -2.1806855438, 2.6203314256, -0.000017975\ O, 3.4597179537, -1.4917233624, -0.0000211004\ O, -0.2055814313, 3.5597009199, 0.0000304827\ O, 3.7098246587, 0.679905963, -0.0000039547\\ Version=AM64L-G09RevD.01\ State=2-A\ HF= -920.2913797\ S2=0.756852\ S2-1=0.\ S2A=0.75004\ RMSD=9.877e-09\ RMSF=3.165e-05\ Dipole =0.1852814, -0.0227185, 0.0000015\ Quadrupole =-8.7528324,-2.5820704,11.3349028,0.7222812, 0.0000195, 0.0000848\ PG=C01 [X(C6H2N3O7)]\\@

VII.2.1.3. *Picrate anion*

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C6H2N3O7(1-)|PCUSER|12-Aug-2020|0| |# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||2,4,6-trinitrofenoxi||-1,1| C,0.6623339596, -1.2992282554, 0.0000180034| C, -0.7068996793, -1.1577727452, 0.0000314525| C,-1.4020179654, 0.1612487061,0.000084227|C,-0.4255188547, 1.2880335016, 0.0000599358| C, 0.9399809337, 1.1143024704, 0.0000250801| C, 1.4906316014, -0.1717594759, 0.0000083234| H, 1.0959675339, -2.2894375867, 0.0000019257| H, 1.587364547, 1.9800769403, 0.0000096943| O, -2.6204355125, 0.301226308, 0.0001875547| N, -1.4690928098, -2.4033584108, -0.0000037112| O, -0.8313935206, -3.4734240244, 0.0003268927| O, -2.6988307972, -2.3636362516, -0.000447013| N, -0.88400985, 2.6745385873, 0.0000714502| N, 2.9179809792, -0.3358886516, -0.0000302896| O, -2.0903950566, 2.9160362639, -0.0001594382| O, 3.3810295609, -1.4880727378, -0.0000657811| O, -0.0190874764, 3.5709536607, 0.0000071762| O, 3.6305452664, 0.6810886265, -0.0000538787|| Version=x86-Win32-G03RevB.03| State=1-A| HF=-920.4523797| RMSD=8.689e-009| RMSF=6.234e-005| Dipole =0.8770828, -0.1005304, 0.0000946| PG=C01 [X(C6H2N3O7)]||@

VII.2.2. 2,4-DINITROPHENOL

VII.2.2.1. *Neutral form of* 2,4-dinitrophenol

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C6H4N2O5|PCUSER|16-Aug-2020|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||AB|| 0,1| C, -0.6353252088, -1.1128308322, 0.5336648949| C, 0.5434757292, -0.5228584689, 0.1024357401| C, 0.511838252, 0.7773972051, -0.3892727668| C, -0.7041658001, 1.4939574842, -0.4735526213| C, -1.8791161056, 0.853798246, -0.03627697| C, -1.8536328549, -0.4346788066, 0.4696359839| H, 1.4813691796, -1.0600873329, 0.1419541381| H, -2.8220456389, 1.3904675704, -0.1006405121| H, -2.7553877186, -0.9265949067, 0.8117271089| N, 1.796222285, 1.3627613973, -0.8073048012| N, -0.5999771423, -2.4793578011, 1.0652409704| O, -0.7309961699, 2.7349250651, -0.9857879617| H, -1.6452170518, 3.0524759945, -1.0091743713| O, 0.4907238547, -3.0445674502, 1.1138634759| O, 1.8873991287, 2.5852214701, -0.8463665504| O, 2.7048242333, 0.5750991826, -1.0716798447| O, -1.6683109018, -2.9717777007, 1.4288177418|| Version=x86-Win32-G03RevB.03| State=1-A| HF=-716.4655787| RMSD=4.557e-009| RMSF=1.085e-005| Dipole =-2.0633156, 1.202169, -0.1823291| PG=C01 [X(C6H4N2O5)]||@

VII.2.2.2. *Neutral Radical of deprotonated 2,4-dinitrophenol*

1|1|UNPC-UNK|FOpt|UB3LYP|6-31G(d,p)|C6H3N2O5(2)|PCUSER|27-May-2021|0||#T B3LYP/6-31G(D,P) FOPT TEST||hydrazide Single Point|| 0,2| C, -1.9192277158, 0.0432310185, -0.4975491833| C, -1.9240659311, 0.0714130021, 0.8770912267| C, -0.6846274184, 0.0104850339, -1.1691430156| C, 0.5514553013, 0.0021545874, -0.5019995114| C, -0.6910972532, 0.0649382923, 1.6543345609| C, 0.548702785, 0.0023055295, 0.8698070419| H, -2.8465741667, 0.1205093163, 1.4451146209| N, -0.6802851381, -0.0128239627, -2.6423305706| H, -2.8321676204, 0.0514874477, -1.07972086| O, -0.7079768462, 0.1575760313, 2.8956184756| H, 1.4759428593, -0.0073546399, -1.06544255| N, 1.8406911639, -0.0697131055, 1.5612531428| O, 2.7511160355, 0.6186590567, 1.1019931226| O, 1.9144962514, -0.8265438134, 2.5203393496| O, -1.7717839049, 0.0121277259, -3.2072595348| O, 0.4132882317, -0.0560749292, -3.2016484044|| Version=x86-Win32-G03RevB.01| State=2-A| HF=-715.8120406| S2=0.792849| S2-1=0.| S2A=0.751298| RMSD=6.257e-009| RMSF=1.510e-005| Dipole= -1.3216093, 0.0035059, -0.3317115| PG=C01 [X(C6H3N2O5)]||@

VII.2.2.3. *2,4-Dinitrophenolate anion*

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C6H3N2O5(1-)|PCUSER|16-Aug-2020|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||ABion||-1,1| C, -1.3618046993, 0.1684042695, 0.0001953007| C, -0.2498854708, -0.6709096134, -0.0017115305| C, 1.0341771439,-0.1460741359, -0.0042217818| C, 1.2984967391, 1.3078401613, -0.0389866175| C, 0.0674616081, 2.1082340439, -0.0362267655| C, -1.1883575552, 1.5802059347, -0.0154872688| H, -0.3848477505, -1.7437393247, 0.0061165108| H, 0.2227122575, 3.1832577775, -0.054083218| H, -2.0729804572, 2.2066801776, -0.0121243562| N, 2.1175705758, -1.1057202855, 0.0200469266| N, -2.6738881747, -0.3892807395, 0.0241662421| O, 2.4118098074, 1.850400716, -0.0928625724| O, -2.8087560338, -1.6277401431, 0.0433980927| O, 3.2528912306, -0.7241307826, 0.3195045426| O, 1.8601682859, -2.2960642081, -0.2529284745| O, -3.6500117216, 0.3891099909, 0.0240422695|| Version=x86-Win32-G03RevB.03| State=1-A| HF= -715.9501459| RMSD=8.023e-009| RMSF=1.051e-005| Dipole =-0.8348538, 0.5126068, 0.0274792| PG=C01 [X(C6H3N2O5)]||@

VII.2.3. 4-NITROPHENOL

VII.2.3.1. *Neutral form of 4-nitrophenol*

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C6H5N1O3|PCUSER|01-Aug-2020|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY|| 4nitrofenol|| 0,1| C, 0.0818964438, -1.1920025941, -0.2086202527| C, 1.4638038227, -1.070129701, -0.27941993| C, 2.0662174394, 0.1848390866, -0.1052372663| C, 1.2782062521, 1.3198987951, 0.140432105|C,-0.1011343377, 1.1998722801, 0.2110814227| C, -0.6879163144, -0.0558138262, 0.0360122467| H, -0.4094120807, -2.147804012, -0.3389805949| H ,2.0773030302, -1.9472524515, -0.4694313411| H, 1.7671422683, 2.2786019086, 0.2714026491| H, -0.7341240691, 2.057754512, 0.3990794556| O, 3.4099591409, 0.365881951, -0.1630881847| H, 3.8463926569, -0.4792838031, -0.3362589826| N, -2.1429056475, -0.1829925873, 0.1106444628| O, -2.7982382317, 0.8380060847, 0.3274791358| O, -2.6308961727, -1.3040195716, -0.0476174983|| Version=x86-Win32-G03RevB.03| State=1-A| HF= -511.9810078| RMSD=2.925e-009| RMSF=2.900e-005| Dipole =2.0622459, -0.3485203, -0.1960645| PG=C01 [X(C6H5N1O3)]||@

VII.2.3.2. *Neutral radical of deprotonated 4-nitrophenol*

1\1\GINC-COPERNICO\FOpt\UB3LYP\6-31G(d,p)\C6H4N1O3(2)\IVAN\20-May-2021 \0\\# opt b3lyp/6-31g(d,p) geom=connectivity\\4-nitrofenolradical\\ 0,2 \ C, 1.1791287473, 1.9586890133,0.1761445348\ C, 2.5521661508,2.0245516974,0.1703609359\ C, 3.2438085421, 3.293939274, 0.3452574063\ C, 2.4240120401, 4.4837837683, 0.525288496\ C, 1.0516027768, 4.4051009812, 0.5292813443\ C, 0.4451041276, 3.1466247183, 0.3551278888\ H, 0.6426982641, 1.0268832518, 0.0482012784\ H, 3.1657977796, 1.1402318987, 0.0361724052\ H, 2.9423348846, 5.427705649, 0.6553845732\ H, 0.4213095059, 5.2755457928, 0.6613519823\ O, 4.4957434572, 3.3598284616, 0.340809973\ N, -1.0229970468, 3.0693561667, 0.3603551548\ O, -1.6468587293, 4.1188692246, 0.5175556074\ O, -1.53412032, 1.9598544422, 0.2071876394\\ Version=AM64L-G09RevD.01\ State=2-A\ HF=-511.3308801\ S2=0.792482\ S2-1=0.\ S2A=0.751254\ RMSD=6.950e-09\ RMSF=3.678e-05\ Dipole=0.3738307, 0.0199784, -0.0013543\ Quadrupole=-11.9561502, 7.6804987, 4.2756516, -1.0355358,0.0305228,0.5138105\ PG=C01 [X(C6H4N1O3)]\\@

VII.2.3.3. *4-Nitrophenolate anion*

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C6H4N1O3(1-)|PCUSER|06-Aug-2020|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||4nitrofenoxido|| -1,1| C, 0.1137651974,-

1.2069145015, 0.1657290927| C, 1.483177623, -1.139297706, 0.1612500771| C, 2.2103915442, 0.115376738, -0.0079234382| C,1.3554455409,1.2873601844,-0.1717796587|C,-0.0136050865, 1.2120682871, -0.166289707| C,-0.6648240273, -0.0346745632, 0.0023654898| H, -0.4087001614, -2.1490223233, 0.2930204813| H, 2.084292847,-2.037044535, 0.2863749184| H, 1.8587738373, 2.2428144048, -0.301040571|H,-0.632083679,2.0947025905,-0.2894811176| O, 3.4620281836, 0.1805638332, -0.0123632814| N, -2.0741448869, -0.1081777, 0.0075403261| O, -2.6295237064, -1.2232616532, 0.1587120964| O, -2.7436761505, 0.9429832113, -0.139069706|| Version=x86-Win32-G03RevB.03| State=1-A| HF=-511.4375775| RMSD=3.208e-009| RMSF=1.660e-005| Dipole= -0.3519237, -0.018298, 0.0010795| PG=C01 [X(C6H4N1O3)]||@

VII.2.4. 3-NITROPHENOL

VII.2.4.1. *Neutral form of 3-nitrophenol*

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C6H5N1O3|PCUSER|18-Jan-2021|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY|| 3-nitrofenol|| 0,1| C, -0.0738346231, -0.1263757884, 1.7937112504| C, -0.1015284921, -0.7723854322, 0.5548497829| C, 0.0201084337, 0.0009329275, -0.5932183178| C, 0.1681676076, 1.3868041688, -0.5648138182| C, 0.1932359087, 2.0099040558, 0.6800683199| C, 0.0736742467, 1.2654726628, 1.8543602531| H, -0.2145990823,-1.8462503762,0.4904306014| H, 0.2582892645, 1.938530863, -1.4906061241| H, 0.3071011827, 3.0873941277 , 0.7406187883| H, 0.0947630375, 1.7651264924, 2.8201152468| O, -0.1957835211, -0.9073850679, 2.9024652242| H, -0.1628571016, -0.353917992, 3.6938587209| N, -0.0093190894, -0.6825666732, -1.9007130284| O, 0.0984449496, 0.0132237688, -2.9097409099| O, -0.139711699, -1.905717697, -1.9051206714|| Version=x86-Win32-G03RevB.03| State=1-A| HF=-511.9778812| RMSD=7.065e-009| RMSF=3.203e-005| Dipole =0.0661595, 1.2184727, 1.9287583| PG=C01 [X(C6H5N1O3)]||@

VII.2.4.2. *Neutral radical of deprotonated 3-nitrophenol*

1\1\GINC-COPERNICO\FOpt\UB3LYP\6-31G(d,p)\C6H4N1O3(2)\IVAN\12-May-2021\0\\# opt b3lyp/6-31g(d,p) geom=connectivity\\3-nitrofenolradical\\0,2\ C, 1.7721709688,-0.5154014737, 0.0000617771\ C, 0.3699758307, -0.8920930298, -0.0000332732\ C, -0.5902790553, 0.0926401118, -0.0000500142\ C,-0.2725661227,1.4614631824,-0.0000690023\ C, 1.0785645685,1.8509115418,-0.000157613\ C, 2.0811359715,0.903164265,-0.0001411054\

H, 0.1042880983, -1.9415555792, -0.0000587977\ H, -1.0754668752, 2.1875951331,-0.0000534955\ H, 1.3222075616, 2.9084900233, -0.0002342583\ H, 3.1308103088, 1.1774101612, -0.0002255609\ O, 2.6772367965, -1.3878652474, -0.0000221857\ N, -2.0191531139, -0.2955034075, -0.0000083657\ O, -2.8496083315, 0.6113817439, 0.000238773\ O, -2.2813346061, -1.4945764249,-0.0001958782\\Version=AM64L-G09RevD.01\State=2- A\ HF=-511.3301508\ S2=0.79235\S2-1=0.\S2A=0.751246\ RMSD=7.835e-09\RMSF= 3.717e-05\ Dipole=0.6144154, 1.3611018, -0.0000692\Quadrupole=-7.1942145, 4.0520518, 3.1421627, 4.0400166, 0.0002738, -0.000814\ PG=C01 [X(C6H4N1O3)]\\@

VII.2.4.3. *3-Nitrophenolate anion*

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C6H4N1O3(1-)|PCUSER|18-Jan-2021|0||#OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||3-nitrofenolato||-1,1|C, 1.8512081567,-0.5658157328, 0.0000696206| C, 0.4371600774, -0.8930966038, -0.0000080386| C,-0.5362364589,0.0976878965,-0.0000430647| C,-0.2501171759,1.4726135287,-0.0000560073| C, 1.105208662, 1.8193784319, -0.0000709384| C, 2.1122279335, 0.8631928566,-0.0000377281| H, 0.1483862225, -1.9365950713, -0.0000280018| H, -1.0464724002, 2.2030124293, -0.0000597438| H, 1.3746771344, 2.8760187344, -0.0001209409| H, 3.1577100107, 1.1660988032, -0.0000740324| O, 2.7598461033, -1.4380691637, 0.0000383661| N, -1.9472053438, -0.30424701, - 0.0000667905| O, -2.8188503019, 0.5792429768, 0.0001901571| O, -2.2310671425, -1.5089948242, -0.0000251242|| Version=x86-Win32-G03RevB.03|State=1-A|HF=-511.4193568| RMSD=4.912e-009|RMSF =5.832e-005| Dipole= -0.8916494, 1.2807308, -0.000143| PG=C01 [X(C6H4N1O3)]||@

VII.2.5. 2-NITROPHENOL

VII.2.5.1. *Neutral form of 2-nitrophenol*

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C6H5N1O3|PCUSER|31-Jul-2020|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||2-nitrofenol||0,1|C, -1.5046333154, -0.2918031095,0.2434818773|C,-0.1162813007,-0.3207115647,0.0359735886| C,0.6262731739, 0.8737137587, -0.1440271054| C, -0.0777922169, 2.0913007569, -0.1074086306| C, -1.4470805247, 2.1102298448, 0.0977404218| C, -2.1718392931, 0.9181811843, 0.2749398176| H, -2.0205540789, -1.2345980675, 0.3748680736| H, 0.4914668877, 3.0037836457, -0.2451504189| H, -1.9658187466, 3.0639749163, 0.1215725965| H, -3.2438722557, 0.9448439048, 0.4349601159| O, 1.945741624, 0.9137632872,-0.3451923622| H, 2.2555077502, -0.0242707883,-0.3383929307| N, 0.5414497473, -1.6077625191,

0.0099025876| O,-0.122596545, -2.625724142, 0.167506716| O, 1.7820103051, -1.6361467952, -0.1749862744| |Version=x86-Win32-G03RevB.03| State=1-A| HF=-511.9882545| RMSD=5.465e-009| RMSF=3.831e-005| Dipole =-0.8960502, 1.0966996, 0.0726271| PG=C01 [X(C6H5N1O3)]||@

VII.2.5.2. *Neutral radical of deprotonated 2-nitrophenol*

1\1\GINC-COPERNICO\FOpt\UB3LYP\6-31G(d,p)\C6H4N1O3(2)\IVAN\20-May-2021\0\\# opt b3lyp/6-31g(d,p) geom=connectivity\\2-nitrofenolradical\\0,2\ C, -0.494743641,-1.4198958554, 0.000136819\ C, 0.2382590605, -0.2541137961, -0.0000484504\ C,-0.4202268924,1.0605667549,-0.0003208259\ C,-1.8791977905,1.0222128077,-0.0001578978\ C, -2.5894297735, -0.1569872484, 0.0000941785\ C, -1.9019904243, -1.3841422922, 0.0002252807\ H, 0.0370584365, -2.3633284745, 0.0002505391\ H,-2.3671769177, 1.9912590162, -0.0003678886\ H, -3.6750048177, -0.1454535302, 0.0001713973\ H,-2.4531955254, -2.3188175292, 0.0004262122\ O, 0.1657887044, 2.1611957891,-0.0009303602\ N, 1.7096743792, -0.3890237226, 0.0001219675\ O, 2.1606155018, -1.5391764023, -0.0018657923\ O, 2.3910187001, 0.627456483, 0.002417821\\ Version=AM64L-G09RevD.01\State=2-A\ HF=-511.320091\ S2=0.788944\ S2-1=0.\ S2A=0.75105\ RMSD =9.461e-09\ RMSF=1.237e-04\ Dipole =-2.3749355, -0.9437842, 0.0004173\ Quadrupole =0.5880223, -1.4950971, 0.9070748, 0.6593935, -0.0009935, -0.004933\ PG=C01 [X(C6H4N1O3)]\\@

VII.2.5.3. *2-Nitrophenolate anion*

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C6H4N1O3(1-)|PCUSER|05-Aug-2020|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||2-nitrofenoxido|| -1,1| C, -0.5021773612,-1.3931373121,0.0000629122|C,0.2545814101,-0.2022767929,0.0000288076|C,-0.3819326856, 1.1249325483,-0.0000637138|C,-1.8461137581,1.043048529,-0.0000916029|C,-2.5501228413, -0.1320924541, -0.0000292482| C, -1.8810367281, -1.3841647903, 0.0000499337| H, 0.0533605965, -2.3237221113, 0.0001130847| H, -2.3536464951, 2.0051829785, -0.000160722| H, -3.6407630265, -0.1075726494, -0.000043179| H, -2.4407452519, -2.3156148429, 0.0001093525| O, 0.1870501954, 2.2347429126, -0.0001511225| N, 1.6782207687,-0.3557958827, 0.0000668294| O, 2.1612800556, -1.5180294183, -0.0002097422| O, 2.4110523217, 0.6450914351, 0.0003322554|| Version=x86-Win32-G03RevB.03| State=1-A| HF=-511.4209472| RMSD=6.883e-009| RMSF=9.789e-005| Dipole =-1.6313287,-1.055641, 0.0001001| PG=C01 [X(C6H4N1O3)]||@

VII.2.6. 2-HYDROXYBENZALDEHYDE

VII.2.6.1. *Neutral form of 2-hydroxybenzaldehyde*

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C7H6O2|PCUSER|12-Aug-2020|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||2-salisaldehido|| 0,1| C, 0.0798718279,-1.5401311881,1.7467116225|C,0.0815776225,-0.1528224434,1.795822251| C,0.0274336411, 0.5878974349, 0.6046040576| C, -0.0288986124,-0.0994678578, -0.6388497314| C,-0.0290844247,-1.5081235278,-0.6548251061| C, 0.0247402714,-2.2318945512, 0.5238976572| H, 0.1222113687, -2.1007769325, 2.6762796869| H, 0.1239853185, 0.3836626636, 2.7374154295| H, -0.0725051361, -2.0174545135, -1.6147940967| H, 0.0244041143,-3.3163914518, 0.5079915189| O, 0.0295080614, 1.9253946966,0.6702067405| H, -0.0126313119, 2.2609645641, -0.2598629362| C, -0.085665008, 0.6526193146,-1.8798923242| H, -0.1278028345, 0.054179002, -2.8108633266| O, -0.0891972395, 1.885524501, -1.9478288449|| Version=x86-Win32-G03RevB.03| State=1-A| HF=-420.8172667| RMSD=4.647e-009| RMSF=2.842e-005| Dipole =0.0050981, -1.1752247, 0.099498| PG=C01 [X(C7H6O2)]||@

VII.2.6.2. *Neutral radical of deprotonated 2-hydroxybenzaldehyde*

1\1\GINC-COPERNICO\FOpt\UB3LYP\6-31G(d,p)\C7H5O2(2)\IVAN\20-May-2021\0\\# opt b3lyp/6-31g(d,p) geom=connectivity\\2-salisaldehidoradical\\0, 2\ C, 2.334205294, 0.3811929691, 0.0000024526\ C, 1.3191706277,1.3119930656, 0.0000023495\ C, -0.0849436626,0.9188302372,-0.0000827011\ C,-0.3668354681,-0.5252061347,-0.0000008131\ C,0.6886138155,-1.423229711,0.0000281494\ C,2.0275077681,-0.9939858963,-0.0000001171\ H, 3.3723697122,0.6999306173, 0.0000145868\ H, 1.5153740002, 2.3792891182, 0.0000804747\ H, 0.4725767006, -2.4897996837, 0.0000475155\ H, 2.8274334834, -1.7277841507, 0.0000168128\ O, -0.9785807092, 1.7913116066, 0.0003396273\ C, -1.7408027589, -1.0873065367, -0.0000367062\ H, -1.7434284957, -2.2029890946, 0.0005248655\ O, -2.781555307, -0.4663724062, -0.0004934966 \\Version=AM64L-G09RevD.01\State=2-A\HF=-420.1500053\ S2=0.791776\S2-1=0.\S2A=0.75125\ RMSD=4.100e-09\ RMSF=6.721e-05\Dipole=2.1639167,-1.0681534,0.0001026\Quadrupole=-2.38308,2.4288941,-0.0458141,2.627718,-0.0011521,-0.0010645\PG=C01 [X(C7H5O2)]\\@

VII.2.6.3. *2-Hydroxybenzaldehyde phenolate anion*

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C7H5O2(1-)|PCUSER|13-Aug-2020|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||2-salisaldehidoxi||-1,1| C, 2.2972388549, 0.380779871, 0.0000195977| C, 1.2936808734, 1.3180155125, 0.0000163995| C, -0.1299176292, 0.9750683333, 0.000166134 |C, -0.3924478794, -0.4754237939, -0.0000008116| C, 0.6827361449, -1.3934383675, 0.0000046862| C, 2.0104895267, -1.0090271976, 0.0000475552| H, 3.3384046323, 0.709081484, -0.0000023247| H, 1.519787437, 2.3829704965, -0.0000505979| H, 0.4327381415, -2.457128324, -0.0000485204| H, 2.8112762604, -1.7444266032, 0.000041245| O, -1.0079222565, 1.8642748411, -0.000111606| C, -1.7222427139, -1.0525097412, -0.0001710937| H, -1.6800538095, -2.1804248384, 0.0001072231| O, -2.8244997093, -0.5106323305, 0.0000438774|| Version=x86-Win32-G03RevB.03| State=1-A| HF=-420.2351836| RMSD=6.328e-009| RMSF=9.209e-005| Dipole=1.8029244,-1.1008971, 0.0000375| PG=C01 [X(C7H5O2)]||@

VII.2.7. 2-HYDROXYACETOPHENONE

VII.2.7.1. Neutral form of 2-hydroxyacetophenone

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C8H8O2|PCUSER|13-Aug-2020|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||2-hidroxiacetofenona||0,1| C, 2.5244040693,0.7146577007,0.0076204576|C,1.4618287137,1.6038295422,0.0120845735| C, 0.1397336132,1.1255966066,0.0074290917|C,-0.1008831694, -0.2788636431,-0.0019153313| C, 1.0072885791, -1.1531342512, -0.0062152182| C,2.3058994943, -0.673179158,-0.0015734255| H,3.5402924166,1.0996783637,0.0113180184| H, 1.6159545694, 2.6774300132, 0.0191958391| H, 0.8362840085, -2.2246559972, -0.0133179266| H, 3.1451299455, -1.3605581308, -0.0049884107| O, -0.8544200291, 2.0206056185, 0.0120493156| H, -1.6991356851, 1.4962238083, 0.007682814| C, -1.4865077103, -0.7694545874, -0.0067511234| O, -2.445259045, 0.0199512427, -0.0027247358| C, -1.7705800464, -2.2576323697, -0.0167932668| H, -1.3370223748, -2.7343825059, -0.901955076| H, -1.3403415594, -2.7456085239, 0.863877564| H, -2.8508299882, -2.4035009575, -0.0197240061|| Version=x86-Win32-G03RevB.03|State=1-A| HF=-460.1431386| RMSD=7.611e-009| RMSF=5.556e-0
06| Dipole=0.7461216,-0.9990386,-0.0055521| PG=C01 [X(C8H8O2)]||@

VII.2.7.2. Neutral radical of deprotonated 2-hydroxyacetophenone

1\1\GINC-COPERNICO\FOpt\UB3LYP\6-31G(d,p)\C8H7O2(2)\IVAN\20-May-2021\0 \\# opt b3lyp/6-31g(d,p) geom=connectivity\\2-hidroxiacetofenonaradical\\0,2\ C, 2.6282275592,-0.3740691658,0.0000591677\ C, 2.0469765898,0.8724238226,-0.0001699961\ C, 0.599486153, 1.0551655015,-0.0002310717\ C, -0.2337875533,-0.1645176829,0.0000995739\ C, 0.4072491507,-1.3964391994, 0.0002963718\ C, 1.8083915385,-1.5177477703, 0.0002863086\ H, 3.7089065148, -0.4817307095,0.0000615636\ H, 2.6346556198, 1.7847079671,-0.0004016406\ H, -0.1797828553, -2.3082351062, 0.0005235017\ H, 2.2565110085,-2.5066283546, 0.0004821919\ O, 0.1381816644, 2.2159811237, -0.0006725363\ C,-1.7360257614, -0.0884009198, 0.0002949953\ O, -2.3323543874, 0.9731251977, 0.0010419434\ C, -2.5215666093, -1.3976821473, -0.000348524\ H, -2.2962592636, -2.0031968078, -0.8848913685\ H, -2.296477038, -2.0038807976, 0.883783653\ H, -3.5822343304, -1.1467399515, -0.0003541339 \\Version=AM64L-G09RevD.01\State=2-A\HF=-459.4729366\ S2=0.791988\ S2-1=0.\ S2A=0.751261\ RMSD=5.052e-09\ RMSF=1.457e-05\ Dipole= 1.2208209, -2.0372389, -0.0002002\ Quadrupole =3.0642565,-2.4509249, -0.6133316, 3.9733892, 0.0026023, -0.0007495\ PG=C01 [X(C8H7O2)]\\@

VII.2.7.3. 2-Hydroxyacetophenone phenolate anion

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C8H7O2(1-)|PCUSER|13-Aug-2020|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||2-hidroxiacetofenoxi||-1,1|C, 2.590542376,-0.3759678588, 0.000088415| C, 2.0247774369, 0.8734922125, -0.0000118149| C, 0.579069719, 1.1121990469, -0.0000681658| C, -0.2404348888,- 0.1189015752, -0.0000358914| C, 0.4065538556, -1.3793695937, 0.0000636926| C, 1.781050648,-1.538998417, 0.0001308352| H, 3.6775074636, -0.4786713142, 0.0001371505| H, 2.6404380648, 1.7712518334, -0.0000431483| H, -0.205105371, -2.2788854221, 0.0001090831| H, 2.2271939724, -2.5307111765, 0.0002164122| O, 0.1381620629, 2.2816853802, -0.0001627865| C, -1.7023094187, -0.0610878554, -0.0000828922| O, -2.3825663377, 0.96782712, 0.0001433433| C, -2.4888900357, -1.3974452948, -0.0000905976| H, -2.2678593893, -2.0096632621, -0.8825688998| H,-2.2680895458,-2.0094791654,0.8825792269|H,-3.5510091498,-1.1434654806,-0.0002357636|| Version=x86-Win32-G03RevB.03|State=1-A| HF=-459.5525485| RMSD= 7.243e-009| RMSF=3.211e-005| Dipole= 0.4476031, -2.1506017, 0.0000048| PG=C01 [X(C8H7O2)]||@

VII.2.8. 3-HYDROXYBENZALDEHYDE

VII.2.8.1. Neutral form of 3-hydroxybenzaldehyde

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C7H6O2|PCUSER|11-Nov-2020|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||3-hidroxibenzaldehido||0,1|C,-1.9733881433, 0.1938085938, 0.0472014776| C, -1.14161827,-0.9358280261, 0.0732960198| C,0.243296804,-0.7803872196, 0.0273678686| C, 0.7908506091, 0.5047258352, -0.0444468343| C, -0.0371682864, 1.6353859744, -0.0706350308| C,-1.4197044913,1.4721934636,-0.0244948015| H, 0.4024454043, 2.6273522376, -0.1265409099| H, -2.0751647495, 2.3374632866, -0.0439608885| C, 2.2625411787, 0.6756033057, -0.0934707361| O, 3.0673529886, -0.2353559793,-0.0762491329| H, 0.89635292,-1.6457500671, 0.0468569287| H, 2.6006840484, 1.7342912804, -0.1494075774| H, -3.0537498536, 0.069346199, 0.0831107238| O, -1.6325350595, -2.2068659673, 0.1427747694| H, -2.597967608, -2.1779389253, 0.1688288513 ||Version=x86-Win32-G03RevB.03| State=1-A| HF=-420.802243| RMSD=2.546e-009| RMSF= 7.211e-006| Dipole=-1.6681758,0.684072,0.0171377| PG=C01 [X(C7H6O2)]||@

VII.2.8.2. Neutral radical of protonated 3-hydroxybenzaldehyde

1\1\GINC-COPERNICO\FOpt\UB3LYP\6-31G(d,p)\C7H5O2(2)\IVAN\12-May-2021\0\\# opt b3lyp/6-31g(d,p) geom=connectivity\\3-hidroxibenzaldehidoradical\\0,2\ C, 1.8691961655, 0.7343645634, 0.0000090679\ C, 1.3842555036, -0.6357924156, 0.0000138067\ C,-0.0499423839, -0.8297899667,-0.0000028949\C,-0.9121940989,0.2572912081,-0.0000003486\ C, -0.395329113,1.5693282782,0.000009533\ C, 0.993752688,1.7990186529,0.0000120955\ H, -1.0836785667, 2.4110104798, 0.0000113801\ H, 1.3680495883, 2.8182779099, 0.0000168634\ C, -2.3852582599, 0.0483752548, -0.0000087795\ O, -2.9210798257, -1.0404505078, -0.0000089551\ H, -0.4405394633, -1.8420493792, -0.0000141135\ H, -2.9866584738, 0.9841256217, 0.00000021\ H, 2.9452883964, 0.8751327905, 0.0000076863\ O, 2.1799608435,-1.6118554901,-0.0000015512\\Version=AM64L-G09RevD.01\State=2-A\ HF=-420.1554392\ S2=0.794448\S2-1=0.\S2A=0.751374\RMSD=7.563e-09\RMSF=1.894e-05\Dipole= -0.002518, 1.8301397, 0.000009\ Quadrupole=-3.677932, 2.1309623, 1.5469697, 0.5529133, 0.0000159, -0.0000011\PG=C01 [X(C7H5O2)]\\@

VII.2.8.3. 3-Hydroxybenzaldehyde phenolate anion

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C7H5O2(1-)|PCUSER|26-Nov-2020|0||#OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||ion-3-hidroxibenzaldehido||-1,1| C, 1.8894748622, 0.6934828401, 0.0000112275| C, 1.4654547043, -0.6990836383, 0.0000610981| C, 0.0264486146, -0.8570619377, 0.0000047453| C, -0.8517859755, 0.2298664163,

0.0000007309| C, -0.3792989578, 1.5618277542, 0.0000164646| C, 1.0043412703, 1.7643174088, 0.0000078497| H, -1.0798518679, 2.3941087129, 0.0000127525| H, 1.3978228164, 2.7824305865, -0.0000011731| C, -2.3049770346, 0.0330354796, -0.0000208114| O, -2.9180368014, -1.0275419893, -0.000019434| H, -0.3802290236, -1.8648455982, -0.0000265297| H, -2.8801214779, 0.9949679665, -0.0000102348| H, 2.9643408513, 0.8703022594, -0.0000110933| O, 2.2780485266, -1.6643667438, -0.0000370097|| Version=x86-Win32-G03RevB.03| State=1-A| HF=-420.2326961| RMSD =7.006e-009| RMSF=1.939e-005| Dipole= -0.9055932 ,1.796123, 0.0000448| PG=C01 [X(C7H5O2)]||@

VII.2.9. 3-HYDROXYACETOPHENONE

VII.2.9.1. Neutral form of 3-Hydroxyacetophenone

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C8H8O2|PCUSER|15-Jan-2021|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||3-hidroxiacetofenona||0,1| C, 1.8556625294,-0.2513739048, -0.0165880337| C,0.578929971,-0.807274684,0.0606315857| C,-0.5507822626, 0.0165054566,0.0101460942|C,-0.3982386201,1.4064291652,-0.1185479711| C, 0.880136363, 1.9549849371, -0.195122209| C,2.0074109133,1.1353785672,-0.14506201| H, 0.4533084039,-1.8791622868,0.1600771112| H, -1.264306015,2.0572200515, -0.1588695628| H, 1.0058403579,3.0289486604,-0.2947602897| H, 3.0030525599,1.5701282725,-0.205518173| O, 2.9193027524, -1.1058641298,0.0378928015| H, 3.7396908446, -0.5994632822, -0.0256029191| C, -1.8973380538, -0.6441995589, 0.0984108779| C, -3.1434285461, 0.2235169605,0.046501559| H,-3.1891633607,0.7899766622,-0.890030177| H,-4.0194451775,-0.4207162751,0.1235699022| H,-3.151483166,0.9489871939,0.8672389995| O, -1.990753779,-1.856600949,0.2098166673||Version=x86-Win32-G03RevB.03| State=1-A| HF=-460.127705|RMSD=5.273e-009| RMSF=1.512e-005 |Dipole= 0.683499, 1.4998609, -0.1501291| PG=C01 [X(C8H8O2)]||@

VII.2.9.2. Neutral radical of deprotonated 3-Hydroxyacetophenone

1\1\GINC-COPERNICO\FOpt\UB3LYP\6-31G(d,p)\C8H7O2(2)\IVAN\12-May-2021\ \\# opt b3lyp/6-31g(d,p) geom=connectivity\\3-hidroxiacetofenonaradical\\0,2\C,-1.8586984901,-0.482623755,-0.000084094\ C,-0.4679377009,-0.8852675469,-0.0000132164\ C, 0.5558170378, 0.0511004244, 0.0000261172\ C, 0.2325859699, 1.4264806008, 0.0000447399\ C, -1.1083414729, 1.8592691355, 0.0000330836\ C, -2.136326684, 0.942514962, -0.000019282\ H, -0.2351912353, -1.9445271719,-0.0000067375\ H, 1.0229545875,

2.1695467508, 0.0000981688\ H, -1.322296351, 2.9239396905, 0.0000589826\ H,-3.1786937364, 1.2445020161, -0.000027803\O,-2.7883499315,-1.3323305491,-0.0000783629\ C, 1.9788366021, -0.4475172306,0.0000897691\C,3.1103025125,0.5638054162,-0.0000683062\ H, 3.0607545442, 1.2105203519, 0.8830834225\ H, 4.0579823764, 0.0254159859, -0.0003655446\ H, 3.0603578391, 1.2108630239, -0.8829377392\ O, 2.2083761327, -1.6448211045, 0.0000858024\\ Version=AM64L-G09RevD.01\ State=2-A\ HF=-459.4817057\ S2=0.79384\S2-1=0.\ S2A=0.751336\ RMSD=4.088e-09\RMSF=6.667e-05\ Dipole=0.6921814,1.9484882,0.0000207\ Quadrupole= -1.8945159, 0.5315209, 1.362995, -0.5799775, -0.0001465, 0.0002005\ PG=C01 [X(C8H7O2)]\\@

VII.2.9.3. 3-Hydroxyacetophenone phenolate anion

N-N= 4.707898566664D+02 E-N=-2.025539549691D+03 KE= 4.554202936505D+02 1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C8H7O2(1-)|PCUSER|15-Jan-2021|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||3-ionehidroxiacetofenona||-1,1|C,-1.9432828225,-0.5263761283,0.0000312827|C,-0.5418622368,-0.8936565244,-0.000009274| C, 0.4989591692, 0.0392565982, 0.0000099032| C, 0.2215742956, 1.4284119191, 0.0000482126| C,-1.1186295653, 1.8295974691, 0.0000442564| C,-2.1589166771, 0.9094754552, 0.0000207979| H, -0.2958525816, -1.951379138,-0.0000511948| H, 1.0157463374, 2.1676459922, 0.0000703922| H, -1.3516087332, 2.8962670075, 0.0000597003| H, -3.1941410283, 1.2483397315, 0.0000034921| O, -2.8839913656, -1.368597303, -0.0000720647| C, 1.89765232, -0.4593009143, -0.0000046632| C, 3.0397657436, 0.5648071472, -0.000036671| H, 2.987045582, 1.2136574804, 0.88077219| H, 3.9880237747, 0.0237091732, -0.0001383176| H, 2.9869139768,1.2137836223,-0.880741739| O, 2.1955302797, -1.652066947, -0.0000026342|| Version=x86-Win32-G03RevB.03 |State=1-A| HF=-459.5540288|RMSD =7.990e-009| RMSF=1.544e-005| Dipole =2.1634994, 1.8192432, 0.0000629| PG=C01 [X(C8H7O2)]||@

VII.2.10. 4-HYDROXYBENZALDEHYDE

VII.2.10.1. Neutral form of 3-hydroxybenzaldehyde

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C7H6O2|PCUSER|09-Nov-2020|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||4-hidroxibenzaldehido||0,1|C,-1.7595159888, 0.2173917603, -0.0006706752| C, -1.1307957952, -1.0387545224, 0.0007345721| C, 0.2538417221, -1.1150486142, 0.0010723559| C, 1.0312912623, 0.0537123669, 0.0001722371| C, 0.3898319696, 1.301884212,-0.0010736418|C,-0.9952353522,1.3922589808,-0.0015022973|

H, -1.733186903,-1.9447399864,0.0014656092|H,0.9884078421,2.2098028775,-0.0017918153| H,-1.5056285773,2.3491342426,-0.0024695222|C,2.5023764831,-0.0285016768, 0.000627314| O, 3.1424284313, -1.0650881733, 0.0015720241| O, -3.1119989781, 0.3554050821, -0.0010063386| H, -3.5251078532, -0.5186127045, -0.0001195616| H, 0.7625479288, -2.0737364883, 0.0021220042| H, 3.0187661312, 0.9579617493, 0.0001086127|| Version=x86-Win32-G03RevB.03|State=1-A|HF=-420.8054316| RMSD=7.693e-009| RMSF=1.538e-005| Dipole =-1.3184172, 0.201205, -0.0002639| PG=C01 [X(C7H6O2)]||@

VII.2.10.2. Neutral radical of deprotonated 4-hydroxybenzaldehyde

1\1\GINC-COPERNICO\FOpt\UB3LYP\6-31G(d,p)\C7H5O2(2)\IVAN\12-May-2021\0 \\# opt b3lyp/6-31g(d,p) geom=connectivity\\4-hidroxibenzaldehidoradical\\0,2\C,-1.8224762492,-0.0686846378, -0.0001032511\ C, -0.9379885366, -1.2293420647, 0.0000114886\ C, 0.4236529184, -1.0764081974,0.0000532401\ C, 0.9966729787, 0.2227706433, 0.0000598609\ C, 0.1720237797, 1.3734782836, 0.0000416814\ C, -1.1961927724, 1.2482819847, -0.0000025544\ H, -1.4104430404, -2.2063333016, 0.0000325106\ H, 0.6381352885, 2.3560953194, 0.0000668705\ H, -1.8572722357, 2.1087335432, 0.0000056954\ C, 2.4659355621, 0.3757825567, 0.0000950185\ O,3.247244664, -0.5589303072, 0.000017822\ O, -3.068029992,-0.1957105139,-0.0000463445\ H, 1.0976012439, -1.9271135208, 0.0000727669\ H, 2.8283383908, 1.4258152125, 0.000072195\\ Version=AM64L-G09RevD.01\ State=2-A\HF=-420.1584107\ S2=0.794543\S2-1=0.\S2A=0.751439\RMSD=4.457e-09\RMSF=1.319e-04\ Dipole = 0.3197101, 0.6931523, 0.0000381\ Quadrupole=-10.6649754, 8.0271006, 2.6378748, 2.5236106, 0.0001823, -0.0000083\ PG=C01 [X(C7H5O2)]\\ @

VII.2.10.3. 3-Hydroxybenzaldehyde phenolate anion

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C7H5O2(1-)|PCUSER|10-Nov-2020|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||ion-4-hidroxibenzaldehido|| -1,1| C, -1.9145608086, -0.0810223296,-0.000139146| C,-1.005665354,-1.2248869751,-0.0000233757| C,0.358250308,-1.0844898687,0.0000061197| C,0.9784992896, 0.19684272,-0.0000000523| C, 0.1231449318, 1.3315105483,0.0000023557| C, -1.245033535,1.2148164919,-0.0000271005| H,-1.4687184425,-2.2102317816,0.0000154101| H,0.584256867, 2.3218055016, 0.0000300376| H, -1.8861363947, 2.0943667893, 0.0000110732| C, 2.4050953444, 0.353375819, 0.0000282133| O, 3.2675927313, -0.5349024124, 0.0000956197| O, -3.1639100092, -0.2045586174, 0.0000011594| H, 1.0123880047,-1.954747314, 0.0000330202| H, 2.7303671307, 1.4276166079,0.0000541402|| Version=x86-Win32-G03RevB.03|State=1-A|HF=-420.2506408|RMSD=2.288e-009|RMSF=4.946e-005|Dipole=0.5938516,0.5680031,

-0.0000943|PG=C01 [X(C7H5O2)]||@

VII.2.11. 4-HYDROXYACETOPHENONE

VII.2.11.1. Neutral form of 4-Hydroxyacetophenone

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C8H8O2|PCUSER|09-Nov-2020|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||4-hidroxiacetofenona||0,1| C, 2.1411598387,-0.1331939444,-0.0636150986|C,1.5322018511,1.1294972597,-0.1033936554| C,0.1487340442, 1.2281252273, -0.0628850709| C, -0.6572148392, 0.0813821878, 0.0176142866| C,-0.0298053823,-1.1754826196, 0.0565109049| C, 1.3541912233, -1.2887701995, 0.0166759386| H, 2.1457612295, 2.0259205927, -0.1657885123| H, -0.6243182429, -2.0811770162, 0.1187105726| H, 1.8446844621, -2.2556797466, 0.046353769| C,-2.138582896, 0.259354026, 0.057576309| O,-2.6373867454, 1.3760507275,0.0209701483|C,-3.0240963922,-0.973813614, 0.1448425467| H,-2.8641385055, -1.6358224429, -0.7132735742| H, -2.8065349319,-1.5525489801, 1.0492323245| H, -4.0656079784, -0.6523552764,0.163690185| O, 3.49169734,-0.2977931892, -0.0999078265| H, 3.918167576, 0.567963472, -0.1548432742| H,-0.3420230505, 2.1950491531, -0.0925370301|| Version=x86-Win32-G03RevB.03|State=1-A|HF=-460.130617|RMSD=8.045e-009|RMSF=3.973e-006|Dipole =0.9350582, -0.4279841,-0.0102855|PG=C01 [X(C8H8O2)]||@

VII.2.11.2. Neutral radical form of deprotonated 4-hydroxyacetophenone

1\1\GINC-COPERNICO\FOpt\UB3LYP\6-31G(d,p)\C8H7O2(2)\IVAN\12-May-2021\ \\# opt b3lyp/6-31g(d,p) geom=connectivity\\4-hidroxiacetofenonaradical\\ 0,2\ C, -2.1956465185, 0.0662878974, 0.0000057624\ C, -1.4880298948, -1.2060156858, 0.000026581\ C,-0.1174953357,-1.2495166483,0.0000241372\C,0.648777434,-0.0537734815,0.0000023488\C,-0.0095157726,1.2023496343,-0.0000224197\C,-1.3823571222, 1.2739125458, -0.0000232618\ H, -2.0931534363, -2.1069611991, 0.0000454371\ H, 0.5747191766, 2.1167912103, -0.0000419826\ H, -1.9088117598, 2.2228378145, -0.0000445127\ C, 2.1409289468, 0.1804097864, 0.0000010154\ O, 2.6594591318, -1.2883228745, 0.0000253039\ C, 2.9912020771,1.0763788244,0.0000312561\H,2.7862349185,1.6916263396,-0.8828938538\ H, 2.7861280419, 1.691667036,0.8829018592\ H,4.0412828287, 0.7842082331, 0.0000979024\O,-3.447656201, 0.1243352852, 0.0000038543\ H, 0.4231094856,-2.1898841449, 0.0000395728\\ Version=AM64L-G09RevD.01\ State=2-A\ HF=-459.4844114\ S2=0.79329\ S2-1=0.\ S2A= 0.751345\ RMSD=8.517e-09\RMSF=2.506e-05\Dipole=0.8092275, 0.8699008,-0.0000116\

Quadrupole =-8.3090954, 5.7782551, 2.5308404,5 .7092192, -0.0000751, -0.0000748\ PG=C01 [X(C8H7O2)]\\@

VII.2.11.3. 4-Hydroxyacetophenone phenolate anion

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C8H7O2(1-)|PCUSER|10-Nov-2020|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||ion-4-hidroxiacetofenona||-1, 1|C,-2.2847945232, 0.0679542802,-0.0002048071| C,-1.5517427121,-1.1922148326,-0.0001050516| C, -0.1808941315, -1.2488441988, 0.000138297| C, 0.6295929268, -0.0777705975, 0.0003301895| C, -0.0578050253, 1.1685606012, 0.0002178952| C, -1.4302134589, 1.2482642911, -0.0000185193| H, -2.1491566915, -2.1026258836, -0.0002304484| H, 0.5182147382, 2.0934730069, 0.000335815| H, -1.933063396, 2.213838103, -0.0000754838| C, 2.0726537508, -0.2025815403, 0.0005844976| O, 2.6760368158, -1.2890665344, -0.0001818264| C, 2.9223908107, 1.0805923611, -0.0000755246| H, 2.7210588394, 1.7002225081, -0.8817490991| H, 2.7218240643, 1.7005920931, 0.8815078943| H, 3.9745567349, 0.7880737093, -0.0004744432| O, -3.539251613, 0.1325848607, -0.0004089162| H, 0.3371582647, -2.2054823337,0.0002098455 ||Version=x86-Win32-G03RevB.03|State=1-A|HF=-459.5711218| RMSD=8.026e-009| RMSF=8.404e-005| Dipole =1.6197099, 0.8598608, 0.0004905| PG=C01 [X(C8H7O2)]||@

VII.2.12. 2,4-DIHYDROXYBENZALDEHYDE

VII.2.12.1. Neutral form of 2,4-hydroxybenzaldehyde

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C7H6O3|PCUSER|17-Nov-2020|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||doscuatrodihidroxibenzaldehido||0,1|C,-0.2547500345,-1.3581907924,-0.0022452661|C,1.1288009156,-1.4258354786,-0.0025515483| C, 1.8676780358,-0.2313890051,-0.0006584001| C, 1.2199661007, 1.0064833078, 0.0014782958| C,-0.1738194266, 1.056404279, 0.0018544919| C, -0.9371248323, -0.1318778077, -0.0000155905| H, -0.8588524431, -2.2598372638, -0.0036867998| H, 1.6407681327, -2.3847898947, -0.00424676| H, 1.8176955989, 1.9135006346, 0.0027544049| O, 3.2270779835, -0.2138828081, -0.0009314116| H, 3.556991911, -1.1224898428, -0.0032349547| O, -0.8438538695, 2.2420337701, 0.0037920999| H, -0.2082476415, 2.9698145035, 0.005547769| C, -2.4104015908, -0.1172507052, 0.0003097793| H, -2.8772832115, 0.8856617071, 0.0023000008| O, -3.0973700332, -1.1271412909, -0.0014187174|| Version=x86-Win32-G03RevB.03| State=1-A| HF=-496.0254681| RMSD

=9.171e-009| RMSF=5.764e-006| Dipole =1.726132, 0.4958171, 0.0005837| PG=C01 [X(C7H6O3)]||@

VII.2.12.2. Neutral radical of deprotonated 2,4-Dihydroxybenzaldehyde

1\1\GINC-COPERNICO\FOpt\UB3LYP\6-31G(d,p)\C7H5O3(2)\IVAN\12-May-2021\ \\# opt b3lyp/6-31g(d,p) geom=connectivity\\doscuatrodihidroxibenzaldehidoradical\\0,2\C,-0.25066163,-1.3777208861,0.0000204141\C,1.1178762107,-1.4512013871, 0.0000009357\ C, 1.9232729944, -0.2334693478, -0.0000023739\ C, 1.2174983135, 1.0359148556, 0.0000390205\ C, -0.1566944329, 1.0820493118, 0.0000670174\ C, -0.919829955, -0.1288847087, 0.0000598954\ H, -0.8732511685, -2.2664342394, 0.0000161336\ H, 1.6502423117,-2.396209971,-0.0000163084\ H, 1.8224773916, 1.9384109889, 0.0000394841\ O, 3.1734802768, -0.2818511069, 0.000006864\ O, -0.8680056385, 2.2426543299, 0.0000758838\ H, -0.2589556917, 2.9935401421, 0.0002399111\ C, -2.3973581302, -0.1045138637, 0.0001190377\ H, -2.8660931167, 0.8943665113, 0.0000988263\ O, -3.0729487352, -1.122240629, -0.0000097414\\ Version=AM64L-G09RevD.01\ State=2-A\ HF=-495.3786548\S2=0.793843\S2-1=0.\S2A=0.751384\RMSD=7.994e-09\RMSF=3.902e-05\Dipole=-0.070248,1.0403394,0.0001749\Quadrupole=-12.0970024,9.9236724,2.173329 9,-1.5631846,-0.0003398,0.0006937\PG=C01 [X(C7H5O3)]\\@

VII.2.12.3. 2,4-Dihydroxybenzaldehyde phenolate anion

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C7H5O3(1-)|PCUSER|19-Nov-2020|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||iondoscuatrodihidroxibenzaldehido||-1,1|C,-0.1874586477,-1.3805352101,-0.0001442764| C, 1.1795584003, -1.4419931168, -0.0000338209| C, 2.0080259078, -0.2387773144, 0.0001044359| C, 1.2523478147, 1.0028848639, 0.0000291547| C, -0.1240584028, 1.0369752642, -0.0000748782| C,-0.9108511659,-0.151450391,-0.0001690608|H,-0.7889854285,-2.2870979373, -0.0002271615| H, 1.7031980704, -2.3957754651, -0.000039774| H, 1.8267942851, 1.9306311959, 0.0000430195| O, 3.2622314599,-0.2722616326, 0.000143787| O, -0.7988641207, 2.2481659241, -0.0001344356| H, -0.1195451851, 2.9351791201, 0.0001627146| C, -2.347183917, -0.1363217286, -0.0002498774| H,-2.7967861799, 0.8811694438, 0.0004018825| O, -3.0942367765, -1.1270043616, 0.0003518057|| Version=x86-Win32-G03RevB.03| State=1-A|HF=-495.4712726| RMSD=7.838e-009| RMSF=9.876e-005| Dipole=-0.4352722,1.2818633,-0.0002148|PG=C01 [X(C7H5O3)]||@

VII.2.13. 3,4-DIHYDROXYBENZALDEHYDE

VII.2.13.1. Neutral form of 3,4-Dihydroxybenzaldehyde

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C7H6O3|PCUSER|17-Nov-2020|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||trescuatrodihidroxibenzaldehido||0,1|C,-0.8479975552,-1.0704136747,0.0037905679| C,0.5372551208,-1.0131438675,-0.078855523| C, 1.2143711895,0.2180480214,-0.0648350104| C,0.4836155665,1.4070981479,0.0338618999| C, -0.9032132376, 1.3586566658, 0.1169044773| C,-1.5796266414, 0.1343836534, 0.1032057826| H, 1.1078571111, -1.9378349495, -0.1557273115| H, 1.0176948083, 2.350779161, 0.0436794512| H, -1.4815044644, 2.2771190238, 0.1939256358| O, -1.5673063976,-2.2291035246,-0.0043797284| O,-2.9312446559, 0.0272426027, 0.1814280516| C, 2.6852037046, 0.2464609081,-0.1539975499|H,3.1620217313,-0.7575110716,-0.2288415623| O, 3.3644017748, 1.2572322365, -0.1500958435| H, -0.9571287329, -2.9748773484, -0.0747488149| H, -3.3133951061, 0.9128155415, 0.2456448986|| Version=x86-Win32-G03RevB.03| State=1-A|HF=-496.019284| RMSD=3.981e-009| RMSF=1.574e-005|Dipole=-0.9277127, -0.4594266,0.0372975| PG=C01 [X(C7H6O3)]||@

VII.2.13.2. Neutral radical of deprotonated 3,4-dihydroxybenzaldehyde

1\1\GINC-COPERNICO\FOpt\UB3LYP\6-31G(d,p)\C7H5O3(2)\IVAN\12-May-2021\0\\# opt b3lyp/6-31g(d,p) geom=connectivity\\trescuatrodihidroxibenzaldehidoradical\\ 0,2\ C, 1.1236057724,0.8038778467,0.000084857\ C, -0.2184767084,1.1564913978,0.0000642924\ C,-1.2100042854,0.1649347329,-0.0000028823\ C,-0.8598624752,-1.2178189984,-0.0000503964\ C, 0.4519492044, -1.5956148057, -0.0000324028\ C, 1.5326289215,-0.6175907822, 0.0000282587\ H,-0.5103091037, 2.2062348161, 0.0000986053\ H,-1.6679240073,-1.9417376555, -0.000100673\ H, 0.754122221,-2.6377594625,-0.0000645428\ O, 2.1334440281, 1.6873613782, 0.0001487925\ O, 2.7331601567, -0.9386759105, 0.0000657293\ C, -2.6304225517, 0.5613591049, -0.000023542\ H, -2.8099663615, 1.6584347943, 0.0000325716\ O, -3.5598511781, -0.226500242, -0.000057594\ H, 1.7812323671, 2.589413786, 0.0002339262\\ Version=AM64L-G09RevD.01\State=2-A\HF=-495.3812316\ S2=0.782888\S2-1=0.\S2A=0.750779\RMSD=7.308e-09\RMSF=4.551e-05\ Dipole=-0.2917425, 1.3335569, 0.0000627\Quadrupole=-14.0776185,11.710589,2.3670295,1.4480013,-0.0001907,0.0006586\PG=C01 [X(C7H5O3)]\\@

VII.2.13.3. 3,4-Dihydroxybenzaldehyde phenolate anion

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C7H5O3(1-)|PCUSER|19-Nov-2020|0||#OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||iontrescuatrodihidroxibenzaldehido||-1,1| C,1.1608731609,0.7511976516,0.0000339328| C,-0.1649373357,1.1000652204,0.0000111947| C,-1.2066336915,0.1252988516,-0.0000078019| C, -0.818074277, -1.2370692749,-0.0000390322|C,0.5076479337,-1.6037366967, -0.000039305|C,1.6033620214,-0.6489150874, 0.000007967| H, -0.4442494157, 2.1584095083,0.0000172559|H,-1.6086187631,-1.9845006621,-0.0000596796| H, 0.7994488673,-2.6522389902,-0.0000611694| O, 2.1785203569,1.6930875217 ,0.0000575019|O,2.8131027151,-0.9736261758,-0.0000120384| C, -2.5834229774, 0.5281290762, -0.0000058638| H, -2.7170761549,1.6430800381,-0.0000057082| O, -3.5881277008, -0.1961568042, -0.0000544722|H, 1.7496434908, 2.5589953284, 0.0004148212||Version=x86-Win32-G03RevB.03|State=1-A|HF=-495.4642418| RMSD=3.671e-009| RMSF=6.613e-005| Dipole=-0.2974217, 1.3097754, 0.0002631| PG=C01 [X(C7H5O3)]||@

VII.2.14. 3-METHOXY-4-HYDROXYBENZALDEHYDE

VII.2.14.1. Neutral form of 3-methoxy-4-hydroxybenzaldehyde

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C8H8O3|PCUSER|18-Nov-2020|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||tresmetoxcuatroihidroxibenzaldehido||0,1|C, 1.5113942999, 0.5955311167, -0.2018637578| C, -0.7176139477,-0.5346699994,0.1198624246| C, 0.660962977, -0.4351799711, 0.1343376775| C, 1.2713475159, 0.79775663, -0.173014947| C, 0.4853913719, 1.9098498313,-0.4897469697| C, -0.9050755615,1.81202536,-0.5049795877| H, 0.964572809, 2.8564115527, -0.7253340112| H,-1.5359947923, 2.6601278232,-0.7474796399| C, 2.7387936789, 0.9045480193, -0.1579201483| O, 3.5014135473, -0.0096820591, 0.1056795146| O, -2.8606051757, 0.4863126079, -0.2130472769| H, -3.0760314006, -0.4306394721, 0.0230026624| H, 1.3030267493,-1.2744559867,0.3748221739| H, 3.1294724935, 1.9149823965, -0.4128977112| O, -1.4593524254, -1.6556026032, 0.3939605232| C,-0.7621240637,-2.8499348594,0.73012532| H,-1.5261144314,-3.6074198916, 0.9076060066| H,-0.1105599964,-3.1716493663,-0.0906529642| H, -0.161745025,-2.7151373844,1.6373913258||Version=x86-Win32-G03RevB.03| State=1-A| HF=-535.3338444| RMSD=8.534e-009| RMSF=9.041e-006| Dipole= -0.9698827,-0.4658409,0.094892| PG=C01 [X(C8H8O3)]||@

VII.2.14.2. Neutral radical of 3-methoxy-4-hydroxybenzaldehyde

1\1\GINC-COPERNICO\FOpt\UB3LYP\6-31G(d,p)\C8H7O3(2)\IVAN\12-May-2021\0\\# opt b3lyp/6-31g(d,p) geom=connectivity\\tresmetoxcuatroihidroxibenzaldehidoradical\\ 0,2\ C, 1.2741955978, -1.156682593, 0.000046895\ C, 0.8940539022, 0.2794547191, 0.0000680992\ C, -0.4385101904, 0.6584642932,0.0000824282\ C,-1.4472232122,-0.3213089027, 0.0000798231\ C, -1.1278598808, -1.7070460318, 0.0000616924\ C, 0.1779508894, -2.1152707665, 0.0000457043\ H, -1.9374831753, -2.4327922813, 0.0000609759\ H, 0.4596770041, -3.1629516685, 0.0000309413\ C, -2.8601553262, 0.1016978776, 0.0000959355\ O, -3.2269814354, 1.264917699, 0.0001126637\ O, 2.4655033959,-1.5081119456, 0.0000253046\ H, -0.7499780303, 1.6964173697, 0.0000955145\ H, -3.597027573, -0.7294657196, 0.0000915349\ O, 1.9396160021,1.1122123115,0.0000710318\ C, 1.6955262372, 2.519180607, 0.0000982421\ H, 2.6786424463,2.9886577034,0.0001096022\ H,1.1405551499,2.8216820375, -0.8946560043\ H, 1.1405511989,2.8216472907,0.8948616155 \\Version=AM64L-G09RevD.01\State=2-A\HF=-534.6884026\S2=0.781861\S2-1=0.\S2A=0.750734\ RMSD = 7.011e-09\ RMSF=1.183e-05\Dipole= -0.4054999, 0.2835784, 0.0000165\ Quadrupole=-8.4237887, 7.0668228, 1.3569658, 11.8467879, 0.0002661, -0.0000231\ PG=C01 [X(C8H7O3)]\\@

VII.2.14.3. 3-Methoxy-4-hydroxybenzaldehyde phenolate anion

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C8H7O3(1-)|PCUSER|19-Nov-2020|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||iontresmetoxcuatroihidroxibenzaldehido||-1,1| C, 1.3261736336, -1.1746256311, -0.0000229944| C,0.9277143234, 0.2464493462, -0.0000076923| C, -0.3846562281, 0.6442138784, 0.0000094191| C, -1.4478950817, -0.3098395316, 0.0000218998| C, -1.1049126164, -1.681283863, 0.0000023481| C, 0.2076102407, -2.0973566022, -0.0000179115| H,-1.9112934218,-2.416948915, 0.0000065372| H, 0.4657519624, -3.1542278878, -0.000030203| C, -2.8202494157, 0.1054377651, 0.0000433963| O, -3.2617432256, 1.2634202772, 0.0000357933| O, 2.5253177824, -1.5337305871, -0.0000669542| H, -0.6733231932, 1.6905885217, 0.000016999| H, -3.5410500871, -0.7537016729, -0.0000064493| O, 2.0068242838, 1.1117025377, -0.0000267806| C, 1.7177053171,2.4854460629,0.0000290382| H,2.6794051506, 3.0080471212, 0.0000528033| H, 1.1441925428, 2.7922664237, -0.8889313502| H, 1.1441852834, 2.7921900387, 0.8890101747|| Version=x86-Win32-G03RevB.03|State=1-A|HF=-534.7712685| RMSD=2.782e-009|RMSF=9.085e-005|Dipole=-0.1051911,0.7649679,0.0000553|PG=C01 [X(C8H7O3)]||@

VII.2.15. 4-HYDROXYBENZOATE METHYL ESTER

VII.2.15.1. Neutral form of 4-hydroxybenzoate methyl ester

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C8H8O3|PCUSER|10-Nov-2020|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||4-hidroxibenzoatodemetilo||0,1|C,-2.5619678741,0.0821146978,0.029076817|C,-1.9656913751,-1.185251798,-0.0193154019|C,-0.5810048095,-1.294997145,-0.0372138711|C,0.2264987994,-0.1504192838,-0.0073496467| C, -0.3816400335, 1.1144316217, 0.0410296679| C, -1.7644753489, 1.2339476405, 0.0592266903| H, -2.587059304, -2.0778749092, -0.0427352892| H, 0.2387090726, 2.0027436117, 0.064250784| H, -2.2477889486, 2.2041910811, 0.0964928113| C, 1.6983265693, -0.3358711522, -0.0286156368| O, 2.260619932, -1.4143458457, -0.0703424832| O, -3.912110235, 0.2569536112, 0.0486169273| H, -4.3466317957, -0.606118685, 0.0242357833| H, -0.1010837418, -2.2668984996,-0.0745483974| C, 3.8005195089, 0.7263158798, -0.0146903909 |H, 4.1357865303, 0.2218754172, -0.9243672305| H, 4.1786507902, 1.7480697253, 0.0175072097| H, 4.1536617742, 0.1591452985, 0.8501407147| O, 2.3705356784, 0.8415477588, 0.0037423368|| Version=x86-Win32-G03RevB.03|State=1-A| HF=-535.362881| RMSD=3.116e-009| RMSF=9.847e-006| Dipole =-0.5083523,0.1568759 ,0.0104787|PG=C01 [X(C8H8O3)]||@

VII.2.15.2. Neutral radical of deprotonated 4-hydroxybenzoate methyl ester

1\1\GINC-COPERNICO\FOpt\UB3LYP\6-31G(d,p)\C8H7O3(2)\IVAN\12-May-2021\0 \\# opt b3lyp/6-31g(d,p) geom=connectivity\\4-hidroxibenzoatodemetiloradical\\0,2\C,-2.6066699574,-0.1548792771, 0.0000818177\ C,-1.9861281349, 1.1614115098, 0.0001544004\ C,-0.6196170497, 1.2963869452,0.0000958325\ C ,0.2132787269,0.150810853,-0.0000731497\ C, -0.3517668219, -1.148289347, -0.0001885533\ C,-1.7169936957, -1.3067114292, -0.0001323235H,-2.6492642588, 2.0203224517,0.0002694992\H,0.3085586169,-2.0076489255, -0.000323297\ H, -2.1808052128, -2.2877250726, -0.0002319871\ C, 1.6861235377, 0.3736974369, -0.0001310599\ O, 2.208142401, 1.4721362861, 0.0001166174\ O, -3.853493452, -0.2927027127, 0.0000831919\ H, -0.1435248113, 2.2709721558, 0.0001730618 \C, 3.8140310645, -0.634725343, 0.0000070181\ H, 4.1422601533, -0.09158308, 0.8892758391\ H, 4.2130649934, -1.6483660423, -0.001059228\ H, 4.1421898653, -0.0896620272, -0.8880963939\ O, 2.3836290353, -0.7825683818, -0.0000712857\ Version=AM64L-G09RevD.01\ State=2-A\ HF=-534.7165245\ S2=0.791293\ S2-1=0.\ S2A= 0.751192\ RMSD=2.562e-09\ RMSF=3.170e-05\ Dipole=1.3075388,-0.5323262,-

0.0001573\Quadrupole=-4.1293323, 2.9559646, 1.1733677, -5.5320509, -0.000485, 0.0002727\ PG=C01 [X(C8H7O3)]\\@

VII.2.15.3. 4-Hydroxybenzoate methyl ester phenolate anion

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C8H7O3(1-)|PCUSER|10-Nov-2020|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||ion-4-hidroxibenzoatodemetilo||-1,1| C, -2.7021047721,-0.1509213875,-0.0000911895|C,-2.0455302669,1.1505863535,0.000169623|C,-0.6796094373,1.2894792526,0.0001698297|C,0.1904078132,0.1650740636,-0.0000216233|C,-0.4133631655,-1.1224693872,-0.0001797005|C,-1.778483063,-1.2787431745,-0.0001846788|H,-2.6952140861,2.0239635996,0.0003496087|H,0.232255035,-1.99737065,-0.0002999049|H,-2.2241503356,-2.2718653152,-0.0002786769| C,1.6163504461,0.3812743735,-0.0000136105| O, 2.2134910672, 1.4576050492, 0.0001770051| O,-3.9509738258, -0.2890692529, 0.000055562| H, -0.2224246301, 2.2767786234, 0.0003179569| C,3.7537160851,-0.6261157557,-0.00003607| H, 4.0934104103,-0.0745111783,0.8842653068| H, 4.1885551894,-1.6299226969,-0.0007411448| H, 4.0933148098, -0.0732423544,-0.8835637417| O, 2.3482267299,-0.8063878036,-0.0000981776|| Version=x86-Win32-G03RevB.03|State=1-A|HF=-534.8013487|RMSD=5.825e-009|RMSF=1.723e-005|Dipole=2.7325792,-0.4888744,-0.0001968|PG=C01 [X(C8H7O3)]||@

VII.2.16. 4-BROMOPHENOL

VII.2.16.1. Neutral form of 4-Bromophenol

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C6H5Br1O1|PCUSER|17-Jan-2021|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||4-bromofenol||0,1|C,0.3126368606, 0., 0.0031672287| C, -0.3720843693, -1.2140933464, -0.0153301327| C,-1.7660794696, -1.2099693302, -0.0480008574| C, -2.4637484865, 0., -0.0591885558| C, -1.7660794696, 1.2099693302, -0.0480008574| C, -0.3720843693, 1.2140933464, -0.0153301327| H, 0.1767812824, -2.1490361071, -0.0072143169| H, -2.3220695389, -2.1415700856, -0.0735674646| H, -2.3220695389, 2.1415700856, -0.0735674646| H, 0.1767812824, 2.1490361071, -0.0072143169| O, -3.8470012141, 0., -0.1449696353| H, -4.2181427502, 0.,0.7472029676| Br, 2.2242675657, 0., 0.0477205006|| Version=x86-Win32-G03RevB.03|State=1-A'|HF=-2878.5750184|RMSD=3.107e-009|RMSF=1.792e-004|Dipole=-0.5963075,0.,0.5835408|PG=CS [SG(C2H1Br1O1),X(C4H4)]||@

VII.2.16.2. Neutral radical of deprotonated 4-Bromophenol

1\1\GINC-COPERNICO\FOpt\UB3LYP\6-31G(d,p)\C6H4Br1O1(2)\IVAN\12-May-202 1\0\\# opt b3lyp/6-31g(d,p) geom=connectivity\\4-bromofenolradical\\0, 2\ C, -0.0059919689,-0.3024755817, 0.\ C,-0.0093059516, 0.3823351232, 1.2323484595\ C, -0.0162760661, 1.757941154, 1.2384030391\ C, -0.0203981764, 2.5193855184, 0.\ C, - 0.0162760661, 1.757941154, -1.2384030391\ C, -0.0093059516, 0.3823351232, -1.2323484595\ H,-0.0063355841, -0.1838627449, 2.1572958154\ H, -0.0189339659, 2.3204460916, 2.1663159819\ H, -0.0189339659,2.3204460916,- 2.1663159819\ H, -0.0063355841,-0.1838627449, -2.1572958154\ O, -0.0272606841, 3.7743567268,0.\Br,0.0031279647,-2.1972809111,0.\\Version=AM64L-G09RevD.01\State=2-A'\HF=-2877.9391244\S2=0.786951\S2-1=0.\S2A=0.750944\ RMSD=5.955e-09\ RMSF=9.939e-06\ Dipole =0.0055893,-0.9955257, 0.\ Quadrupole=1.2385239,-8.5955659,7.357042,0.0532116,0.,0.\PG=CS [SG(C2Br1O1),X(C4 H4)]\\@

VII.2.16.3. 4-Bromophenolate anion

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C6H4Br1O1(1-)|PCUSER|17-Jan-2021|||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||4-bromofenolato||-1,1| C,0.0013883294,-0.2549887013,0.| C,-0.0018724898, 0.4399567018, 1.2132989554| C,-0.0086333341, 1.82708524, 1.2144815129| C, -0.0132744107, 2.6243153282, 0.|C,-0.0086333341, 1.82708524, -1.2144815129| C, -0.0018724898, 0.4399567018, -1.2132989554| H, 0.001004492, -0.1123843521, 2.1508049484| H, -0.011270734, 2.3684755366, 2.1590326978| H, -0.011270734, 2.3684755366, -2.1590326978| H, 0.001004492, -0.1123843521, -2.1508049484| O, -0.0206932004, 3.88658557480 .| Br, 0.0109561275, -2.2007237152,0.||Version=x86-Win32-G03RevB.03|State=1-A'|HF=-2878.0100302|RMSD=3.527e-009|RMSF=4.564e-005| Dipole =0.0166232,-3.1390615,0.|PG=CS [SG(C2Br1O1),X(C4H4)]||@

VII.2.17. 4-CHLOROPHENOL

VII.2.17.1. Neutral form of 4-chlorophenol

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C6H5Cl1O1|PCUSER|11-Nov-2020|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||p-clorofenol|| 0,1| C,-0.0152932215,-0.2731448669,1.2143304853| C,0.0212070612,1.1208742585,1.2096235628| C,0.0444516734, 1.818738812, 0.| C, 0.0212070612, 1.1208742585, -1.2096235628| C, -0.0152932215,-0.2731448669, -1.2143304853| C,-0.0304865284, -0.9582725437, 0.| H, -0.0340588004,-

0.8228172986, 2.1487681391| H, 0.0234635092, 1.6773983165, 2.1412981803| H, 0.0234635092, 1.6773983165, -2.1412981803| H,- 0.0340588004, -0.8228172986,-2.1487681391| H, 0.9355232562, 3.5317556134, 0.| Cl, -0.0753445646, -2.7182719286, 0.| O, 0.0264709972, 3.2042693535, 0. ||Version=x86-Win32-G03RevB.03|State=1-A'|HF=-767.0661635| RMSD=3.884e-009| RMSF=1.689e-005|Dipole=0.6146073,0.6132529,0.|PG=CS [SG(C2H1Cl1O1),X(C4H4)]||@

VII.2.17.2. Neutral radical of deprotonated 4-chlorophenol

1\1\GINC-COPERNICO\FOpt\UB3LYP\6-31G(d,p)\C6H4Cl1O1(2)\IVAN\12-May-2021\0\\# opt b3lyp/6-31g(d,p) geom=connectivity\\p-clorofenolradical\\0,2\ C,-0.0103274528,-0.2632203068, 1.2327943473\ C, -0.0179030923, 1.1122072934, 1.2383290384\ C, -0.0223494411, 1.8735938522, 0.\ C, -0.0179030923, 1.1122072934, -1.2383290384\ C, -0.0103274528, -0.2632203068, -1.2327943473\ C,-0.006720381, -0.9485920138, 0.\ H,-0.0070917608, -0.8307886794, 2.1571204599\ H,-0.0208107371,1.6750243204,2.1659559093\ H,-0.0208107371,1.6750243204, -2.1659559093\ H, -0.0070917608, -0.8307886794,-2.1571204599\ Cl, 0.0024529047, -2.6917606072, 0.\ O, -0.0297319966, 3.1286095134, 0.\\ Version=AM64L-G09RevD.01\ State=2-A'\ HF=-766.4303117\ S2=0.787312\S21=0.\ S2A =0.750961\RMSD=4.399e-09\ RMSF=1.162e-05\ Dipole= 0.005489, 0.8959848, 0.\ Quadrupole=0.7919166,-7.8139717,7.0220552,0.0498014,0.,0.\PG=CS [SG(C2Cl1O1),X(C4H4)]\\@

VII.2.17.3. 4-Chlorophenolate anion

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C6H4Cl1O1(1-)|PCUSER|11-Nov-2020| ||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||p-clorofenolato||-1,1| C,0.001467876,-0.2080895168, 1.2121134158|C,-0.0058518901,1.1795010929,1.213727591|C,-0.0109109262, 1.9771393728,0.| C, -0.0058518901, 1.1795010929, -1.213727591| C, 0.001467876, -0.2080895168, -1.2121134158| C, 0.005057519, -0.9054268664, 0.| H, 0.0046046026, -0.7610638845, 2.1497491488| H, -0.0087323731, 1.7206836427, 2.1584029202| H, -0.0087323731, 1.7206836427, -2.1584029202| H, 0.0046046026, -0.7610638845, -2.1497491488| Cl, 0.0145870135, -2.7015628926, 0.| O, -0.0189993846, 3.2400144633, 0. ||Version=x86-Win32-G03RevB.03|State=1-A'|HF=-766.4999276|RMSD=3.148e-009| RMSF =5.152e-005|Dipole=0.0120822,-2.0324666,0.|PG=CS [SG(C2Cl1O1),X(C4H4)]||@

VII.2.18. 2-CHLOROPHENOL

VII.2.18.1. Neutral form of 2-chlorophenol

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C6H5Cl1O1|PCUSER|15-Jan-2021|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||2-clorofenol|| 0,1| C, 2.1941393846,-0.8651318348,0.0000535399|C,1.0070102522,-1.5904605785,0.0000790235| C,-0.2274266179, -0.9292487951, 0.0000402054| C, -0.2305951098, 0.4736700335, -0.0000233992| C, 0.9542578025, 1.2047441065, -0.0000488047| C, 2.1749869301, 0.5322694294, -0.0000106222| H, 3.1415279243, -1.3952696891, 0.0000839825| H,1.0029592135, -2.6752428975, 0.0001281433| H,0.9108712163, 2.2882544444, -0.0000971883| H, 3.1010801501, 1.0973638339, -0.0000307973| O, -1.3579138932, -1.67805925, 0.000067142| H, -2.1256530763, -1.0855787405, 0.0000403352| Cl, -1.7883358901, 1.3082289931, -0.0000706628|| Version=x86-Win32-G03RevB.03| State=1-A| HF=-767.0747381| RMSD =4.323e-009| RMSF=6.012e-005| Dipole =0.3417075, 0.1077038, 0.0000004| PG=C01 [X(C6H5Cl1O1)]||@

VII.2.18.2. Neutral radical of deprotonated 2-chlorophenol

1\1\GINC-COPERNICO\FOpt\UB3LYP\6-31G(d,p)\C6H4Cl1O1(2)\IVAN\12-May-2021\0\\# opt b3lyp/6-31g(d,p) geom=connectivity\\2-clorofenolradical\\0,2\ C,-2.3731702687, 0.0263327287, 0.0000544211\ C,-1.5499986718,1.1262666998,0.0000798127\C,-0.1004234755,0.9988781149, 0.0000411944\ C,0.4180992996, -0.3740058978, -0.0000246414\ C, -0.4290028434, -1.467016402,-0.0000491749\C,-1.818554379,-1.2725535339,-0.0000101236\ H, -3.4520379969, 0.1476564455, 0.0000836761\ H, -1.9376732809, 2.1397331105, 0.0001294743\ H, -0.0162152719, -2.4699632325, -0.0000984106\ H, -2.4725050977, -2.1390445372, -0.0000300203\ O, 0.6462984511, 1.9993256921, 0.0000652621\ Cl, 2.1366925351, -0.5940611881, -0.0000714699\\ Version=AM64L-G09RevD.01\State=2-A\HF=-766.4287527\ S2=0.787355\S2-1=0.\ S2A=0.750974\ RMSD= 6.311e-09\ RMSF=8.420e-05\ Dipole=-1.352505,-1.0515633,-0.0000119\ Quadrupole = 2.6527802, -0.9957307, -1.6570495, -1.526613, -0.0001585, 0.0000604\ PG=C01 [X(C6H4Cl1O1)]\\@

VII.2.18.3. 2-Chlorophenolate anion

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C6H4Cl1O1(1-)|PCUSER|15-Jan-2021|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||2-clorofenolato||-1,1|C,-2.3418028862,

0.038819621, 0.0000541169| C, -1.5080329494, 1.1460876439, 0.0000803903| C, -0.0571347956, 1.0702993169, 0.0000487584| C, 0.3995492091, -0.3110795337, -0.0000206028 |C, -0.4332119356, -1.4195029494, -0.0000469298| C,-1.8264256163, -1.26677738,-0.0000085181| H, -3.4231891127, 0.1878301616, 0.0000830305| H, -1.9225004167, 2.1528762744, 0.0001282485| H, 0.0113043407, -2.4126606211, -0.0000977695| H, -2.478561238, -2.136396168, -0.0000291109| O, 0.6925456146, 2.0787752027, 0.0000656467| Cl, 2.1691138444, -0.5864077401,-0.0000736977|| Version=x86-Win32-G03RevB.03|State=1-A|HF=-766.5008705|RMSD=6.266e-009|RMSF=4.785e-005|Dipole=-0.7007711,-1.3573639,-0.0000358|PG=C01 [X(C6H4Cl1O1)]||@

VII.2.19. PHENOL

VII.2.19.1. Neutral form of phenol

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C6H6O1|PCUSER|31-Jul-2020|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||fenol||0,1| C, -1.1557552414, -1.2074308884, 0.0187578252| C, 0.239796842,-1.2114272392, 0.008698004| C, 0.935096279, -0.0000705394, -0.0017585128| C, 0.2399766236, 1.2114019975, 0.0071103598| C,-1.1555760365, 1.2076259429, 0.0171752741| C, -1.8567291258, 0.0001509733, 0.0201409381| H, -1.695618063, -2.1502038881, 0.0274011197| H,0.8016403397,-2.1402900658, 0.0173941428| H, 0.801957965, 2.1401920319,0.0145892061| H,-1.6952989379, 2.1504895693, 0.0245829389| H, -2.9425884202, 0.0002374254, 0.0291109513| O, 2.3232374535, -0.0001454078, 0.0411787281 |H,2.6631514437, -0.0007632903, -0.8632515139|| Version=x86-Win32-G03RevB.03|State=1-A'|HF=-307.4721197|RMSD=5.748e-009|RMSF=7.110e-005|Dipole=-0.150108,-0.0003798,-0.596575|PG=CS [SG(C2H2O1),X(C4H4)]||@

VII.2.19.2. Neutral radical of deprotonated phenol

1|1|UNPC-UNK|FOpt|UB3LYP|6-31G(d,p)|C6H5O1(2)|PCUSER|03-May-2021|0||#OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||fenolradical|| 0, 2| C, 0.0063833717, -1.0878429593, 1.2253441895| C, -0.0014804723,0.2901380859,1.2395260559| C, -0.0060706566, 1.0475123501, 0.| C, -0.0014804723, 0.2901380859, -1.2395260559| C, 0.0063833717, -1.0878429593, -1.2253441895| C, 0.0102520978, -1.7851247231, 0.| H, 0.0096500217, -1.6456463577,2.1573934601|H,-0.0045440562, 0.8579460936, 2.1644143093| H, -0.0045440562, 0.8579460936, -2.1644143093| H, 0.0096500217, -1.6456463577, -2.1573934601| H, 0.0162202529, -2.8709673111, 0.| O, -0.013794453, 2.3055625697, 0.|| Version=x86-Win32-G03RevB.03|State =2-A'|HF=-306.8353851|S2=0.789782|S2-1=0.| S2A=

0.751098| RMSD=3.715e-009 |RMSF=8.861e-006|Dipole=0.0086787,-1.4375889,0.|PG=CS [SG(C2H1O1),X(C4H4)]||@

VII.2.19.3. Phenolate anion

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C6H5O1(1-)|PCUSER|05-Aug-2020|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY|| fenoxido|| -1,1| C,0.0065616936 ,-1.101722992, 1.2008349296| C, -0.0011183312, 0.2863689345, 1.2128907591| C, -0.0063559979, 1.0841484279, 0.| C, -0.0011183312, 0.2863689345, -1.2128907591| C,0.0065616936, -1.101722992, -1.2008349296| C, 0.0105232043, -1.8306254115, 0.| H, 0.0097767133, -1.6412383118, 2.1514971539| H, -0.0041751592, 0.8315747093, 2.1566703659| H, -0.0041751592, 0.8315747093, -2.1566703659| H, 0.0097767133, -1.6412383118, -2.1514971539| H, 0.0163929766, -2.918774967, 0.| O,-0.0147399589, 2.3501515955, 0.|| Version=x86-Win32-G03RevB.03|State=1-A'|HF=-306.8923984| RMSD= 9.571e-009| RMSF=4.128e-005| Dipole= 0.0097652, -1.5637012, 0.| PG=CS [SG(C2H1O1),X(C4H4)]||@

VII.2.19.4. Phenol radical cation

1|1|UNPC-UNK|FOpt|UB3LYP|6-31G(d,p)|C6H6O1(1+,2)|PCUSER|07-Jan-2001|0||# B3LYP/6-31G(D,P) FOPT TEST||FFF||1,2| C,0.0086576972,0.03475637,0.9410036549| O,-0.0613559964,0.0823508386,2.2500919949| C,1.2526145686,0.0139798777,0.2296632411| C,-1.2514411546, 0.0039949515, 0.249771044| C,-1.2539047032, -0.046725808, -1.1217668462| C, 1.2231327816, -0.0366452934, -1.1401249604| C, -0.0247710255, -0.0675648612, -1.8280472417| H, -2.1611644228, 0.0218379322, 0.8403078822| H, 2.147135427,-0.0532766186, -1.7078983354| H, -0.0308271581, -0.1078140052, -2.9129211123| H, 2.1902041249, 0.0385362957, 0.778003567| H, 0.8096193861, 0.1021871165, 2.6875048289| H, -2.1898483722, -0.0710488495, -1.6687261395|| Version=x86-Win32-G03RevB.01|State=2-A|HF=-307.1838584|S2=0.764456|S2-1=0.|S2A=0.750118|RMSD=8.526e-009|RMSF=8.4 09e-005|Dipole=0.5701765,0.0029014,0.0106276|PG=C01 [X(C6H6O1)]||@

VII.2.20. 4-AMINOPHENOL

VII.2.20.1. Neutral form of 4-aminophenol

N-N= 3.439851129748D+02 E-N=-1.532619679557D+03 KE= 3.594463108380D+02 1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C6H7N1O1|PCUSER|22-Aug-2020|0||# OPT

B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||p-aminofenol|| 0,1| C,-0.2102540634,-0.6647914799, 1.1963599487| C, -0.1130360375, 0.7229003859, 1.2001992379| C, 0.0948925005, 1.4178589341, 0.0056868384| C,0.2039954845,0.7017412529,-1.1879199939| C, 0.1064451902,-0.6898484381,-1.1883763069| C,-0.1018843538,-1.39802653, 0.002989437| H, -0.3774425742, -1.1905300935, 2.1332999803| H, -0.1953380156, 1.2828366328, 2.1259807149| H, 0.3686511281, 1.2281013174, -2.1261407235| H, 0.188988073,-1.2304377502, -2.128020214| O, 0.1857553772, 2.7873046232, 0.0705583364| H, 0.3182545392, 3.132159734, -0.8216384037| N, -0.2644827499, -2.794823618,-0.0026699892| H, 0.1973218985, -3.2574095215, -0.7752400328| H, -0.0160511406, -3.2383967288, 0.8723469445|| Version=x86-Win32-G03RevB.03| State=1-A| HF=-362.8334204| RMSD=5.372e-009|RMSF=7.632e-006| Dipole= 0.4902723, -0.4744569, -0.4527083| PG=C01 [X(C6H7N1O1)]||@

VII.2.20.2. Neutral radical of deprotonated 4-aminophenol

1\1\GINC-COPERNICO\FOpt\UB3LYP\6-31G(d,p)\C6H6N1O1(2)\IVAN\20-May-2021\0\\# opt b3lyp/6-31g(d,p) geom=connectivity\\p-aminofenolradical\\0,2\C,-0.6814137003, 1.2291770886, 0.0143295127\ C, 0.6896794247, 1.2493993387, -0.0017361835\ C, 1.474158652, 0.0254368465, -0.0096523878\ C,0.7149213239 ,-1.2144795854, -0.0014779737\ C,-0.6562258806,-1.2224392248, 0.0145553373\ C, -1.3881275616,-0.0039668262, 0.0255505662\ H, -1.2474328159, 2.1582604238, 0.0178025971\ H, 1.2387459596, 2.1855648566, -0.0070318139\ H, 1.2833248321, -2.1390350006, -0.0066347295\ H, -1.2031191205, -2.1629076001, 0.0181273407\ O, 2.7288657916, 0.038254115, -0.0214291167\ N, -2.7599056477, -0.0181467273, 0.0066793021\ H, -3.2410686738, -0.8758393627, 0.2289205256\ H, -3.2586465834, 0.8296586579, 0.2281160235 \\Version=AM64L-G09RevD.01\State=2-A\ HF=-362.2039793\S2=0.773305\ S2-1=0.\ S2A=0.750352\ RMSD=7.590e-09\ RMSF=2.407e-05\ Dipole=-2.5613419, -0.0261878, 0.2942505\ Quadrupole=-1.3189093, 4.0289561,-2.7100467,-0.0554777,-1.7737557,-0.0195776\PG=C01 [X(C6H6N1 O1)]\\@

VII.2.20.3. 4-Aminophenolate anion

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C6H6N1O1(1-)|PCUSER|22-Aug-2020|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY|| p-aminofenolato|| -1,1| C,-0.6371530797, 1.1906592209, -0.023603212| C, 0.7543030042, 1.2139931542, 0.0043091794| C, 1.568656997, 0.0158945984, 0.0211861886| C, 0.7787454554, -1.1983944158, 0.0053599138| C, -0.612958423, -1.2031761435, -0.0221854491| C, -1.3548100091, -0.0136728263 ,-

0.0348513302| H, -1.1910342621, 2.133851367, -0.0370944042| H, 1.2817056635, 2.1672820473, 0.0201805812| H, 1.3253046417, -2.1408156952, 0.0221091874| H, -1.1476024191, -2.1574589514, -0.0342500679| O, 2.8374015207, 0.028851509,0.0525363045| N, -2.8030752776, -0.028038392, -0.1214710483| H, -3.1549162116, -0.8456031266, 0.3742901833| H, -3.1718463041, 0.7763795044, 0.3834796797 ||Version=x86-Win32-G03RevB.03|State=1-A|HF=-362.240306| RMSD=2.726e-009| RMSF=2.786e-005|Dipole=-2.4894226,-0.0277356, 0.5062159|PG=C01 [X(C6H6N1O1)]||@

VII.2.20.4. 4-Aminophenol radical cation

1|1|UNPC-UNK|FOpt|UB3LYP|6-31G(d,p)|C6H7N1O1(1+,2)|PCUSER|02-Jan-2001| 0||#T B3LYP/6-31G(D,P) FOPT TEST||ggg||1,2|C,0.0203222856,-0.0400883132,1.4071329875|O,-0.0400907439,-0.0803758698,2.7307360924| C,1.2432477567,0.0181858235,0.6839472396|C,-1.2262766971,-0.0577487548,0.7180778551| C,-1.2510251839,-0.0189664153,-0.6481554327| C,1.2229147686,0.0572022535,-0.6853574563|C,-0.0254673144,0.039471351,-1.3886099661| H, -2.138021839, -0.1021569836, 1.3031578261| H, -2.1965098062, -0.0321349365,-1.1812064203| H,2.1889001624,0.0316674353,1.2180328562| H,2.1511988032,0.1018021479,-1.2462705269| N, -0.045264696, 0.0768247894, -2.7278119418| H, 0.8372693978,-0.0658832971, 3.1470902115| H,-0.9157724077,0.0652726894,-3.244080008| H,0.8082208201, 0.1183307083,-3.2701404475||Version=x86-Win32-G03RevB.01|State=2-A|HF=-362.5872368| S2=0.758799|S2-1=0.|S2A=0.750038|RMSD=9.932e-009| RMSF=2.247e-005|Dipole= 0.5500134, 0.0508871,-1.1874344|PG=C01 [X(C6H7N1O1)]||@

VII.2.21. 3-AMINOPHENOL

VII.2.21.1. Neutral form of 3-aminophenol

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C6H7N1O1|PCUSER|13-Jan-2021|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||3-aminofenol||0,1|C,0.077223719, -0.3286422727, 1.2056772487| C, 0.0553369075, -0.9996039169, -0.0174918353| C,-0.0498616663, -0.2779890898, -1.2143641757| C, -0.1295689235, 1.1266177209, -1.1657319709| C, -0.1052740498, 1.7778377418, 0.0628608422| C, -0.0018143, 1.067136842, 1.2594405859| H, 0.1160125436, -2.0836307703,-0.0217436558| H,-0.217021801, 1.6942061108, -2.0879226702| H, -0.1655985931, 2.8622006345, 0.0919309043| H, 0.0180691502, 1.5843192033, 2.2154980745| O, 0.1832323334, -1.1004454435, 2.3315116726| H, 0.1849360821, -0.5213144343, 3.1046383964| N, -0.1302242373, -0.9488628969, -2.4363199624| H, 0.158571076, -0.4072701253, -3.2392778159| H, 0.2744924138, -

1.8750489431, -2.4433210473|| Version=x86-Win32-G03RevB.03| State=1-A| HF=-362.8373837| RMSD=6.539e-009| RMSF=5.125e-005| Dipole=0.4030379,0.2188927,-0.1973693|PG=C01 [X(C6H7N1O1)]||@

VII.2.21.2. Neutral radical of deprotonated 3-aminophenol

1\1\GINC-COPERNICO\FOpt\UB3LYP\6-31G(d,p)\C6H6N1O1(2)\IVAN\12-May-2021\0\\# opt b3lyp/6-31g(d,p) geom=connectivity\\3-aminofenolradical\\0,2\C,-1.2497997365,-0.3746246414,0.0008924759\C,0.0394266069,-1.0276682555,0.0018474815\C,1.2169438502,-0.3012002074, -0.0023251688\ C, 1.1453581756, 1.1235701941, -0.0034453841\ C,-0.0879489055, 1.791855477,0.0025047115\C,-1.2707135347, 1.0815629297, 0.0026166276\ H, 0.0420149231, -2.1135977371, 0.0035994002\ H, 2.0691790829, 1.6961717484, -0.0175393295\ H, -0.0975321451, 2.8779753464, 0.0045646176\ H, -2.2413112464, 1.5654560595, 0.0051787539\ O, -2.3225252626,-1.0311548918, 0.0070978509\ N, 2.4663058988, -0.9108509734, -0.064624506\ H, 3.2345226202, -0.3852706152, 0.3280937284\ H, 2.4892366732, -1.8848984332,0.2026557409\\Version=AM64L-G09RevD.01\State=2-A\HF=-362.1948797\S2=0.789962\S2-1=0.\S2A=0.751083\RMSD=8.934e-09\RMSF=2.10 2e-05\ Dipole=1.7738867, 0.5960954, 0.3973937\ Quadrupole= -0.6405042,3.1679589,-2.5274548,-4.614068,2.4144809,-0.8284702\PG=C01 [X(C6H6N1O1)]\\@

VII.2.21.3. 3-Aminophenolate anion

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C6H6N1O1(1-)|PCUSER|13-Jan-2021|0| |# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||3-aminofenolato||-1,1|C,-1.3318662639,-0.4091642865,0.012224342|C,-0.0135467446,-1.0110890573,-0.0172710283|C,1.1616345696,-0.2689215902,-0.0369950186| C,1.1304142986,1.13795606,-0.0219356959|C,-0.1276224783, 1.763080489,0.0091610733| C,-1.310980481,1.0432165539,0.0271801768|H,0.0307974053,-2.1012964022,-0.0223565808| H,2.053206371,1.7145202111,-0.0558794532|H,-0.1677156779, 2.8549483317, 0.0228442308| H, -2.2736965071, 1.5514155171, 0.0562984056| O,-2.3998218206, -1.0876778556, 0.0346103351| N, 2.4324810787, -0.9349462772, -0.1163958472| H, 3.1249223627, -0.4324354424, 0.4328357093| H, 2.3554956589, -1.8715744437, 0.2699628417|| Version=x86-Win32-G03RevB.03|State=1-A|HF=-362.2482686| RMSD=8.471e-009| RMSF=9.823e-005| Dipole= 2.1031871, 0.4825329, 0.4859397|PG=C01 [X(C6H6N1O1)]||@

VII.2.21.4. 3-Aminophenol radical cation

1|1|UNPC-UNK|FOpt|UB3LYP|6-31G(d,p)|C6H7N1O1(1+,2)|PCUSER|04-Jan-2001 0||#T B3LYP/6-31G(D,P) FOPT TEST||ggg||1,2| C,-0.3536659243,0.018424971,1.2073288071| O,-0.5290242249,0.0329221628,2.5274996522| C,0.8726409364,-0.0182970438,0.5712046677| C,-1.5769749698,0.0443727861,0.4470668089| C,-1.5401795541,0.0323905953,-0.949098813| C, 0.9043770553,-0.0297685631 ,-0.8430614071| C, -0.3252883084, -0.0042318438, -1.6061760809| H, -2.5129907851, 0.0731621591, 0.9946231592| H, -2.4652327356, 0.0517381835, -1.5140463082| H,1.7989164326,-0.0383337086, 1.1371314121| N, 2.0636927775, -0.0648981707,-1.5105807724| H, 0.3101564727,0.0143438817,3.0139702251| H, -0.2750417245, -0.0145293608, -2.6904132692| H, 2.9538092315, -0.0820068064,-1.0286198719| H, 2.0912720549, -0.0708098649, -2.5221610549|| Version=x86-Win32-G03RevB.01|State=2-A| HF=-362.5771178| S2=0.770857| S2-1=0.| S2A=0.750237| RMSD=9.768e-009| RMSF=2.827e-005|Dipole=1.3324101,-0.0384423,-0.8353172| PG=C01 [X(C6H7N1O1)]||@

VII.2.22. 2-AMINOPHENOL

VII.2.22.1. Neutral form of deprotonated 2-aminophenol

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C6H7N1O1|PCUSER|23-Aug-2020|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||o-aminofenol||0,1|C,-0.0639044831,-1.2767915987,0.8647297861| C,0.0083003941,0.1159591457,0.8404872134| C, 0.0399260046, 0.7901357358,-0.3955926815| C,-0.0008937374, 0.0661137474, -1.5913133801| C,-0.0729484533, -1.3247381172, -1.5480645131| C, -0.1048644744, -2.0037284406,-0.3265068263| H, -0.0879366189, -1.7901868352, 1.8233109724| H, 0.0244851961, 0.6045750792, -2.5327835176| H, -0.104536413, -1.8846621687, -2.4784044415| H,-0.1610175944, -3.0873340644, -0.3017410442| O, 0.1100624914, 2.1424032882, -0.412650213| H, 0.1254676965, 2.3893840549, 0.5356473753|N,0.0559073815, 0.9725432353, 2.0033257446| H, -0.7681677092, 0.8522022949, 2.5869036129| H, 0.866162338, 0.7672898518, 2.5825509438|| Version=x86-Win32-G03RevB.03|State=1-A|HF=-362.837236|RMSD=9.227e-009|RMSF=1.653e-006|Dipole=-0.0191633,-0.4190078, 0.9647124| PG=C01 [X(C6H7N1O1)]||@

VII.2.22.2. Neutral radical of deprotonated 2-aminophenol

1\1\GINC-COPERNICO\FOpt\UB3LYP\6-31G(d,p)\C6H6N1O1(2)\IVAN\12-May-2021\0\\# opt b3lyp/6-31g(d,p) geom=connectivity\\2-aminofenolradiical\\0,2\ C,-1.9549222232,

0.5701134974, -0.0053452193\ C,-0.8199026461,1.3344719978, 0.1034955372\ C,0.48979905,0.7288636562,0.1110969115\ C,0.5393367707,-0.7450203309,-0.0043284865\ C, -0.6437480988, -1.4942227687, -0.1137923044\ C, -1.8686001672, -0.8446101732, -0.114029153\ H,-2.9331597097,1.0417398775, -0.0094792349\ H,-0.8588843485, 2.4156188605, 0.1877562945\ H,-0.5931480884, -2.5768191095, -0.1974874706\ H,-2.7804317243,-1.4280320446,-0.1988798059\ O,1.5644381486, 1.3700812341, 0.2079118658\ N,1.7820088446,-1.2683188769,0.006301224\H,2.5407733533,-0.6032685229,0.0917724337\ H,1.9613098391,-2.2552442967,-0.0640935921\\Version=AM64L-G09RevD.01\State=2-A\ HF= -362.2118834\S2=0.766616\S2-1=0.\S2A=0.750187\RMSD=9.124e-09\RMSF=2.640e-05\Dipole=-0.2831058,-1.3341115,-0.1178826\Quadrupole=2.3240791,1.2418147,-3.5658938,-5.7834177,-0.2095962,0.1344384\PG=C01 [X(C6H6N1O1)]\\@

VII.2.22.3. 2-Aminophenolate anion

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C6H6N1O1(1-)|PCUSER|23-Aug-2020|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||o-aminofenolato||-1,1|C,-0.5005071371,-1.3907385441,-0.0000230987|C,0.640291948,-0.5907745064,-0.0000239219| C, 0.5472022452, 0.8700656554, 0.0000160594| C, -0.8252769173, 1.353799882, 0.0000256776| C,-1.9369193652,0.5269437523,0.0000097359| C,-1.8028418949, -0.8711489891, -0.0000146781| H, -0.3601622516, -2.4764462496, -0.0000410888| H, -0.9421801198, 2.4373450514, 0.0000441073| H,-2.9350518189, 0.9718023868, 0.0000168407| H, -2.6703402614,-1.5277463001, -0.0000271394| O, 1.5372919789, 1.6503506773, 0.0000447015| N, 1.9671630314, -1.1961362814, -0.0000692143| H, 2.0539314186, -1.8116056376, 0.8085793139| H, 2.0536327106, -1.8120842, -0.8083837916|| Version=x86-Win32-G03RevB.03|State=1-A|HF= -362.2337583|RMSD=3.410e-009|RMSF=1.292e-004|Dipole=-0.963071,-1.6526958,0.0001674|PG=C01 [X(C6H6N1O1)]||@

VII.2.22.4. 2-Aminophenol radical cation

1|1|UNPC-UNK|FOpt|UB3LYP|6-31G(d,p)|C6H7N1O1(1+,2)|PCUSER|05-Jan-2001 0||#T B3LYP/6-31G(D,P) FOPT TEST||ggg||1,2|C,-0.4426591928,0.0767588322,1.1701813859|O,-0.623250965, 0.1699988916, 2.4647408241| C, 0.93812963, 0.069952647, 0.5943299648|C,-1.5898503597, -0.0141453541, 0.3731652677| C,-1.4694918353, -0.1165033857,-1.0191688852| C, 1.007617374, -0.0433378885, -0.9271371553| C, -0.2308679432,-0.1320762465, -1.6603483687| H, -2.5601037765, -0.0032181966, 0.858230727| H, -2.374878174, -0.1857578595, -1.6142585401| H, 1.4989592048,-0.763068252, 1.0451994763| N, 2.1001502448,-0.065905915,-1.6153166004|H,0.2038107045, 0.2306186351,2.9745182482|

H, -0.1547688139, -0.2118499386, -2.7396950064| H, 2.9425084026, 0.0008677487, -1.033193102| H, 1.4521624217, 0.9898665089, 0.9123545511|| Version=x86-Win32-G03RevB.01|State=2-A|HF=-362.5233411|S2=0.776794|S2-1=0.|S2A=0.750374|RMSD=9.02 7e-009| RMSF=1.364e-005| Dipole= 0.020877, 0.087524, 1.1503612| PG=C01 [X(C6 H7N1O1)]||@

VII.2.23. 4-METHOXYPHENOL

VII.2.23.1. Neutral form of 4-Methoxyphenol

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C7H8O2|PCUSER|13-Jan-2021|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||4-metoxifenol||0,1| C, 0.9704982704,-0.0000003454, 0.1689823634| C,0.2731572524, -1.2106987125, 0.1679788685| C, -1.1214511451,-1.2101584767, 0.1709224786| C, -1.8193206201, 0.0000005017, 0.1748122429| C, -1.1214504131,1.2101590589,0.1709218607| C,0.2731579816,1.2106984432, 0.1679782422| H, 0.8310878279,-2.1418379737,0.1770758566| H, -1.6804188108,-2.1407126762,0.1664188144| H, -1.6804175323, 2.1407135818, 0.1664177503| H, 0.8310891131, 2.1418373781, 0.1770747769| O,-3.2071099712, 0.0000009473, 0.1259185258| H, -3.5509955147, 0.0000005806, 1.0287592568| O, 2.3516825287,-0.0000007858, 0.2141588267| C, 2.9808979091, -0.0000005737, -1.064853808| H, 2.7111271176, 0.8918263847, -1.6462850622| H, 4.0578852464, -0.0000008634, -0.8842481571| H, 2.7111266815, -0.8918270766,-1.646285545 ||Version=x86-Win32-G03RevB.03|State=1-A|HF=-421.99166|RMSD=6.067e-009 |RMSF=1.946e-005|Dipole=0.0550943,-0.0000001,0.0836256|PG=C01 [X(C7H8O2)]||@

VII.2.23.2. Neutral radical of deprotonated 4-Methoxyphenol

1|1|UNPC-UNK|FOpt|UB3LYP|6-31G(d,p)|C7H7O2(2)|PCUSER|27-May-2021|0||#T B3LYP/6-31G(D,P) FOPT TEST||hydrazide Single Point||0,2|C,-1.3534771143, 0.1596508446,-0.2600607098| C, -1.4498068018, 0.0645727286, 1.1024748925| C,-0.0874490803, 0.0780549974, -0.8974577922| C, 1.0875241211, -0.1019416371, -0.1331286769| C,-0.2713506555,-0.1214191886,1.9349702035| C,0.9999085211, -0.1986414598, 1.2389877159| H, -2.4079989649, 0.1245866885, 1.6082461278| O, -0.1166281118, 0.1850160545, -2.2445560828|H,-2.2272265501,0.2983886645, -0.8890257535|O,-0.3472105338,-0.2097190569,3.1854371314| H, 2.0547520937, -0.1642959827,-0.618357293| H, 1.8867320549, -0.3370305204, 1.8489945233| C,1.1054319432,0.115524601,-2.9748971056| H, 1.6037814804, -0.849219605,-2.8271079953|H,1.785891799,0.9262491282,-2.6911553288| H,0.8300916505,0.224140331,-4.0239738343||Version=x86-Win32-G03RevB.01|State=2-A|

HF=-421.3664318|S2=0.777947|S2-1=0.|S2A=0.750526|RMSD=9.387e-009|RMSF=2.354e-005|Dipole=0.6654342,0.0843938,-1.9844064|PG=C01 [X(C7H7O2)]||@

VII.2.23.3. 4-Methoxyphenolate anion

N-N= 4.097117745482D+02 E-N=-1.814535249777D+03 KE= 4.176630656200D+021|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C7H7O2(1-)|PCUSER|14-Jan-2021|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||4-metoxifenolato||-1,1| C, 0.8891264234, 0.0000000832, -0.3311875215| C, 0.1860785226, 1.2059383162, -0.2208322514| C,-1.1865848136,1.2132659449,-0.0076089078|C,-1.9742589859,-0.000000054,0.1199040254| C, -1.1865848242, -1.2132659575, -0.0076096161| C, 0.1860785141, -1.2059382049, -0.2208329677| H, 0.7382126071, 2.1418567, -0.3182119528| H,-1.7248590388, 2.1572030803, 0.0677438261| H, -1.7248590454, -2.157203141, 0.0677425478| H, 0.7382126006, -2.1418565324 ,-0.3182131976| O, -3.2242813864, -0.0000000929, 0.3179690809| O, 2.2806346387, 0.0000001456, -0.5696973921| C, 3.042044656,-0.0000001208, 0.6185840934| H, 2.8419030051, -0.8885962254, 1.2384576122| H, 4.1032640057, 0.0000000193,0.335348446| H, 2.8419028922, 0.888595628, 1.2384580815|| Version=x86-Win32-G03RevB.03|State=1-A|HF=-421.4138148|RMSD=8.982e-009|RMSF=4.959e-005|Dipole=2.7915884,0.,0.2479319|PG=C01 [X(C7H7O2)]||@

VII.2.23.4. 4-Methoxyphenol radical cation

1|1|UNPC-UNK|FOpt|UB3LYP|6-31G(d,p)|C7H8O2(1+,2)|PCUSER|03-Jan-2001|0| |#T B3LYP/6-31G(D,P) FOPT TEST||ggg||1,2|C,0.0871712345,-0.3121744245, 1.8171496122| O,-0.0371874304,-0.5036946192,3.1191364637|C,1.3289940912, 0.4128051199,1.1274163393|C,-1.1144784247,0.0092480231,1.1144724538| C,-1.0841582276,0.2252004214,-0.2379015705| C,1.3626500024,-0.1978283236,-0.222666461|C,0.1586684168,0.1252188752,-0.9326901358| H,-2.0366553099,0.0749754355,1.6813990718| H,-1.995898085,0.4687061045,-0.7688272136| H, 2.2362034806, -0.6577628443, 1.6721031041| H, 2.2845814406, -0.2635424449, -0.7898270603|O,0.3142361827,0.3097671045,-2.2246836794|H,0.8062275034,-0.7194160541, 3.5520528917| C, -0.8000156683, 0.6434130833, -3.0925150422| H, -1.5405785172, -0.1593611379, -3.0724850733| H, -1.2393622664, 1.5950241516, -2.7848562311| H, -0.3638968108, 0.7311616972, -4.0847729376|| Version=x86-Win32-G03RevB.01|State=2-A|HF=-421.7376583|S2=0.756942|S2-1=0.|S2A=0.750018|RMSD=4.676e-009|RMSF=7.920e-006|Dipole=0.1010092,-0.038571,0.1302214|PG=C01 [X(C7H8O2)]||@

VII.2.24. 3-METHOXYPHENOL

VII.2.24.1. Neutral form of 3-Methoxyphenol

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C7H8O2|PCUSER|13-Jan-2021|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||3-metoxifenol||0,1|C,-0.0041928069,-0.3289463371,1.6497203293|C,-0.0368277826,-0.980561308,0.419474819|C,-0.0133702376,-0.2325046343,-0.7627944191|C,0.0425870131,1.167692714,-0.7178603052| C,0.0744975227, 1.7987528156,0.5275619911|C,0.0520116633,1.0707892616,1.713223516|H,-0.080101366,-2.0623344907,0.3736844065| H, 0.0611245547,1.7606303618,-1.6233162563| H, 0.1179803365, 2.8832697345, 0.5700606234|H,0.0774862416,1.5763192374,2.6755005401|O,-0.0485989081,-0.9656462363,-1.9145719481|O,-0.0290523753,-1.1117359262, 2.7707842349| H, -0.0022889119, -0.5416671986, 3.5501653881| C, -0.0283057561, -0.2726831232, -3.152034451| H, 0.8883996377, 0.3189025739, -3.2712416506| H,-0.0624736419, -1.0399901267, -3.9269098652| H, -0.8973142785, 0.3886908766, -3.2613903604|| Version=x86-Win32-G03RevB.03|State=1-A|HF=-422.0035472|RMSD=6.577e-009| RMSF= 1.160e-005| Dipole=0.0296001,0.7673916,-0.1078609|PG=C01 [X(C7H8O2)]||@

VII.2.24.2. Neutral radical of deprotonated 3-Methoxyphenol

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C7H7O2(1-)|PCUSER|13-Jan-2021|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||3-metoxifenolato||-1,1|C,1.770908776,-0.4350031684,-0.0001508018|C,0.4399333728,-1.0059368042,-0.0000904432|C,-0.7089629241, -0.227867044, -0.0000227576| C, -0.6618374975, 1.1768851967,0.0000292088| C, 0.618108275, 1.7664521895, 0.000076604| C,1.7813263273, 1.0199347521, 0.0000218575| H, 0.3448203364,-2.0889825292,-0.00011186| H, -1.5540239349,1.7919266353,0.0000962236| H, 0.6836987069,2.8566510222,0.0001596754| H,2.7557579547,1.5061986078,0.0000888576| O,-1.9147282968, -0.9425989251,-0.0000610084| O,2.8254520672,-1.1319897852,-0.0000486772| C, -3.104152905, -0.1999470837, 0.0001438937| H, -3.2003468182, 0.4434211987, -0.8889504535| H, -3.9275004377, -0.9228661011, 0.0001681079| H, -3.2001365171, 0.4432526207, 0.8893815647|| Version=x86-Win32-G03RevB.03|State=1-A|HF=-421.41819|RMSD=6.132e-009|RMSF=6.749e-005| Dipole= -2.8130632, 0.9976408, 0.0001092| PG=C01 [X(C7H7O2)]||@

VII.2.24.4. 3-Methoxyphenol radical cation

1|1|UNPC-UNK|FOpt|UB3LYP|6-31G(d,p)|C7H8O2(1+,2)|PCUSER|04-Jan-2001|0 |#T B3LYP/6-31G(D,P) FOPT TEST||ggg||1,2|C,-0.6644647614,0.3329029982,1.3204804653|O,-

0.7603298417,0.4924333247,2.6319031301|C,0.4903135684,-0.0828659845,0.6610480263|C,-1.8823165589,0.6306116404,0.6003585629| C,-1.9195332977,0.5044743016,-0.7825458879| C,0.4355051679, -0.2047182959 ,-0.7317061628| C, -0.7811719413, 0.0917569686, -1.461209241| H, -2.7438737333, 0.9491441045, 1.1774401023| H ,-2.8301486221, 0.7265633418,-1.3270364371| H,1.3946858693,-0.3019009502,1.215651604|O,1.4287601066,-0.5831809084, -1.5074025773| H,0.0669183963,0.2881322345,3.0987577857| H,-0.75747377 7, -0.0226377689, -2.5395826077| C, 2.7237432523, -0.9215736148, -0.9549529498| H, 2.6264737077, -1.7706265353, -0.2734647756| H, 3.148310875, -0.0534851028,-0.4441889136| H, 3.3352125893,-1.1927367363,-1.8124180584||Version=x86-Win32-G03RevB.01|State=2-A|HF=-421.72925|S2=0.767629|S2-1=0.|S2A=0.750136|RMSD=6.689e-009|RMSF=4.420e-005|Dipole=0.4718019,-0.1073274,0.3608199|PG=C01 [X(C7H8O2)]||@

VII.2.25. 2-METHOXYPHENOL

VII.2.25.1. Neutral form of 2-Methoxyphenol

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C7H8O2|PCUSER|14-Jan-2021|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||2-metoxifenol||0,1| C,2.1226301175,-1.0652120762,-0.0502080293| C, 0.9092326635, -1.7599915512, -0.0143223977| C, -0.2913109962,-1.059214781, 0.0135349555| C,-0.2775352259, 0.3510787798, 0.0053087695| C,0.9298926835, 1.0417509808,-0.0302312817| C,2.1347283666,0.3265431197,-0.0579647414|H,3.055566129,-1.619825665,-0.0717604727| H,0.8755363221,-2.8444470029,-0.0075659883|H,0.9445249107, 2.1256383463, -0.0365079757| H, 3.0748125044, 0.8682736815, -0.0855544293| O,-1.477222786, -1.729830131,0.0482425599| H, -2.1788265589,-1.0605330961, 0.0630505568| O, -1.534161097,0.9131111903,0.0354384967| C,-1.6344655487,2.3284740907, 0.0304911645| H, -1.1929910123, 2.7575819034, -0.8775785921| H, -2.7003074738, 2.5593617858, 0.0571386446| H, -1.1462809782, 2.7671301973, 0.9096791674|| Version=x86-Win32-G03RevB.03|State=1-A|HF=-422.0049569|RMSD=7.707e-009|RMSF=2.117e-005|Dipole=-0.2075813,1.0487668,-0.0001803|PG=C01 [X(C7H8O2)]||@

VII.2.25.2. Neutral radical of deprotonated 4-Methoxyphenol

1\1\GINC-COPERNICO\FOpt\UB3LYP\6-31G(d,p)\C7H7O2(2)\IVAN\12-May-2021\ 0 \\#opt b3lyp/6-31g(d,p) geom=connectivity\\2-metoxifenolradical\\0,2\ C,-2.3103291794,-0.5739722067, 0.0000210134\ C, -1.8807829454, 0.7314421602, -0.0000051964\ C,-0.471077914, 1.0705471282,-0.0000136923\ C, 0.4729368261,-0.0643136301, 0.0000215228\ C, 0.007450086, -1.3767662263,0.000048213\ C,-1.3693476241,-1.6280267424, 0.0000446238\

H, -3.3713608575, -0.8048553479, 0.0000220769\ H, -2.5722516052, 1.5678833464, -0.000019196\ H, 0.6990780278, -2.2113635409, 0.0000744833\ H, -1.7163238826, -2.6569478329, 0.0000661409\ O, -0.0654726578, 2.2523049488, -0.0000236535\ O, 1.7643291462, 0.3003410674, 0.0000276459\ C, 2.7625685022,-0.7148096454, 0.0000260333\ H, 2.6894202141, -1.344203287, -0.8946768401\ H, 3.7183941379, -0.1911307534, -0.0000089192\ H, 2.6894657256,-1.3441654381,0.8947597442\\Version=AM64L-G09RevD.01\State=2-A\HF=-421.3630731\S2=0.779672\S2-1=0.\S2A=0.75061\RMSD=7.243e-09\RMSF= 3.886e-05\ Dipole=0.1635729, -1.7863084, 0.0000209\ Quadrupole=6.8764503,-4.5318612,-2.3445891,-2.545551,0.0000168,0.0000023\PG=C01 [X(C7H7O2)]\\@

VII.2.25.3. 2-Methoxyphenolate anion

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C7H7O2(1-)|PCUSER|14-Jan-2021|0||#OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||2-metoxifenolato||-1,1|C,-2.2724379377,-0.5831904154, 0.0000222018| C, -1.8413025135, 0.7425536965, -0.0000139151| C, -0.4526220902, 1.1299679801,-0.0000780434|C,0.4565657728,-0.017959632,-0.000018368| C, 0.0162632809,-1.3331665208,0.0000168501| C,-1.3617259917,-1.6409420184,0.0000265542| H, -3.3437480316, -0.7954262347, 0.0000502193| H, -2.5619430449, 1.5593922514, 0.0000030885| H, 0.7342876802, -2.1510845574, 0.0000409561| H, -1.6916436118, -2.6774192814, 0.0000578397| O, -0.0437749709, 2.3247936658, -0.000016896| O, 1.8044916197, 0.3426984699, -0.0000029057|C,2.7421779039,-0.6918648062,0.0000277456| H, 2.6612994631, -1.3419669398,-0.8888863547|H,3.733180637,-0.2239248011,-0.0000011228| H, 2.66132317, -1.3418972259, 0.8889956362|| Version=x86-Win32-G03RevB.03|State=1-A|HF=-421.4115051| RMSD=4.815e-009| RMSF=2.638e-005| Dipole =0.8533684,-1.9266937,0.000009|PG=C01 [X(C7H7O2)]||@

VII.2.25.4. 2-Methoxyphenol radical cation

1|1|UNPC-UNK|FOpt|UB3LYP|6-31G(d,p)|C7H8O2(1+,2)|PCUSER|05-Jan-2001|0||#T B3LYP/6-31G(D,P) FOPT TEST||FFF||1,2|C,-0.7280936323,0.0362335189, 0.840504966|O,-0.6241386451,0.0859175458,2.1497889251|C,0.4759467387,- 0.0021879297,0.0153427399|C,-2.00439952, 0.0211517016, 0.2411303407| C, -2.084924876, -0.0300604902,-1.1299495294| C, 0.3636860899, -0.0539438125, -1.3808470278| C, -0.9027534529, -0.0674194452, -1.9391251062| H, -2.8798865351, 0.0503588805, 0.8795792999| H, -3.054558522, -0.0428228999, -1.61583327| O, 1.587145652, 0.0180584526, 0.7309361202| H, 1.2454160389,-0.0826531814, -2.0085337595| H, 0.3120871712, 0.0895252639, 2.4275711514| H, -1.0077074017, -0.1070812466,-3.0183455732|C,2.8921657434,-0.0155705929, 0.0892518372|

H ,2.99362599,-0.9398706019,-0.4835246004|H,3.0072174711,0.862269711,-0.5501841625|H, 3.6099871866,0.0092483873,0.9056212301||Version=x86-Win32-G03RevB.01|State=2-A|HF=-421.733422|S2=0.759832|S2-1=0.|S2A=0.750061|RMSD=5.987e-009|RMSF=2.489e-005|Dipole=0.624194,-0.0250565,-0.5249618|PG=C01 [X(C7H8O2)]||@

VII.2.26. 4-METHYLPHENOL

VII.2.26.1. Neutral form of 4-methylphenol

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C7H8O1|PCUSER|11-Nov-2020|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||4-hidroxitolueno||0,1| C,0.0038234066,-0.6584996249, 1.200684555| C,-0.0085740451, 0.735996518,1.2074002928| C,-0.0116527301, 1.4361975565, 0.0000070992| C,-0.0090903457,0.7360043056,-1.207391805| C, 0.0033099195, -0.6584918866,-1.200690352| C, 0.0087321546, -1.3806757884,-0.0000063436| H, 0.0090285471, -1.1952051184,2.1463370636| H,-0.0195771728,1.2918598902, 2.1399369403| H, -0.0204921952,1.2918737047,-2.1399200664| H,0.0081106642,-1.1951912837,-2.14634846| O,-0.0724982082,2.8241097236,0.0000245151|H,0.8276569754,3.1747580917,-0.0001652812| C,-0.0124719506,-2.891511278,-0.0000066603| H,0.4856517102,-3.2994006143, 0.8847806588| H, -1.0401242699,-3.2762963586,0.0002120325| H,0.4852729523,-3.299394914, -0.8850097348|| Version=x86-Win32-G03RevB.03|State=1-A|HF=-346.7923608| RMSD=7.819e-009| RMSF=2.252e-005| Dipole=0.5813359,-0.2776209,-0.0001242| PG=C01 [X(C7H8O1)]||@

VII.2.26.2. Neutral radical of deprotonated 4-methylphenol

1\1\GINC-COPERNICO\FOpt\UB3LYP\6-31G(d,p)\C7H7O1(2)\IVAN\12-May-2021\0\\# opt b3lyp/6-31g(d,p) geom=connectivity\\4-hidroxitoluenoradical\\0,2\ C, -0.6515624902,-1.2190555708,-0.0056932364\C,0.7236497783,-1.2352763479, 0.0216836815\ C, 1.4871616398, 0., 0.0380644512\C,0.7236497783,1.2352763479,0.0216836815\C,-0.6515624902, 1.2190555708, -0.0056932364\ C, -1.3730847926, 0., -0.0171761942\ H,-1.2055427002, -2.1545802966, -0.0202313389\ H, 1.2858414858, -2.1636925106, 0.0285271305\ H, 1.2858414858, 2.1636925106, 0.0285271305\ H,-1.2055427002, 2.1545802966, -0.0202313389\ O,2.7437994314, 0.,0.0623528772\C,-2.8771921378,0.,-0.0084850343\ H, -3.2824913512, -0.8876171736, -0.5027389824\ H, -3.2599855857, 0., 1.0211533914\ H, -3.2824913512, 0.8876171736, -0.5027389824\\Version=AM64L-G09RevD.01\State=2-A'\HF=-346.1581657\S2=0.786743\S21=0.\S2A=0.750931\ RMSD=

3.406e-09\ RMSF=7.586e-06\Dipole=-1.7092573,0.,-0.0060288\Quadrupole=-4.1820432, 4.5669102, -0.384867,0.,-0.2112961,0.\PG=CS [SG(C3H1O1),X(C4H6)]\\@

VII.2.26.3. 4-methylphenolate anion

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C7H7O1(1-)|PCUSER|11-Nov-2020|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||ion-4-hidroxitolueno||-1,1|C, -0.5996059813,-1.1951848663,-0.0206608651|C,0.7876747029,-1.2097084523 ,0.0059605717| C, 1.5882483023, 0.,0.0251316254| C, 0.7876747029, 1.2097084523, 0.0059605717| C,-0.5996059813, 1.1951848663, -0.0206608651| C, -1.3431784816, 0., -0.0324559939| H,-1.1394087087, -2.1465372037,-0.0354643415| H,1.3283303754,-2.1559212175, 0.0056260175| H, 1.3283303754, 2.1559212175, 0.0056260175| H, -1.1394087087, 2.1465372037, -0.0354643415| O, 2.8540043321, 0., 0.0483554042|C,-2.853217921,0.,-0.0121134191| H,-3.2659547439, -0.8831659526, -0.5192905922| H, -3.2859045605, 0., 1.0044448448| H,-3.2659547439, 0.8831659526, -0.5192905922||Version=x86-Win32-G03RevB.03|State=1-A'| HF=-346.2117014| RMSD=3.038e-009| RMSF=5.251e-005| Dipole= -2.2991193, 0.,-0.0397921| PG=CS [SG(C3H1O1),X(C4H6)]||@

VII.2.26.4. 4-methylphenol radical cation

1|1|UNPC-UNK|FOpt|UB3LYP|6-31G(d,p)|C7H8O1(1+,2)|PCUSER|03-Jan-2001|0 |#T B3LYP/6-31G(D,P) FOPT TEST||ggg||1,2| C,-0.0651047576,-0.0240039675,1.4336955174| O,-0.2031143447,-0.049482311,2.7416430631| C,1.2080175608,-0.0059482132,0.7846653408| C, -1.2792336436, -0.0141481858,0.6733699239| C,-1.2100383571,0.0139706428,-0.6943709034| C,1.2514277195,0.0216928544,-0.5831665916| C,0.0490784923,0.0327876111,-1.3668966764| H, -2.2218966686, -0.0274279212, 1.2097135816| H, -2.1213463011, 0.0240133294,-1.2830824433| H,2.1187514506,-0.0124374775,1.377023044|H,2.2091788291,0.0371567635,-1.0937535587| C, 0.1283651805, 0.0389200773, -2.8519988437| H, 0.6459904022,-0.0548026643, 3.2184080264| H,0.9201230308,0.7071031514,-3.207416839| H,0.3986792264,-0.9685382564,-3.2073563025|H,-0.81963838,0.3111666474,-3.3184666158|| Version=x86-Win32-G03RevB.01|State=2-A|HF=-346.5166644|S2=0.75963|S21=0.|S2A=0.750043| RMSD= 8.787e-009| RMSF=9.305e-006| Dipole =0.5912739, -0.0406127, 0.1996267| PG=C01 [X(C7H8O1)]||@

VII.2.27. 3-METHYLPHENOL

VII.2.27.1. Neutral form of 3-methylphenol

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C7H8O1|PCUSER|15-Jan-2021|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||3-metilfenol||0,1|C,0.0001442678, -0.2765002237, 1.2400403513| C, 0.0004093092, -0.9828169594, 0.0354074196| C,0.0001028575,-0.3049938177, -1.1884039021| C, -0.0004766927, 1.0959536255, -1.1871339026| C,-0.000741582, 1.7995643305, 0.0176663321| C,-0.0004320058, 1.1230602487, 1.2357902447| H, 0.0008484206,-2.0683092083,0.0719003213| H,-0.0007227029,1.6350377899,-2.1300571221| H,-0.0011899728,2.8857953168,0.010777581| H,-0.000634016, 1.672788595, 2.1747479085| O, 0.0004881941,-1.0083302081,2.3966260056|H,0.0002108808,-0.403997324, 3.1503889732| C, 0.0003707065, -1.0835494204, -2.4836851339| H, 0.8817174195, -1.7307846978,- 2.5591543968| H, -0.8806719997, -1.7311877416, -2.5592792069| H, 0.0002752552, -0.417007766, -3.3504205573||Version=x86-Win32-G03RevB.03|State=1-A|HF=-346.7990989| RMSD=4.531e-009| RMSF=9.043e-005| Dipole=-0.0001924, 0.3644072, 0.1714787| PG=C01 [X(C7H8O1)]||@

VII.2.27.2. Neutral radical of deprotonated 3-methylphenol

1\1\GINC-COPERNICO\FOpt\UB3LYP\6-31G(d,p)\C7H7O1(2)\IVAN\12-May-2021\ \\# opt b3lyp/6-31g(d,p) geom=connectivity\\3-metilfenolradical\\0,2\C,1.2602227243,-0.4033481089, 0.0000045629\ C,-0.0594995111,-1.0038196351,-0.0000072777\C,-1.2133865756, -0.2394866099, -0.0000059981\ C,-1.0822310219,1.1682132147,-0.0000018029\ C, 0.1794901451, 1.7984604752, 0.0000034325\ C,1.3322858234,1.0469434518,0.0000048468\ H, -0.0979068418, -2.0897209755, -0.0000161004\ H, -1.980262426, 1.7803560497, -0.0000052644\ H, 0.2295709761, 2.8835252487, 0.0000042394\ H, 2.3196813305, 1.4968274451,0.0000056864 \O,2.300932303,-1.1116640891,-0.0000048316\C,-2.5800870055, -0.8860112477, 0.0000074133\ H, -2.7162938741, -1.5217914383, -0.8812782062\ H, -2.7164449608, -1.5214264012,0.881535159\H,-3.3775940855,-0.1384303793,-0.000211859 \\Version=AM64L-G09RevD.01\State=2-A\ HF=-346.1560676\ S2=0.790199\S2-1=0.\ S2A=0.751121\ RMSD=7.969e-09\ RMSF=4.472e-05\ Dipole=-1.3523152, 0.7168255, 0.000016\ Quadrupole=-1.9728191,2.6804904,-0.7076712,4.0227665,-0.0000265,-0.0000162\PG=C01 [X(C7H7O1)]\\@

VII.2.27.3. 3-Methylphenolate anion

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C7H7O1(1-)|PCUSER|15-Jan-2021|0||#OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||3-metilfenolato||-1,1| C,1.3391034661,-0.4440282193, 0.0000066042| C, -0.0004125482, -0.9981411139, -0.0000102251| C, -1.1568644004, -0.2229020819,-0.0000102769|C,-1.0695436891,1.1809318998,-0.0000038246| C, 0.2057534094,1.7712389442,0.0000040465| C,1.3625843214, 1.0083572565,0.000006474| H, -0.0738916537, -2.0868473638, -0.0000217552| H, -1.9710406955, 1.7915495013,-0.0000056877| H, 0.2845282188, 2.8611858151, 0.0000040659| H, 2.3428229979, 1.4843781209, 0.0000072197| O, 2.3867088173, -1.1547144013, -0.0000062779| C,-2.5187803771,-0.8929655897, 0.000009794| H, -2.658222466, -1.5361817543, -0.8799007027| H, -2.6583845107, -1.5358134838,0.880166221|H,-3.3305235214,-0.1555021986,-0.0002146907||Version=x86-Win32-G03RevB.03|State=1-A|HF=-346.212368| RMSD=3.018e-009|RMSF=7.598e-005|Dipole=-1.9970451,0.6349442,0.0000168|PG=C01 [X(C7H7O1)]||@

VII.2.27.4. 3-Methylphenol radical cation

1|1|UNPC-UNK|FOpt|UB3LYP|6-31G(d,p)|C7H8O1(1+,2)|PCUSER|03-Jan-2001|0#T B3LYP/6-31G(D,P) FOPT TEST||ggg||1,2|C,-0.4174306268,0.0581541181, 1.1983805011|O,-0.5638603597,0.1205665763,2.5038126312| C,0.8474422851,0.0237473603,0.558115139| C, -1.6493975805, 0.0263765448, 0.4474785883| C, -1.582852172, -0.0387170945, -0.9229881581|C,0.914042978,-0.0417253221,-0 .8188221452|C,-0.3236995659,-0.072650999,-1.557063867|H,-2.5851382259,0.0552239945,0.9951701716|H,-2.4884991758,-0.0641002206, -1.5186457031| H,1.7530512279,0.0493561881,1.158909952|C,2.2272373943,-0.0804302211,-1.5450139994| H, 0.2830216132, 0.1407976481, 2.9851451298| H, -0.2755926876,-0.1239181996, -2.6407760372| H, 2.8236265051, 0.8084427358,-1.3111571343| H, 2.8147218632, -0.9511394559,-1.2331214797| H, 2.0936354839, -0.1277216199, -2.6265423008||Version=x86-Win32-G03RevB.01|State=2-A|HF=-346.5113552| S2=0.765245| S2-1=0.|S2A=0.750122|RMSD=6.305e-009|RMSF=2.083e-005|Dipole =0.2863685, 0.0087773, 0.2089757| PG=C01 [X(C7H8O1)]||@

VII.2.28. 2-METHYLPHENOL

VII.2.28.1. Neutral form of 2-methylphenol

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C7H8O1|PCUSER|20-Jan-2021|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||2-metilfenol||0,1|C,1.9486796381, -0.6190114673,-

0.000064612| C, 0.7552920056, -1.3466815325, -0.0000740986| C, -0.4922163803,-0.7191742089, -0.0000177904| C, -0.5150848895, 0.6876529837, 0.0000403689| C, 0.6687426434, 1.4280449126,0.0000341472| C,1.9014584666, 0.7729766542, -0.000008873| H, 2.9026149184,-1.1369006511,-0.0000994867| H, 0.7890159262,-2.4334019887,-0.0001130945| H, 0.6246634426,2.5155990064,0.000057626| H,2.8178570859,1.355782959,-0.0000048188| O,-1.7503726917,1.2829731626,0.0000530304| H,-1.635907498, 2.2422069301, 0.0004454277| C, -1.7852617153, -1.4932199582, -0.0000178486| H, -2.3948230782, -1.2503567493, 0.8775294052| H, -2.3947653218, -1.2504709001, -0.8776386078| H,-1.5953325531, -2.569768208, 0.000051544|| Version=x86-Win32-G03RevB.03|State=1-A|HF=-346.7997119| RMSD=3.100e-009| RMSF=5.573e-005| Dipole= 0.0765948, 0.4397011,0.0002416| PG=C01 [X(C7H8O1)]||@

VII.2.28.2. Neutral radical of deprotonated 2-methylphenol

1\1\GINC-COPERNICO\FOpt\UB3LYP\6-31G(d,p)\C7H7O1(2)\IVAN\12-May-2021\0\\# opt b3lyp/6-31g(d,p) geom=connectivity\\2-metilfenolradical\\0,2\C ,-1.8250282008,-0.8830220188, 0.0000620623\ C, -0.5417351513,-1.4579702304, 0.0000601673\ C, 0.5993494028, -0.6738405235,0.0000125624\ C,0.4567531871, 0.7849056883,-0.0000444692\ C,-0.8869068247,1.3371237008,-0.000029042\ C,-1.9919209159,0.5181277724,0.0000188038\ H, -2.698655409, -1.5282471376, 0.0000999343\ H, -0.4468252158, -2.5408437125, 0.0000965167\ H,-0.9679818338, 2.4194335352, -0.0000615711\ H, -2.9924712921, 0.9405075407, 0.0000230303\ O,1.466570497,1.532226974,-0.0000762264\ C,1.9845327673,-1.2463767978, 0.0000226955\ H, 2.5464083375, -0.9005024212, -0.8741763738\ H, 2.5463486584, -0.90061738, 0.874308094\ H, 1.9657889932, -2.3389299895, -0.0000421841\ \Version=AM64L-G09RevD.01\State=2-A\HF=-346.1598998\S2=0.786956\S2-1=0.\S2A= 0.750952\ RMSD=9.265e-09\ RMSF=7.914e-05\ Dipole =-0.9213655,-0.8917382, 0.0000525\ Quadrupole=1.3106752,0.1412045,-1.4518797,-3.4967444,0.0000999,-0.0000255\PG=C01 [X(C7H7O1)]\\@

VII.2.28.3. 2-Methylphenolate anion

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C7H7O1(1-)|PCUSER|20-Jan-2021|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||2-metilfenolato||-1,1|C,-1.834523089,-0.8646281844, 0.0000523173| C, -0.5379705608, -1.4071218496, 0.0000561898| C, 0.6012757261, -0.6112864802, 0.0000070463| C,0.5094128415, 0.8431292727,-0.0000679903| C, -0.8406947632,1.3576487371,-0.0000386584| C,-1.9587580333,0.5319736943,0.000010784| H, -2.7108777449, -1.5097481664, 0.0000895197| H, -0.4165461229, -2.4940058061,

0.0000948108| H, -0.9504962696, 2.4417944239, -0.0000579038| H,-2.9545622399, 0.9817504966, 0.0000186731| O,1.5446098978,1.5779076678,-0.000054145|C,1.9897866287,-1.1922393799, 0.0000176489| H, 2.5643706726, -0.8487160253, -0.8716235404| H, 2.5643392074, -0.8488026813, 0.8717163163| H, 1.9757208138, -2.2903884442, -0.0000287408||Version=x86-Win32-G03RevB.03|State=1-A|HF=-346.2154659|RMSD=3.014e-009| RMSF=3.833e-005|Dipole=-0.7022628,-1.1567356,0.0000276|PG=C01 [X(C7H7O 1)]||@

VII.2.29. 2-ISOPROPYLPHENOL

VII.2.29.1. Neutral form of 2-isopropylphenol

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C9H12O1|PCUSER|18-Nov-2020|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||dosisopropilfenol||0,1|C,-0.1588932796,-1.4807631456,2.234189067|C,-0.2953885618,-0.0958104849,2.2200156159|C,-0.2620742667, 0.5980394681, 1.0076652129| C, -0.0991212643, -0.0809452275, -0.2179501541| C, 0.0319118995, -1.4745355511,-0.1684617449| C,0.0054047982, -2.1768031446, 1.0364918771| H, -0.1843574492, -2.0134366227, 3.1803606785| H,-0.4288886277,0.4720439159, 3.1349525755| H, 0.1562420366, -2.0263932314, -1.0944298557| H, 0.1101307955, -3.2572821062, 1.0368307503| O,- 0.3904384405,1.9613881035,1.0894828437|H,-0.4321919307, 2.3358230697, 0.2010213934| C, -0.0304934307,0.7074365109,-1.5231424146| H, -0.7928931254, 1.5040833987,-1.4723897548| C,1.3472542547,1.3867674031,-1.6874693718| H, 1.3717204636, 2.0145775737, -2.5849413196| H, 1.5966586075, 2.0126813629, -0.8250097718| H, 2.1321153004, 0.6290764739, -1.7797316924| C,-0.3760472723, -0.1165457863,-2.7715360736| H, -1.3405468131, -0.6221111369, -2.6668775012| H, -0.4257927376, 0.5350082829, -3.6495539648| H, 0.3859937412, -0.8762160615,-2.9749063701||Version=x86-Win32-G03RevB.03|State=1-A|HF=-425.429147|RMSD=6.411e-009|RMSF=2.968e-006|Dipole=0.0308773,0.0546605,-0.6854336|PG=C01 [X(C9H12O1)]||@

VII.2.29.2. Neutral radical of deprotonated 2-isopropylphenol

1\1\GINC-COPERNICO\FOpt\UB3LYP\6-31G(d,p)\C9H11O1(2)\IVAN\12-May-2021\0\\# opt b3lyp/6-31g(d,p) geom=connectivity\\dosisopropilfenolradical\\ 0,2\C, -2.6575709533,-0.4570638923,0.1522368486\C,-2.1305464662,0.7933358935,-0.069528669\C,-0.698928059, 0.9906673231, -0.2104795641\ C, 0.1772300684, -0.1845251232, -0.1077944045\ C, -0.4037129022, -1.4222708066, 0.1160910987\ C, -1.7960709169, -1.5698088763, 0.2465532606\ H, -3.7299566396, -0.5954399985, 0.2545566326\ H,-2.7526660192,

1.6786577186, -0.1532894438\ H, 0.220807241,-2.3069902204,0.1917270506\H,-2.2123581297,-2.5576320238, 0.4215251695\ O,-0.2280026648, 2.137762754,-0.4183446895\ C,1.6691876273,0.0440653695, -0.2235573878\ H,1.795440276,0.8437397993,-0.9625004271\ C,2.2303682881, 0.5858310054, 1.1109918808\ H, 3.2983669212, 0.8064091998, 1.010033004\ H,1.717312735,1.505701382,1.400394922\ H,2.1100070635,-0.1497552669, 1.9142219489\ C, 2.4552120848, -1.1879112425, -0.6912944609\ H, 2.0546321116, -1.5952379416, -1.6251139009\ H, 3.5019424391, -0.9184824179 ,-0.8632785834\ H, 2.4483758948,-1.9875926351, 0.0581847145\\ Version=AM64L-G09RevD.01\ State=2-A\ HF=-424.7915474\ S2=0.78619\S2-1=0.\S2A=0.750913\RMSD=8.197e-09\RMSF=6.837e-06\Dipole=-0.3093937, -1.1777475,0.2112861\ Quadrupole= 4.9264399,- 3.156542, -1.769898, 0.5827655,-0.5304637,0.4775747\PG=C01 [X(C9H11O1)]\\@

VII.2.29.3. 2-Isopropylphenolate anion

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C9H11O1(1-)|PCUSER|19-Nov-2020|0| # OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||iondosisopropilfenol||-1,1|C,-2.63703105,-0.4378002484,0.1257681006| C,-2.0872486714,0.8285246378,- 0.0279513112|C,-0.667559492, 1.0514953407, -0.1507088541| C,0.1495636107, -0.1580025922, -0.1155359734| C, -0.4383717465, -1.4096946257,0.0378689702 |C,-1.8271954066,-1.5805635802, 0.1631036498| H, -3.7204396678, -0.5430674311, 0.2177129889| H, -2.7226735564, 1.7128336551, -0.0569371671| H,0.196026356,-2.2970695545,0.0598817516|H,-2.2571619157,-2.5731575341, 0.2806495951| O,-0.1544771996,2.2087290835,-0.2817987148| C,1.6479327859,0.059878 6916,-0.2477458282| H, 1.7665781343, 0.8241314711,-1.0297762261| C, 2.2267541866, 0.6908146158, 1.0357726513| H, 3.2930174836, 0.9380971046, 0.9211526352| H,1.6726162122,1.6084496594,1.246040982|H,2.1275168,0.0059452345,1.8884678838|C,2.4490354496,-1.1829460884,-0.6542524123|H,2.0538811414,-1.6347279941,-1.5714835113| H, 3.5031811675, -0.9275661315, -0.8263358714| H, 2.4279974435,-1.9539380531, 0.1271027021|| Version=x86-Win32-G03RevB.03| State=1-A| HF=-424.8505143| RMSD= 9.422e-009| RMSF=3.669e-005| Dipole=0.8492382, -1.3999239, 0.1451658| PG=C01 [X(C9H11O1)]||@

VII.2.29.4. 2-Isopropylphenol radical cation

1|1|UNPC-UNK|FOpt|UB3LYP|6-31G(d,p)|C9H12O1(1+,2)|PCUSER|09-Jan-2001|0 ||#T B3LYP/6-31G(D,P) FOPT TEST||ddd||1,2| C,-1.0003672069, 0.3228227599,0.5970468917| O,-1.0574678874,0.5416914887, 1.8923318033| C,0.2577657177,0.0867702889, -0.0966911996| C, -2.2616022415, 0.3401566552, -0.0782223165| C, -2.2916104253, 0.1266123808, -

1.4288701539| C, 0.1687194287, -0.119530778, -1.4624600004| C, -1.0721058817,-0.1050292579, -2.1283967201| H, -3.1530290161, 0.5262656372, 0.5105836224| H, 1.0691831088,-0.2926830068,-2.0393140961| H,-1.0997622644,-0.2727806692,-3.2007007961|C,1.5528163199,0.0372416081,0.6863351977| H,-0.1806718308, 0.5340412803, 2.3169329029| H,-3.2311689963,0.1337181855,-1.9701777483| H, 1.51314389, 0.8349479501, 1.447422736| C,1.6781832881,-1.3252451827,1.4242231588| C,2.8005296843,0.3140967545,-0.1653369031| H, 0.8214737781, -1.5445272183, 2.069839896| H, 1.7668292016,-2.1408949129,0.7015942805| H, 2.576976003,-1.3194813841,2.0459222191| H, 2.989064884,-0.494393166, -0.8782578404| H, 2.7186928518, 1.2560839645, -0.7143462113| H, 3.6750393892, 0.3788000567,0.4860788817|| Version=x86-Win32-G03RevB.01| State=2-A|HF=-425.1466767|S2=0.763846|S2-1=0.|S2A=0.750108|RMSD=3.351e-009|RMSF=1.824e-005|Dipole=-0.4544892,0.0967773,-0.3154912|PG=C01 [X(C9H12O1)]||@

VII.2.30. 4-HYDROXYPHENOL

VII.2.30.1. Neutral form of 4-hydroxylphenol

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C6H6O2|PCUSER|14-Aug-2020|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||hidroquinona||0,1|C,-0.6976834375 ,-1.2083548711,0.0207277986| C,0.6990732272,-1.2088130147,0.009758426| C ,1.3964082899,-0.0010585621,-0.0083836806| C,0.6976834222,1.208354883,- 0.020727797| C,-0.6990732514, 1.2088130303, -0.0097583634| C,-1.3964083132 ,0.0010585795, 0.0083836779| H, 1.2257574652, -2.15810281, 0.0100181715| H, 2.4818598143,0.0174297815,-0.0075857667| H, -1.225757476, 2.1581028309, -0.0100181906| H,-2.4818598358,-0.0174297785,0.0075859236| O, 1.39183859, 2.4106620549,0.0141170168| H,1.5594901306,2.7000014149,-0.8924146565| O, -1.3918386611, -2.4106620143, -0.0141170716| H, -1.559489145, -2.7000020366, 0.8924145871|| Version=x86-Win32-G03RevB.03|State=1-A|HF=-382.6853783 |RMSD= 1.740e-009| RMSF=5.100e-005|Dipole=0.0000012,-0.0000007,0.|PG=C01 [X(C6H6O2)]||@

VII.2.30.2. Neutral radical of deprotonated 4-hydroxylphenol

1\1\GINC-COPERNICO\FOpt\UB3LYP\6-31G(d,p)\C6H5O2(2)\IVAN\20-May-2021\0\\# opt b3lyp/6-31g(d,p) geom=connectivity\\hidroquinonaradical\\0,2\ C, 1.4498042336, 0., 0.0405277705\ C,0.688563022,-1.2383453851,0.0198278037\ C,-0.6867011373,-1.228214207, -0.0096321976\ C,-1.3838213546, 0., -0.0155706191\C,-0.6867011373,1.2282142069,-0.0096321976\ C,0.6885630212,1.2383453851,0.0198278037\H,1.2535071082,-2.1648465114, 0.0269834514\ H, -1.2627587804, -2.1482719423, -0.0343549981\ H, -1.2627587804,

2.1482719423, -0.0343549981\ H, 1.2535071082, 2.1648465114, 0.0269834514\ O,-2.757130914, 0.,-0.095547622\ H,-3.1432836028,0.,0.7911030336\ O,2.7059262144,0.,0.0727013181\\Version=AM64L-G09RevD.01\State=2-A'\HF=-382.0512059\S2=0.785711\S21=0.\S2A=0.750878\ RMSD=3.356e-09\ RMSF=8.714e-06\ Dipole= -1.4500836, 0., 0.5688691\ Quadrupole =-5.1531591, 4.7100873, 0.4430718, 0., -4.0353496, 0. \PG=CS [SG(C2H1O2),X(C4H4)]\\@

VII.2.30.3. 4-Hydroxylphenolate anion

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C6H5O2(1-)|PCUSER|14-Aug-2020|0||#OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||ionhidroquinona||-1,1| C, 1.5493293515, 0., 0.0319070884|C,0.7510480799,-1.2119171157,0.0051492204|C,-0.6384146338, 1.2036260355, -0.033987921| C, -1.3529583596, 0.,-0.0517278342| C, -0.6384146338,1.2036260355,-0.033987921|C,0.7510480799,1.2119171157,0.0051492204|H, 1.2934252837, 2.1566960585, 0.0164956653| H, -1.1985087877, -2.1399743595, -0.0548494342| H, -1.1985087877, 2.1399743595, -0.0548494342| H, 1.2934252837,2.1566960585,0.0164956653|O,-2.7699256411,0.,-0.1071003496|H,-3.0821372479, 0., 0.8073093291| O, 2.8152352601, 0., 0.073898736 ||Version=x86-Win32-G03RevB.03|State=1-A'|HF=-382.1057769|RMSD=7.190e-009|RMSF=4.358e-005|Dipole=-2.1392765,0.,0.5201046|PG=CS [SG(C2H1O2),X(C4H4)]||@

VII.2.30.4. 4-Hydroxylphenol radical cation

1|1|UNPC-UNK|FOpt|UB3LYP|6-31G(d,p)|C6H6O2(1+,2)|PCUSER|02-Jan-2001|0||#T B3LYP/6-31G(D,P) FOPT TEST||ggg||1,2| C,0.0194131158,0.0247755862, 1.3884691555|O,-0.0501075767,0.0471290441,2.7058344676| C,1.2523080771,0.0132934812,0.6709421685| C,-1.2328384274,0.0108519344,0.6965913023| C,-1.2522547147,-0.0134084773,-0.6710143961| C, 1.2328805308, -0.0107079178, -0.6966759949| C,-0.0193392418, -0.0243202174, -1.3884830525| H, -2.1447732058, 0.0198959623, 1.2834035969| H, -2.1944764609,-0.024098434, -1.2112414847| H, 2.1945837821,0.0238900145,1.2110882776| H, 2.144786356,-0.019721731,-1.2835365819| O,0.0500108708,-0.0475369552,-2.7056892456|H,0.8227705059, 0.0559654202,3.1347338362| H,-0.8231333691,-0.0555742786,-3.1345845158|| Version=x86-Win32-G03RevB.01| State=2-A|HF=-382.4257054|S2=0.756732|S2-1=0.| S2A=0.750015| RMSD=3.137e-009| RMSF=7.798e-005| Dipole=-0.0000716,0.000737,-0.0003783|PG=C01 [X(C6H6O2)]||@

VII.2.31. 3-HYDROXYLPHENOL

VII.2.31.1. Neutral form of 3-hydroxylphenol

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C6H6O2|PCUSER|12-Nov-2020|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||resorcinol|| 0,1| C, 0.0092723765,-0.8962267845, 0.8638008712| C,0.0287930347, 0.4987635779, 0.8889853818| C, 0.0085304188, 1.2043111643, -0.3146779667| C, -0.0314081087, 0.5272662374, -1.5407493352| C, -0.0505925464, -0.8662486721, -1.5439824736| C,-0.0306603263,-1.5897616746, -0.353019023| H, 0.0592267818, 1.0287184553, 1.8335655598| H,-0.0472242632,1.0835931146,-2.4746185096| H,-0.0815356934,-1.3974274009,-2.4907437417| H, -0.0458960338, -2.676723992, -0.3649426827| O, 0.0295629671, 2.5685163371, -0.2329157178| H, 0.0126465444,2.9359140312,-1.1261807025| O, 0.0310132851,-1.5374428828,2.0706780129| H, 0.0145635544,-2.4912849341, 1.918676989|| Version=x86-Win32-G03RevB.03|State=1-A'|HF=-382.6989259| RMSD=4.281e-009| RMSF=1.915e-005| Dipole=-0.0250694,-0.4355385,-0.7762945|PG=CS [SG(C2H2),X(C4H4O2)]||@

VII.2.31.2. Neutral radical of deprotonated 3-hydroxylphenol

1\1\GINC-COPERNICO\FOpt\UB3LYP\6-31G(d,p)\C6H5O2(2)\IVAN\12-May-2021\0\# opt b3lyp/6-31g(d,p) geom=connectivity\\resorcinolradical\\0,2\C,0.0001658139,-0.3434959205, 1.210968702\ C,0.0005731028,-1.0452461919,0.022168123\C,0.0002599114,-0.3472828705,-1.2454643876\ C, -0.000341723, 1.1075999917, -1.2186104924\ C, -0.0007214879, 1.7808299712, -0.0170207751\ C, -0.0004812565, 1.0718681482, 1.1987885831\ H, 0.0011197792, -2.1291035428,0.0156634681\ H, -0.0005031033, 1.6228426976, -2.1728472216\ H, -0.0012079688, 2.8663104423, 0.0079899944\ H,-0.0007599786, 1.6158963969, 2.1408962649\ O, 0.0005653786,-0.9727028317,-2.3373164858\ O, 0.0003953309, -1.048093609,2.3789550643\ H,-0.0000347986,-0.4371296815,3.1273261626\\ Version=AM64L-G09RevD.01\ State=2-A\ HF= -382.0542939\S2=0.79084\S2-1=0.\ S2A= 0.751151\ RMSD=5.852e-09\RMSF=7.538e-05\Dipole=-0.0006488,1.2210903,1.5318752\Qua drupole=-1.345119,1.0164587,0.3286602,-0.0011116,-0.0004317,-0.7877686\PG=C01 [X(C6H5O2)]\\@

VII.2.31.3. 3-Hydroxylphenolate anion

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C6H5O2(1-)|PCUSER|19-Nov-2020|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||resorcinolato||-1,1| C,0.000094018,-

0.3297589096,1.1455381508| C,0.000490192,-1.0361129331,-0.0448162169| C,0.0002788803,-0.3758372206, -1.3372573178| C,-0.0004031992, 1.0769434732, -1.2569575172| C,-0.0007801804, 1.7519705995, -0.0488058529| C,-0.0005466495, 1.0750155647, 1.1839852476| H, 0.0009784139, -2.1231670105, -0.0237673129| H, -0.000607663, 1.6224065681,-2.1993280285| H, -0.0012810155, 2.8440994521, -0.0451089589| H, -0.0008186365, 1.6114889796, 2.1330044987| O, 0.0005301767, -1.0051000271,-2.4336261125| O, 0.0003490841, -1.0598909482, 2.3379520306| H, -0.0001035518, -0.4082236324, 3.0504734957|| Version=x86-Win32-G03RevB.03| State=1-A| HF=-382.1140903| RMSD= 7.465e-009| RMSF=1.448e-004| Dipole= -0.0005847, 1.0186337, 2.1277574| PG=C01 [X(C6H5O2)]||@

VII.2.31.4. 3-Hydroxylphenol radical cation

1|1|UNPC-UNK|FOpt|UB3LYP|6-31G(d,p)|C6H6O2(1+,2)|PCUSER|04-Jan-2001|0|#T B3LYP/6-31G(D,P) FOPT TEST||ggg||1,2|C,-0.3128657814,0.1150441816, 1.1943509589|O,-0.4530104015,0.2255085438,2.5037474476|C,0.9097134689,-0.0263192741,0.5389996241|C,-1.561919696, 0.1518140522,0.46158728|C,-1.5580666096,0.0451025564,-0.9232823045| C, 0.8919452996, -0.1316881136, -0.8512589561| C, -0.3506044016, -0.0963059236 ,-1.5948648799| H, -2.4772098321, 0.2641547534, 1.0330678298| H, -2.4903450897, 0.0720542634, -1.4756912019 | H,1.8439618611,-0.0539137393,1.09217737| O,1.9680710434,-0.2695688885,-1.6058796914| H,0.3929451654,0.1996725147,2.9826363842| H,-0.29323477,-0.1834693482,-2.6747223401| H,2 .7941838509,-0.2919005592,-1.0936004263|Version=x86-Win32-G03RevB.01| State=2-A| HF=-382.4167383| S2=0.767378 |S2-1=0.| S2A=0.750121| RMSD =3.214e-009|RMSF=6.131e-005|Dipole=0.6496798, -0.0186301, 0.3854655|PG=C01 [X(C6H6O2)]||@

VII.2.32. 2-HYDROXYLPHENOL

VII.2.32.1. Neutral form of 2-hydroxylphenol

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C6H6O2|PCUSER|08-Jan-2021|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||2-hidroxifenol||0,1|C,-0.1430354612,-1.3328563431, 1.5143993296| C,-0.0567893327,0.0611854626,1.5654060095| C,0.0354858838, 0.7979575725, 0.387676393| C,0.0409297057,0.1275692248,-0.8481954498| C,-0.0448665063,-1.2592547417, -0.8990672075| C,-0.1372842143,-1.994365349,0.287641053| H,-0.2146041723,-1.898064061, 2.4383125975| H, -0.0595096795, 0.5955351314, 2.5096941025| H, -0.0395666937,-1.7636533663, -1.8631703159| H, -0.2041012338, -3.0766168468, 0.2444653444| O,

0.1196696533, 2.1581492178, 0.4342997269| H,0.17535976,2.4769035131,-0.4791293765| O, 0.1355267302, 0.9481039044, -1.9519656299| H, 0.1342105012, 0.4144556951, -2.7560058947||Version=x86-Win32-G03RevB.03|State=1-A|HF=-382.6992864|RMSD=8.815e-009| RMSF=2.328e-005| Dipole=0.0089088,-0.4162392,-0.8854174|PG=C01 [X(C6H6O2)]||@

VII.2.32.2. Neutral radical of deprotonated 2-hydroxylphenol

1\1\GINC-COPERNICO\FOpt\UB3LYP\6-31G(d,p)\C6H5O2(2)\IVAN\12-May-2021\ \\# opt b3lyp/6-31g(d,p) geom=connectivity\\2-hidroxifenolradical\\0,2\ C,1.889693087 ,-0.6730426678, 0.0000223068\ C, 0.7269368698, -1.4390202677 ,0.0000542539\ C,-0.4993793752, -0.780533311,0.0000170516\ C,-0.5870865022,0.6849885551,-0.0000524182\ C,0.6513878725,1.4212351141,-0.0000772184\ C,1.8490221532,0.748723023,-0.0000433408\ H, 2.8536222211, -1.1726507361, 0.0000504431\ H, 0.7583747584, -2.5231685739, 0.000103509\ H,0.5932718287, 2.5045339416,-0.0001214773\H,2.7839468709,1.3006997468,-0.0000633448\ O, -1.6669621598, -1.4226211923, 0.0000369813\ H, -2.3322230977, -0.6947666407, -0.0000192743\ O, -1.7402875268, 1.190493009, -0.000065472\\ Version=AM64L-G09RevD.01\State=2-A\ HF=-382.0730705\ S2=0.771388\ S2-1=0.\ S2A=0.750312\RMSD=7.837e-09\RMSF=8.676e-05\ Dipole= 1.0200815, -0.2735228, -0.0000028 \Quadrupole=1.8381003,-0.3943424,-1.4437578,1.4971507,0.0000518,-0.0000486\PG=C01 [X(C6H5O2)]\\@

VII.2.32.3. 2-Hydroxylphenolate anion

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C6H5O2(1-)|PCUSER|08-Jan-2021|0||#OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||2-hidroxifenolato||-1,1|C,1.913608011,-0.6153530952,0.0000714934|C,0.7173500222,-1.3732949229,0.000041531| C,-0.4987134854,-0.721011713,0.0000285993| C,-0.6216855325,0.725233765,-0.0000087699| C, 0.5996800503,1.4431982195,-0.0000223374| C,1.8372442164, 0.7750825547,0.000041109| H, 2.8778179626,-1.1204076403,0.0001047199| H,0.7432667773,-2.4623589943, 0.0000676156| H, 0.5569256111,2.5313506452, -0.0001013794| H, 2.7562897962, 1.3632974425, 0.0000369108| O, -1.7177072303, -1.3430493794, 0.0000542111| H, -2.283799548,-0.5143260971, 0.000273761| O, -1.824217806,1.1929638539,-0.0002156336||Version=x86-Win32-G03RevB.03|State=1-A|HF=-382.1315098|RMSD=8.290e-009|RMSF=5.512e-005|Dipole=0.9942666,-0.422629,0.0002695|PG=C01 [X(C6H5O2)]||@

VII.2.32.4. 2-Hydroxylphenol radical cation

1|1|UNPC-UNK|FOpt|UB3LYP|6-31G(d,p)|C6H6O2(1+,2)|PCUSER|05-Jan-2001|0||#T B3LYP/6-31G(D,P) FOPT TEST||ggg||1,2|C,-0.3704294498,0.0772906124, 1.1849446129|O,-0.5126811913,0.1737111874,2.4781640173|C,0.9785328577,-0.0367358585,0.5626761101|C,-1.5564826016,0.0834898342,0.4225701442| C,-1.5009389206,0.0024500888,-0.9761977004| C, 0.9940749771,-0.0904296257, -0.9713482184| C,-0.2971025358,-0.0815868801,-1.6714626871| H,-2.5041378067,0.1582650971,0.9460207807| H, 2.4353549017, 0.0125225694, -1.5297919826| H, 1.6149365238, 0.7998799678, 0.886522726| O,2.0505059383,-0.1460532368, -1.5731421218| H, 0.3288216805, 0.1664962967, 2.9708510398| H, -0.2674733944, -0.1384366064,-2.7551574134|H,1.4746839608,-0.9468599562, 0.9342861182|| Version=x86-Win32-G03RevB.01|State=2-A|HF=-382.3874514|S2=0.773849| S2-1=0.|S2A=0.75031|RMSD=9.885e-009|RMSF=2.770e-005|Dipole=-0.9375976,0.0678623,1.2141013|PG=C01 [X(C6H6O2)]||@

VII.2.33. 4-ACETAMIDEPHENOL

VII.2.33.1. Neutral form of 4-acetamidephenol

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C8H9N1O2|PCUSER|14-Aug-2020|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||4-hidroxiacetanilida||0,1|C,-0.1390441331,0.5460384091,0.9374804687|C,0.0430622964,1.9164394089,0.7847620971|C,0.7600685012,2.4108446709,-0.3097574003|C,1.2835521212,1.5191471551,-1.251474535| C, 1.0713769183, 0.1496861318,-1.1084975127|C,0.3559723995,-0.3553874308,-0.0161456646| H, -0.6573937589, 0.1696323172,1.8124345676| H,-0.3435957084,2.6161391236,1.51787741| H,1.8456712502,1.8934312002,-2.1042093441| H,1.4600774399,-0.537002102,-1.8549041587| O,0.9199607813,3.7648195936,-0.3991340932|H,1.4344306828,3.9731638899,-1.189890529| N,0.1991729648,-1.758708816,0.1250708817|H,1.0119738897,-2.3379570225,-0.0465507825| C, -0.9346178726, -2.5184796456, 0.3458675436| C, -2.2630922665, -1.7984111168, 0.4897840557| H,-2.4331180099,-1.5263635425, 1.5368074508| H,-2.3246358175,-0.8883221183,-0.1105375371| H,-3.045624653,-2.4984890898,0.1954602146| O,-0.8456687632, -3.7363866487,0.416121871||Version=x86-Win32-G03RevB.03|State=1-A|HF=-515.494922|RMSD=2.831e-009|RMSF=2.403e-006|Dipole=0.5168653,1.3783309,-0.6163634|PG=C01 [X(C8H9N1O2)]||@

VII.2.33.2. Neutral radical of deprotonated 4-acetamidephenol

1\1\GINC-COPERNICO\FOpt\UB3LYP\6-31G(d,p)\C8H8N1O2(2)\IVAN\20-May-2021\0\\# opt b3lyp/6-31g(d,p) geom=connectivity\\4-hidroxiacetanilidaradical\\0,2\C,-0.3364360595,0.913375062,-0.2532139215\C,-1.6911536592,1.143288934,-0.2398966708\C,-2.6552350425,0.0746068751,-0.0445695683\C,-2.1000225498,-1.2586243185, 0.1223605068\ C, -0.7478113691, -1.4736735388, 0.1121073425\ C, 0.1703911452, -0.3982907115,-0.0583739151\ H, 0.3389919497, 1.7362327244, -0.4423660682\ H, -2.0886453915, 2.1407581482, -0.396831965\ H, -2.8010166892, -2.0749117672, 0.2623449066\ H, -0.3522300952, -2.4771689979, 0.2516338211\ O,-3.8903038327,0.2879288143,-0.031224026\ N, 1.5215734233, -0.7273982195, -0.0664930035\ H, 1.7283844603, -1.7144716236,-0.1756285203\ C, 2.7128253025, -0.0231240552, 0.1387778634\ C, 2.6696148916, 1.4460754325, 0.4916317958\ H, 2.5020957034,2.053994106,-0.4036566248\ H,1.8860303622, 1.6786462684,1.2166928092\ H,3.64536417,1.7059957734,0.9015934325\ O,3.7603642705,-0.641721886, 0.0475548156\\ Version=AM64L-G09RevD.01\ State=2-A\HF=-514.8577281\S2=0.778837\S2-1=0.\S2A=0.750569\RMSD=4.738e-09\RMSF=5.140e-06\Dipole=0.8461369,0.1192247,0.0737657\Quadrupole=-16.836422, 12.0407922, 4.7956298, 5.7026841, 0.3119475,-0.3112932\PG=C01 [X(C8H8N1O2)]\\@

VII.2.33.3. 4-Acetamidephenolate anion

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C8H8N1O2(1-)|PCUSER|15-Aug-2020|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||4-hidroxiacetanilidaion||-1,1|C,-0.4862593886,0.7593959403,-0.9792868818|C,-1.8284892971,1.0119315972,-0.7558441944| C, -2.654986997,0.1824439902,0.106426719|C,-1.9335745441,-0.9308128194,0.7021812951| C, -0.5898356972, -1.1663365436, 0.4690255478| C, 0.1688034174, -0.3277129138, -0.3697436891| H, 0.0894295397, 1.4067125284, -1.6426831354| H, -2.3164368181, 1.8593481621, -1.2343423679| H,-2.5027673933, -1.5898164944, 1.3555705698| H, -0.0934723022, -2.0174208308, 0.9377544997| O,-3.8787191245, 0.40508636,0.3149455513| N,1.5574380847,-0.5974669599,-0.6267068569| H, 1.8215305289,-1.2233605153,-1.380932499| C,2.6417288865,-0.0755938877,0.013467046| C, 2.3431045449, 0.8836307215, 1.1571655666|H,1.8674617443,1.7944447783,0.7812665775|H,1.6434797107,0.4408025311,1.8708140689| H, 3.2853643314, 1.13355099, 1.6472967426| O, 3.796268939, -0.3605449772,-0.3159636655|| Version=x86-Win32-G03RevB.03| State=1-A| HF=-514.9272616| RMSD =3.999e-009| RMSF=3.287e-005| Dipole=2.1442427,-0.1321445,-0.0564881| PG=C01 [X(C8H8N1O2)]||@

VII.2.33.4. 4-Acetamidephenol radical cation

1|1|UNPC-UNK|FOpt|UB3LYP|6-31G(d,p)|C8H9N1O2(1+,2)|PCUSER|07-Jan-2001|0||#T B3LYP/6-31G(D,P) FOPT TEST||FFF||1,2|C,-1.0891737863,-0.0866915668,1.2131393558|H,-0.9704469547,-0.1513055651,2.2907430599|C,0.0766184276,-0.0221999058, 0.3786482858| C, -2.3439065078, -0.0676596011, 0.6677015892| C, -2.4882183288, 0.0174802329,-0.7456828685| C, -0.0818247287, 0.0638579791, -1.0439423055| C, -1.3393732666, 0.0824990913, -1.5843553055| H, -3.2226125238, -0.1167430474, 1.3041480979| O, -3.6636968423, 0.0411027104, -1.3527054247| N, 1.2882143667, -0.0468509733, 0.9962301707| H, 0.7968768352, 0.1128283882, -1.6703640047| H, -1.4896735949, 0.1467715276, -2.6563731778| C, 2.6084884374, 0.0039876499, 0.4152125407| O, 2.7569934436,0.0794332009,-0.7792771333| C,3.7086653672,-0.0470024038,1.4414075337| H, 1.2677564924,-0.1093099005, 2.0093991513| H, 3.6358306613,0.798419415,2.1345879275| H,3.6550371829,-0.972191897,2.0259851671| H,4.6655902588,-0.0048084691,0.9232506628| H,-4.4098854183,-0.0056197834,-0.7319005682||Version=x86-Win32-G03RevB.01|State=2-A|HF=-515.236792|S2=0.756888|S2-1=0.|S2A=0.750024|RMSD=6.875e-009|RMSF=3.084e-005|Dipole=-1.3483697,-0.1179612,1.6696009|PG=C01 [X(C8H9N1O2)]||@

VII.2.34. 2-ACETAMIDEPHENOL

VII.2.34.1. Neutral form of 2-acetamidephenol

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C8H9N1O2|PCUSER|12-Jan-2021|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||doshidroxiacetanilida||0,1|C,2.5980583887,-1.438101534,0.5589293717|C,1.4025852571,-2.1606729164,0.5887787782|C,0.1969272897,-1.5167864424,0.3343012416| C,0.1624459846,-0.1366159075, 0.0446975215| C,1.3649811113, 0.5785756805, 0.0170872931| C,2.5726149736,-0.0752776339,0.2738240424| H,3.537175946,-1.9445163887,0.7581612451| H,1.4042985385,-3.2260257927,0.8098280874| H,1.3313298091, 1.6354726503, -0.2054382821| H, 3.4967745294, 0.4934592841, 0.2486453997| O,-1.0196422568, -2.1623544503, 0.3460612979| H, -0.8845046877,-3.0953648733,0.5531482053| N, -1.1089969275, 0.4160526014, -0.1974557177| H, -1.8651245668, -0.2503043285,-0.135200743| C, -1.4315419153, 1.7181072266, -0.4999337713| C,- 2.9200653188, 1.9663429171, -0.7009670382| H, -3.2454515312, 2.7296187529, 0.0110189113| H,-3.0734038012, 2.3719657328,-1.7046464715| H,-3.5440061254,1.0770342961,-0.5781760913| O,-0.6141257736,2.622712465,-0.6054931568||Version=x86-Win32-G03RevB.03|State=1-A|HF=-515.5028322|RMSD=3.007e-009|RMSF=3.189e-006|Dipole=-0.6559715,-1.4946316,0.2439945|PG=C01 [X(C8H9N1O2)]||

VII.2.34.2. Neutral radical of deprotonated 2-acetamidephenol

1\1\GINC-COPERNICO\FOpt\UB3LYP\6-31G(d,p)\C8H8N1O2(2)\IVAN\12-May-2021 \0\\# opt b3lyp/6-31g(d,p) geom=connectivity\\doshidroxiacetanilidaradical\\0,2\C,2.9361391293,-0.6831280666,0.0001239146\C,2.5803848916,0.6416338426,0.0000959312\C,1.1888318855,1.0306044005,-0.0000221152\C,0.1857933242,-0.052393664,-0.000112952\C,0.5794727473,-1.3915893551,-0.0000842195\C,1.9403015544,-1.6947206336, 0.0000348524\ H, 3.9836969572, -0.9690631357,0.0002128515\ H,3.3129738781,1.4417846128,0.0001601269\ H,-0.1727495332,-2.1679415903,-0.0001557068\ H,2.2447911959,-2.7369653313, 0.0000570563\ O,0.8052890246,2.2264896795,-0.0000522919\N,-1.1078642066, 0.420879201, -0.0002351693\ H, -1.1288468109, 1.4391312475, -0.000205289\ C, -2.2955406089,-0.2924904628, -0.0002833898\ C, -3.5474446706, 0.566499084, 0.0001442152\ H,-4.1450822516, 0.3131745925, -0.8796935864\ H,-4.1435583844, 0.3146263825,0.8814492628\ H,-3.3473562191,1.6404452202,-0.0008741548\ O,-2.3409459028,-1.5126780239,-0.0000103359 \\Version=AM64L-G09RevD.01\State=2-A\HF=-514.8743952\S2=0.774299\S2-1=0.\S2A=0.750411\ RMSD=4.360e-09\ RMSF=5.177e-05\ Dipole= 0.1060884, -0.0789262, 0.0000557\ Quadrupole= 7.0866535, -5.3785271, -1.7081264, -8.0098547, 0.0000371, 0.0003255\PG=C01 [X(C8H8N1O2)]\\@

VII.2.34.3. 2-Acetamidephenolate anion

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C8H8N1O2(1-)|PCUSER|13-Jan-2021|0 |# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||iondoshidroxiacetanilida||-1,1| C,2.9681061598,-0.6281370706,0.0000792456|C,2.5616364973,0.7064112 596,0.0000235031| C,1.1814635474,1.074163928,-0.0000495426|C,0.2560311091,-0.0507600538,-0.0000591484| C,0.6680683,-1.3763636644,-0.0000048374| C,2.041129468,-1.6761230916, 0.0000661434| H,4.0350098808,-0.8568308, 0.0001327407| H,3.2924503881,1.5129472066,0.0000330367| H,-0.083904553, -2.157677964, -0.0000181295| H,2.3722714534, -2.7121178868, 0.000108425| O, 0.7249978878, 2.2701949725, -0.0001072151| N,-1.0737612749, 0.4174608059,-0.0001324612| H, -1.0198748916, 1.4443387193, -0.0001346036|C,-2.2492059788,-0.2420029208,-0.0001132285| C, -3.4811907994, 0.6672886018, 0.0001481558| H,-4.0917231944, 0.4389991467,-0.8799697226| H, -4.0907796147, 0.439863209, 0.8811541064|H,-3.2424702856,1.7348086468,-0.0004753755|O,-2.3913578976,-1.4718722034, 0.0000515907|| Version=x86-Win32-G03RevB.03|State=1-A|HF=-514.9412476|RMSD=4.973e-009|RMSF= 2.928e-005|Dipole=-0.9150045,-0.2075319,0.0000617|PG=C01 [X(C8H8N1O2)]||@

VII.2.34.4. 2-Acetamidephenol radical cation

1|1|UNPC-UNK|FOpt|UB3LYP|6-31G(d,p)|C8H9N1O2(1+,2)|PCUSER|06-Jan-2001|0||#T B3LYP/6-31G(D,P) FOPT TEST||FFF||1,2|C,-1.3579384495,-0.0388374338,0.8744435059|O,-1.2282775449,0.0265875483,2.2057338565|C,-0.19833226,0.0259016673,-0.0138075699|C,-2.6391150205,-0.2184977298,0.3507486039| C,-2.8101090771,-0.2108892961,-1.0221271055|C,-0.4158978583,0.089863717,-1.418834806|C,-1.6956226398,-0.0377735969,-1.9005073776| H, -3.4732846327, -0.3009073391, 1.0378378774| H, -3.8064731877, -0.3084555899,-1.4405727619| N,1.0302562279,-0.0329582519,0.5681070206| H, 0.43238724, 0.1957378221, -2.0784779104| H, -0.4995066852, 0.5959532854, 2.4981407709| H, -1.8649883413, -0.0255407395,-2.9718551479| C,2.3316519229,0.1141463807,-0.0580834479| O, 2.4193242022,0.4249937539,-1.2175627517| C, 3.4734968646,-0.1507258371, 0.8851341219| H,1.057856875,-0.3240703065,1.5404203418|H,3.4312613386, 0.5144669973, 1.7546338967| H, 3.4463484257, -1.1854784428, 1.2453053462| H, 4.4074312169, 0.0172244319, 0.3506540567|| Version=x86-Win32-G03RevB.01|State=2-A|HF=-515.217457|S2=0.760615|S2-1=0.|S2A=0.750076|RMSD=7.411e-009|RMSF=7.174e-006|Dipole=-0.4474003,-0.0897154,0.999306|PG=C01 [X(C8H9N1O2)]||@

VII.2.35. 3-BROMOPHENOL

VII.2.35.1. Neutral form of 3-bromophenol

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C6H5Br1O1|PCUSER|16-Jan-2021|0||#OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||3-bromofenol||0,1|C,2.104867751,-0.3578476124,-0.0000011839|C,0.7716295142,-0.7847539982,0.0000007008|C,-0.23579189, 0.1724685404,-0.0000017509|C,0.0396489859,1.5399783286,-0.0000034645| C, 1.3743808564,1.9430386891,-0.000005375|C,2.4087696406 ,1.0076618847,-0.0000053574| H, 0.5479297698, -1.8442176554,0.0000077277| H,-0.7663601141,2.2632346104,-0.0000034562| H,1.612640578,3.002461678, -0.0000072695| H,3.4456843192,1.3349857316,-0.0000067507| O,3.0628114865,-1.3294878947,-0.0000029863|H,3.9358088043,-0.91538606,0.0000127847| Br,-2.0588349828,-0.4093842897,0.0000034126||Version=x86-Win32-G03RevB.03|State=1-A|HF=-2878.5816276|RMSD=4.445e-009| RMSF=9.973e-005| Dipole =1.0683152, 0.563908, 0.0000109| PG=C01 [X(C6H5Br1O1)]||@

VII.2.35.2. Neutral radical of deprotonated 3-bromophenol

1\1\GINC-COPERNICO\FOpt\UB3LYP\6-31G(d,p)\C6H4Br1O1(2)\IVAN\12-May-2021\0\\# opt b3lyp/6-31g(d,p) geom=connectivity\\3-bromofenolradical\\0,2\C,-2.0934840008,-0.590234902,0.0000000548\C,-0.6651240033,-0.8688477181,-0.0000014863\ C,0.2353361781, 0.1680675877,-0.0000003913\ C,-0.189886293,1.5124284244,0.0000027283\C,-1.5656237349, 1.8120838229, 0.0000055021\ C, -2.5041967212, 0.8028526918, 0.0000048164\ H,-0.3539032658, -1.9065769353,-0.0000040095\ H, 0.5469074243, 2.3073242293,0.0000033869\ H, -1.8753584132, 2.8526878723, 0.0000081775\ H, -3.5700194168, 1.0045226809, 0.0000073429\ O,-2.9334687642, -1.5235284696, 0.0000015996\ Br, 2.1138750108,-0.1884812843, -0.0000037213\\Version=AM64L-G09RevD.01\State=2-A\HF=-2877.9368549\S2=0.791716\S2-1=0.\S2A=0.751206\RMSD=3.844e-09\RMSF=9.162e-05\ Dipole=0.3204174,1.1737961,0.0000009\Quadrupole=-2.8449764,2.9720098,-0.1270334,-6.2108049,-0.0000037,0.0000187\PG=C01 [X(C6H4Br1O1)]\\@

VII.2.35.3. 3-Bromophenolate anion

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C6H4Br1O1(1-)|PCUSER|17-Jan-2021|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||3-bromofenolato||-1,1|C,-2.1845383929,-0.6420088664, 0.0000040464| C, -0.7438066661, -0.8777218496, -0.0000001465| C, 0.1412370375, 0.176922697,0.0000007651|C,-0.2209182586,1.5252208509,0.0000041228|C,-1.6047062721,1.7780740702,0.000006531| C,-2.5469684289,0.7629910523,0.0000059096| H,-0.401387665,-1.9065713649,-0.0000031875| H,0.5171967178,2.31733362,0.0000041465| H,-1.9400967541, 2.8165721182,0.0000085267| H,-3.6104197433, 0.9945110355, 0.0000070706| O, -3.0234180241,-1.582245466,0.0000000673| Br, 2.0737216435,-0.2258499831,-0.0000041276|| Version=x86-Win32-G03RevB.03|State=1-A|HF=-2878.0124375| RMSD= 2.910e-009| RMSF=4.272e-005| Dipole = 2.401925, 1.0650322, -0.0000001| PG=C01 [X(C6H4Br1O1)]||@

VII.2.36. 3-CHLOROPHENOL

VII.2.36.1. Neutral form of 3-bromophenol

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C6H5Cl1O1|PCUSER|16-Jan-2021|0||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||3-clorofenol||0,1|C,-0.0000188404,-0.1418404807,1.5740105376|C,0.0003475321,-0.8495366735,0.3661806686|C,0.0000961642,-0.1340196127,-0.8256510029|C,-0.0005111723,1.2612606206,-0.8550021769|C,-0.000876666,

1.9446302032,0.3602382428|C,-0.0006359544, 1.2570227007, 1.5734673603| H, 0.0008034277,-1.9325061129,0.3783698056| H,-0.0006964616,1.790670105,-1.7999998424| H,-0.0013548297,3.0303867091,0.3626783031| H,-0.0009282351, 1.8024792094, 2.5141654057| O,0.0002545824,-0.8814464062,2.72059487|H,-0.0000669708,-0.2874133948, 3.4826777654|Cl,0.0005764724,-1.0221850478,-2.3448301279||Version=x86-Win32G03RevB. 03| State=1-A|HF=-767.0728344| RMSD=6.019e-009|RMSF=1.259e-004| Dipole=-0.0004259,0.80604,0.9584184|PG=C01 [X(C6H5Cl1O1)]||@

VII.2.36.2. Neutral radical of deprotonated 3-bromophenol

1\1\GINC-COPERNICO\FOpt\UB3LYP\6-31G(d,p)\C6H4Cl1O1(2)\IVAN\12-May-202 1\0\\# opt b3lyp/6-31g(d,p) geom=connectivity\\3-clorofenolradical\\0,2\C,1.5387519866,-0.5194336254,0.0000007374\C,0.1428250574,-0.927672901,0.0000071024\C,-0.849599253, 0.0229181693, 0.0000050517\C,-0.5484073003,1.4015269883,0.0000000384\ C,0.7940609821, 1.8247267477,-0.0000013489\ C,1.8208629008,0.9052526328,0.000000519\H,-0.0744024418,-1.9893015972, 0.0000128385\ H,-1.3560616427,2.1247921098,-0.0000013436\ H, 1.0080214269, 2.8890754059,-0.0000039888\H, 2.8637437454,1.2034806939,0.0000002161\ O, 2.4608744798, -1.3720422695, 0.0000027064\ Cl, -2.5388889412, -0.4620863546, 0.0000074714 \\Version=AM64L-G09RevD.01\State=2-A\HF=-766.4279339\S2=0.791884\S2-1=0.\ S2A=0.751216\RMSD=4.801e-09\RMSF=8.824e-05\Dipole=-0.3652167,1.1645661,-0.0000014\ Quadrupole=-3.7186842,3.680112,0.0385723,4.096245,0.0000003,-0.0000188\ PG=C01 [X(C6H4Cl1O1)]\\@

VII.2.36.3. 3-Chlorophenolate anion

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d,p)|C6H4Cl1O1(1-)|PCUSER|16-Jan-2021|0 ||# OPT B3LYP/6-31G(D,P) GEOM=CONNECTIVITY||3-clorofenolato||-1,1|C,1.6285124653,-0.5655612158,0.0000021241|C,0.2168162235,-0.9300427846,0.0000025986|C,-0.7662924761, 0.036501419,0.0000000625|C,-0.523678396, 1.4128156702,-0.0000031241| C,0.8307065578, 1.7915602901, -0.0000049267| C, 1.8618853759, 0.8669003563, -0.0000033159| H,-0.0318422813, -1.98616002, 0.0000069345| H,-1.3317821138, 2.1343674826, -0.0000044044| H, 1.0700795996, 2.8563649101, -0.0000077791| H, 2.8997938447, 1.1946586443,-0.0000055291| O, 2.5508613262, -1.4252887969, -0.0000013868| Cl, -2.5000493036,-0.4982331207, 0.0000036096||Version=x86-Win32-G03RevB.03|State=1-A|HF=-766.5025538| RMSD =9.750e-009| RMSF=6.258e-005| Dipole=-1.483195,1.0573724,0.000002| PG=C01 [X(C6H4Cl1O1)]||@