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Phenol: A Succinct Essay About Its Bonding Ability in Three Examples[*]

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The present essay represents an effort to focus on some aspects of the bonding abilities of phenol throughout a theoretical study of the three potential energy surfaces of the interaction of phenol with the HCN, HOCN, and HF (including HCl) molecules. The studied surfaces clearly demonstrate the existence of the alternative bonding of phenol *via* its π cloud, largerly localized in the vicinity of the para carbon atom, leading to the formation of metastable π hydrogen-bonded complexes with sufficiently large lifetimes comparable with experimental timescales.

Key words: phenol, hydrogen bond, π-hydrogen bond, HCN, HOCN, HF, HCl

1. Foreground: The Bonding Abilities of Phenol

Phenol belongs to the class of alcohols due to the presence of the OH group attached to the aromatic benzene ring. During nearly 170 years since its discovery by Runge [1,2] in 1834, who isolated phenol from a coal tar and named as *karbolsäure* (it was renamed to *phénol* by Gerhardt [3] nine years later), phenol and its substituted derivatives played and pursue to play the gross role in the theory of hydrogen bonding, primarily due to the well established fact of an almost smooth variation of their hydrogen bonding abilities over a wide pK_a domain from 10.2 to 0.4. This has been discussed at length in [4–14].

The OH group is the unique site of phenol (PhOH) actually responsible for its hydrogen bonding ability (a possible weak bonding with the phenolic C-H groups is not treated here). It acts bifunctionally: either it **d**onates the proton to the the "outsider" acceptor molecule X, forming that way the **d**-type hydrogen-bonded bridge O–H···X, or (and) it **a**ccepts the proton from the X-H group, thanks to its oxygen lone electron pair. The latter then results in the appearance of the **a**-type hydrogen bond X–H···O. As commonly suggested, the majority of cases in the chemistry of phenols (the pres-

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ent treatment is only confined to neutral X or X–H systems) falls to the former category [4–14]. In other words, the **d** hydrogen bonding favors over the **a** that is usually argued in terms of the stretching vibrational mode ν_{OH} of phenol as its most accepting mode. However, there might exist a high enough energetic barrier, separating these forms from each other, such that, if the **a**th bridge was initially prepared, it remains so for a rather long timescales, sufficient to conduct the appropriate measurements. It has been also always assumed that the aromatic ring of phenol is less favorable for hydrogen bonding (precisely, of the π type [15,16]), so its possible bonding with the X–H molecules was even neglected or not considered, because it was previously unseen in experiments. That might be true, on the one side, like, for example, with X–H = H_2O or NH_3, where the ground electronic state potential energy surface (PES) of PhOH-X-H shows no minima within the ring area (see comments in [17]). Though, on the other side, we cannot rule out, generally speaking, that there could exist such X-Hs for which the corresponding PESs of PhOH-X-H have the least π energetic minimum. This raises the following questions: **(i)** Whether such systems do actually exist?, **(ii)** How then π is energetically comparable with **d** and **a**?, **(iii)** Whether it is well separated from them to be experimentally detected? and finally, **(iv)** Does always **d** dominate over **a**?

As a matter of fact, such questions have not been addressed at all (except partly **(iv)**) in the past theoretical and experimental studies of phenols [4–13]. We nevertheless believe that they are worth to be investigated, and this is actually a key goal undertaken in this paper, whose computational methodology is outlined in [20] and whose arguments are extremely simple. We will study the three different PESs of PhOH-HCN, PhOH-HOCN, and PhOH-FH (partly PhOH-HCl) and show that they all have three energetic minima of the **d**, **a**, and π types, thus **(i)** and **(iv)** will be easily answered in that way. Their landscape dispositions will shed then a light on **(ii)** and **(iii)**.

2. Example I: Phenol-Hydrogen Cyanide Complex

The ground electronic state PES of the complex PhOH-HCN is shown in Figure 1. Its **d** and **a** structures fit the canonical fingerprints of hydrogen bond [22,23]. In **d**, as expected, the harmonic ν_{OH} stretching vibration downshifts by 115 cm^{-1} mirroring, say energetically, its modest binding energy of 2.8 kcal/mol after ZPVE and, geometrically, the elongation of the OH bond by 0.006 Å compared to that of a bare phenol. The IR activity of ν_{OH} is enhanced about ten times. A sharing of the proton within the O–H···N hydrogen bond strengthens the triple CN bond, which is contracted by 0.001 Å and whose harmonic stretching vibrational mode ν_{CN} is blue shifted by 23 cm^{-1}. The **a** structure is formed thanks to the almost linear C–H···O hydrogen bond, accomodating the elongation of the C–H bond by 0.006 Å (interestingly, it is precisely of the same magnitude as that of the O–H bond in **d**). The corresponding stretching mode ν_{CH} undergoes a red shift by 99 cm^{-1} and its IR activity grows by a factor of 6. A marked difference of the **d**onor and **a**cceptor functionings of the phenolic OH group consists in a strengthening of the C–O group in the former case, that is seen from its compressing by 0.008 Å, and its weakening in the latter, accompanied by the elonga-

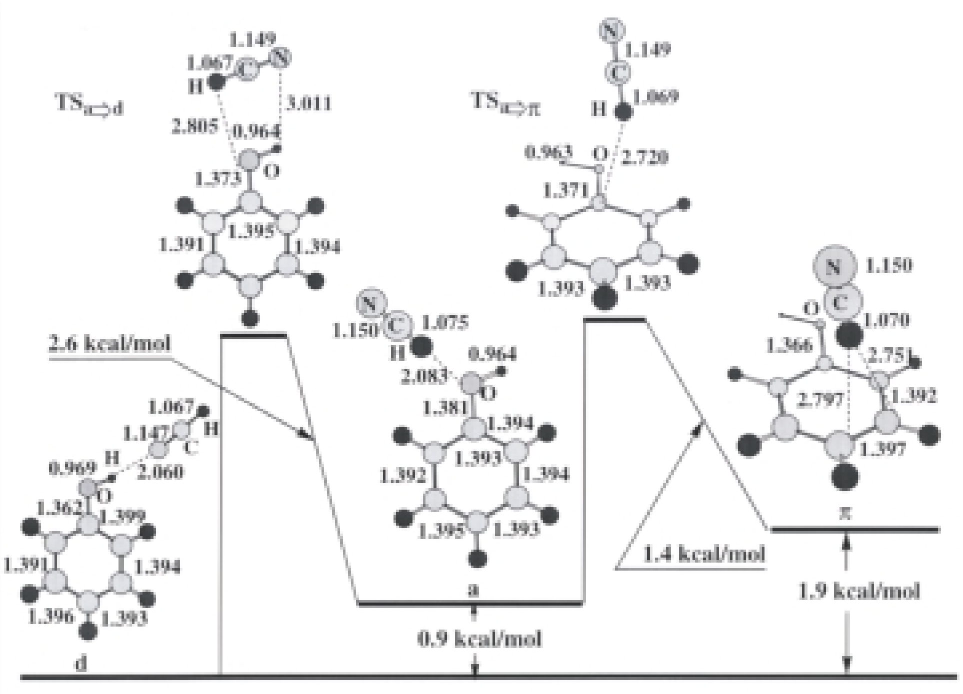

Figure 1. The potential energy surface of the interaction between phenol and hydrogen cyanide. Bond lengths in Å.

tion by 0.011 Å. This is physically obvious: in **d**, the proton of the OH group becomes shared with the N atom of HCN and releases the partial electronic charge directed then to enhance the C–O bond, while in **a**, the partial lone-pair charge of the oxygen participates in the formation of the C–H···O hydrogen bond. Notice, finally, that the HCN molecule in **a** is placed out of the phenol ring (this is also true for all other studied complexes due to the particular spatial direction of the oxygen lone pair except PhOH-HOCN which reveals two quasi isomers of this kind). The transition state TS$_a$ linking two symmetrical dispositions of **a**, say, above and below the phenolic plane, is characterized by a tiny barrier of 0.1 kcal/mol, easily accessible at $T > 100$ K.

The π structure demonstrated in Figure 1 is remarkable for several reasons. First of all due to the fact that, to our knowledge, this is the first structure with the anchor π hydrogen bonding with phenol reported so far (see also [14]). According to the present computational results, the π bond is only formed between the C–H group of the HCN molecule and the carbon atom placed in the trans meta position. Such bond is rather weak, that is primarily indicated by a very small (≈ 0.001 Å) elongation of the C–H bond and a red shift of ν_{CH} by 21 cm^{-1}. It is worth also mentioning a somewhat higher polarity of **d** and **a** (the total dipole moments are equal to 5.3 and 5.1 D, respectively) compared to that of π (3.8 D).

Comparing the electronic energies (after ZPVE) of the **d**, **a**, and π structures collected in Table 1, we place them in the following order: **d** is stronger by 0.9 kcal/mol than **a** which, in turn, is stronger than π by 1.0 kcal/mol. This implies that the energies of all these forms are rather close to each other, although **d** somewhat dominates. This is actually the order at 0 K. As seen in Table 1, the π form possesses a larger entropy than both **d** and **a** which, in terms of Gibbs energy at T = 298.15 K, diminishes the difference between **a** and π to 0.1 kcal/mol, though still keeps the latter less stronger than **d** by 0.6 kcal/mol. The energetic barriers associated with $TS_{\mathbf{a}\Rightarrow\mathbf{d}}$ and $TS_{\pi\Rightarrow\mathbf{a}}$, which separate, respectively, **a** from **d**, and π from **a**, are equal to 2.6 and 1.4 kcal/mol. We may, therefore, conclude that **d**, **a**, and π are somewhat separated from each other, particularly, **d** from **a**, and, thus, they all are likely good candidates for experimental determination by, for instance, rotational spectroscopy, which could be facilitated by the knowledge of the rotational constants. The latters are collected in Table 1 and show a distinction between the studied forms.

Table 1. Key features of the PES of the interaction between phenol and hydrogen cyanide. Total electronic energies and enthalpies in hartree, ZPVE in kcal/mol, entropies in cal/mol·T, total dipole moments in D, rotational constants in MHz.

Form	Energy +401	ZPVE kcal/mol	Enthalpy +400	Entropy cal/mol·T	Rotational constants, MHz			Dipole D
d	–0.0209	76.40	–0.8897	100.65	4169.5434	693.0442	594.2675	5.3
a	–0.0196	76.49	–0.8883	100.81	3959.3196	636.9127	595.4124	5.1
π	–0.0173	76.03	–0.8862	104.80	1838.0962	1058.9500	881.9349	3.8
$TS_{\mathbf{a}}$	–0.0195	76.28	–0.8893	94.21	4339.9269	620.4890	542.8733	5.2
$TS_{\mathbf{a}\Rightarrow\mathbf{d}}$	–0.0169	75.91	–0.8869	100.10	5101.3286	613.9606	548.0064	2.1
$TS_{\pi\Rightarrow\mathbf{a}}$	–0.0164	75.89	–0.8864	99.22	2167.8732	866.9513	788.2955	4.0

3. Example II: Phenol-HOCN Complex

The interaction of phenol with the HOCN molecule looks drastically different in many aspects from what we have seen in Example I. Let us have a look at Figure 2. We observe that, first, the energetic order, revealed in Example I between **d**, **a**, and π, completely changes in a sense that **a** becomes significantly favored over **d**. This seems to be readily understandable in terms of the canonical hydrogen bond theory, bordering a stronger O–H···O bond from a less stronger O–H···N. Second. There exists a near degeneracy in **a**. That is, in the other words, there are two different structures, say, $\mathbf{a}_1$ and $\mathbf{a}_2$, non-planar and planar with respect to the phenol ring. In terms of the electronic energy, they are practically iso-energetic although a small difference of 0.06 kcal/mol in their ZPVEs makes $\mathbf{a}_2$ slightly more dominant. At room temperature, the order, in terms of Gibbs energy, reverses, due to a larger entropy of $\mathbf{a}_2$ (see Table 2). The binding energy of $\mathbf{a}_1$ amounts to 8.5 kcal/mol, so this is not a weak hydrogen bond (see also a further discussion of its properties). Third and the last worth indeed to be

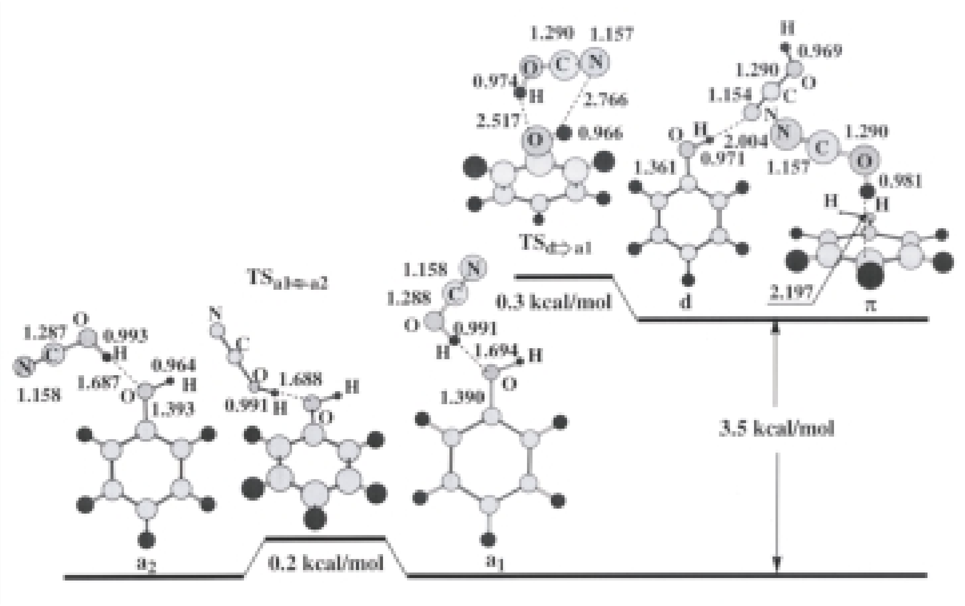

Figure 2. The potential energy surface of the PhOH–HOCN interaction. Bond lengths in Å.

mentioned now. **d** appears to be almost iso-energetical to π. Both **d** and π distance from $\mathbf{a}_1$ by 3.5 kcal/mol. We have already noticed that the hydrogen bonding in $\mathbf{a}_{1,2}$ is not too weak. Their key features are the following: 1. The O–H···O_{ph} (O_{ph} belongs to PhOH) bond is quite short (1.694 Å in $\mathbf{a}_1$ and 1.687 Å in $\mathbf{a}_2$) and practically linear (177.1° and 178.6°, respectively). 2. The OH bond of HOCN elongates rather spectacularly, by 0.023 and 0.025 Å, to be exact. 3. The H-stretching ν_{OH} of HOCN undergoes the enormous red shifts of 466 and 485 cm^{-1} and IR enhancement (by factors of 14 and 13) and the phenolic H-stretching mode is also redshifted by 7 and 13 cm^{-1}, due to a weakeness of this bond as a consequence of forming the O–H···O_{ph} one.

As we have already emphasized, the **d** and π forms are almost iso-energetical, that is, to say, their binding energies are very close to each other. Though, by the nature of their bonding, they are absolutely different: the former is a typical weak hydrogen bond, whose formation is accompanied by the elongation of the phenolic O–H bond by 0.008 Å and by the red shift of its harmonic streching vibration by 151 cm^{-1}. The latter, however, refers to the alternative π hydrogen bond, where the hydrogen atom of the HOCN molecule points down to the carbon atom in the para position. Its formation induces a lengthening of the O–H bond of HOCN by 0.013 Å and redshifting of the corresponding stretch by 281 cm^{-1}. There is still another feature, making these two forms rather distinct from each other. We mean the transition state structure $TS_{\mathbf{d}\Rightarrow\mathbf{a}_1}$, which separates **d** from $\mathbf{a}_1$. The corresponding barrier is so small (0.3 kcal/mol) on the **d** side that it actually supresses the stability of the **d** form of the PhOH–HOCN complex at room temperature, say the least, thus, predicting its existence only in three forms, namely, $\mathbf{a}_1$, $\mathbf{a}_2$, and π. Though, precisely, since $\mathbf{a}_1$ is separated from $\mathbf{a}_2$ by the transition state $\mathrm{TS}_{\mathbf{a}_1 \Leftrightarrow \mathbf{a}_2}$ with a small barrier, just 0.2 kcal/mol, we may actually observe a "free" walk over the rather flat **a** portion of PES.

Table 2. Key features of the PES of the PhOH–HOCN interaction. Total electronic energies and enthalpies in hartree, ZPVE in kcal/mol, entropies in cal/mol·T, total dipole moments in D, rotational constants in MHz.

Form	Energy +476	ZPVE kcal/mol	Enthalpy +476	Entropy cal/mol·T	Rotational constants, MHz			Dipole D
$\mathbf{a}_2$	–0.2682	80.26	–0.1304	103.58	2816.5914	643.4520	532.5254	6.6
$\mathbf{a}_1$	–0.2682	80.20	–0.1303	107.06	3533.3647	510.2954	471.0877	6.4
d	–0.2617	79.65	–0.1240	110.76	4077.5918	419.9378	380.9088	6.2
π	–0.2618	79.65	–0.1244	108.94	1879.5331	820.3508	718.0418	4.2
$\mathrm{TS}_{\mathbf{d} \Rightarrow \mathbf{a}_1}$	–0.2612	79.65	–0.1246	100.11	2315.5893	781.4887	754.2424	3.4
$\mathrm{TS}_{\mathbf{a}_1 \Leftrightarrow \mathbf{a}_2}$	–0.2680	80.15	–0.1310	98.93	3538.8236	523.2471	475.0342	7.0

4. Example III: Interaction of Phenol with HF

This is another, much simpler and obvious example, when the **d** form becomes less favorable than **a**: 3.6 kcal/mol is the difference between them after ZPVE. It appears, however, not because of that the donor ability of the OH group of phenol is weaker than its acceptor one. Rather of that the acceptor ability of HF is substantially weaker than its donor one, even to a π cloud of the phenol ring in the vicinity of the trans meta-para carbon atoms, where the bonding occurs in π, and this is precisely the reason why the π complex is more stable than **d** by 0.4 kcal/mol. π is placed 3.2 kcal/mol above **a** and separated from the latter by the barrier of 1.2 kcal/mol formed by the transition state $\mathrm{TS}_{\pi \Rightarrow \mathbf{a}}$. Clearly, it is not quite easily accessible at room temperature. These three forms, lying on the PES of the interaction of phenol with hydrogen fluoride together with the transition structure $\mathrm{TS}_{\pi \Rightarrow \mathbf{a}}$, governing the transition $\pi \Rightarrow \mathbf{a}$, are shown in Figure 3.

Let us deal first with the **a** form. It is stabilized by 6.2 kcal/mol (ZPVE included) relative to the infinitely separated PhOH and HF due to formation of the almost linear hydrogen bond F–H···O. This hydrogen bond is indeed quite strong: the F–H bond therein undergoes an elongation by 0.016 Å compared to the equilibrium distance in the diatomic HF molecule. This, on the one hand, weakens its harmonic force constant: ν_{HF} downshifts by 379 cm^{-1} and, on the other one, strengthens its dipole moment derivative: IR activity of ν_{HF} raises by a factor of 9. The corresponding elongation in the π form is less (only 0.008 Å). A similar tendency is predicted for the ν_{FH} stretching mode in π: its downshift amounts to 208 cm^{-1}.

In **d**, the key bond is the phenolic OH one. Relative to its length in a bare phenol, it is elongated by only 0.003 Å that, in turn, is manifested spectroscopically: the ν_{OH} is redshifted by 48 wavenumbers. It is then worth to compare these structures of

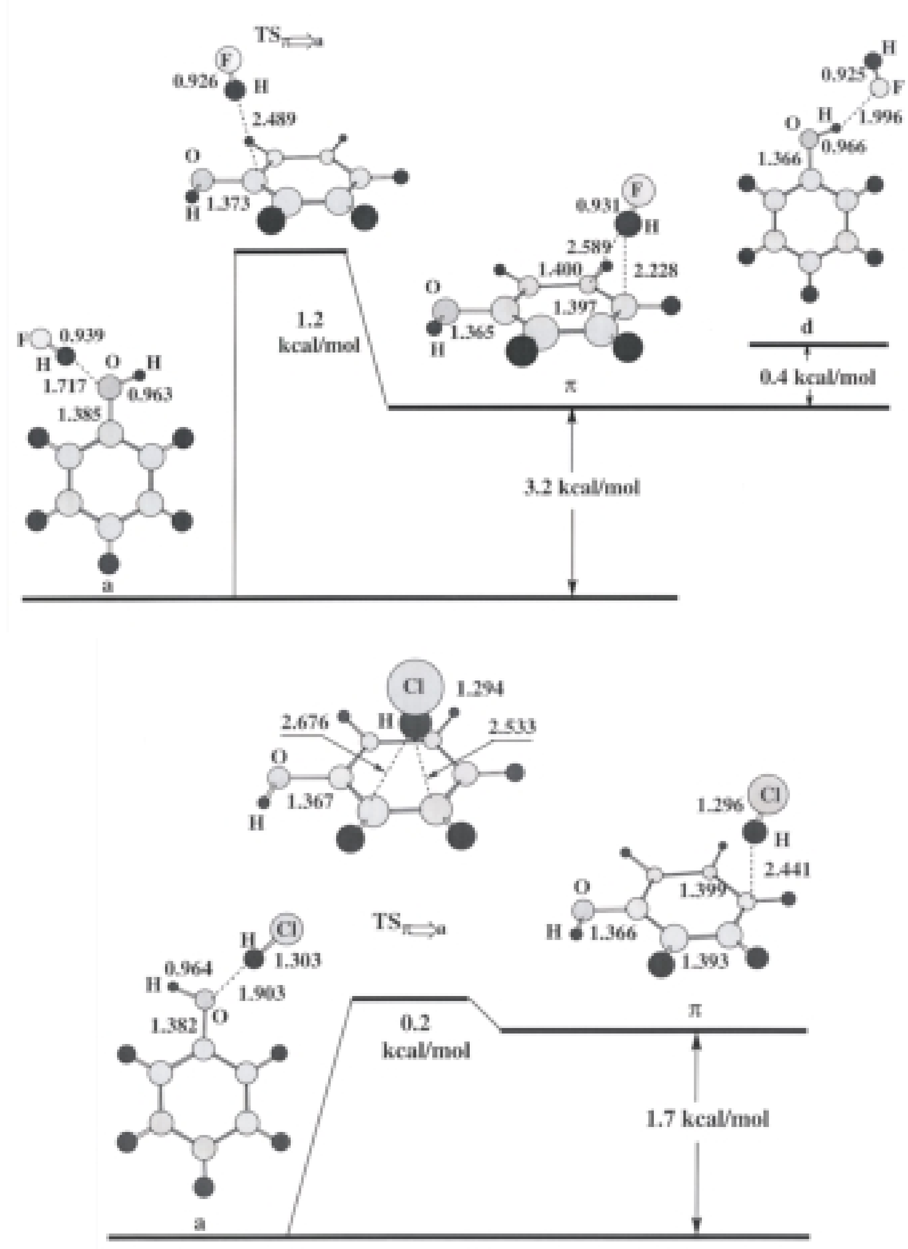

Figure 3. The potential energy surfaces of the interaction of phenol with hydrogen fluoride and hydrogen chloride molecules. Bond lengths in Å.

PhOH–HF with their analogues formed on the PES of PhOH–HCl (continue to see Figure 3). There appear three interesting points in that comparison. 1) Surprisingly, PhOH–HCl is not realized as the **d** form, at least, we would say precautiously, at the present, rather high computational level. 2) The binding energy of **a** of PhOH–HCl amounts to 3.4 kcal/mol after ZPVE, that is lower by 2.8 kcal/mol from that was predicted for the same form on the PhOH-HF PES. An analogous bonding trend has been revealed for benzene-HF and benzene-HCl interactions [24], although, interestingly, the difference is much smaller: only 0.9 kcal/mol. Notice further the red shifts of the harmonic stretching mode ν_{HCl} in **a** and π: 217 *vs.* 127 cm^{-1}. Nevertheless, they will not certainly fit the experimental shifts, due to the well known large anharmonicity of such mode of HCl [25]. 3) On the PES of PhOH–HCl, the transition state $TS_{\pi\Rightarrow\mathbf{a}}$ determines a very small barrier of 0.2 kcal/mol, that means that **a** can be only experimentally detectable on this PES.

Table 3. Key features of the PESs of the interactions between phenol and HF and phenol and HCl. Total electronic energies and enthalpies in hartree, ZPVE in kcal/mol, entropies in cal/mol·T, total dipole moments in D, rotational constants in MHz. E_0 = 408 and H_0 = 407 hartree for HF and E_0 = H_0 = 768 hartree for HCl.

Form	Energy +E_o	ZPVE kcal/mol	Enthalpy +H_o	Entropy cal/mol·T	Rotational constants, MHz			Dipole D
HF								
d	–0.0469	72.07	–0.9229	98.83	4613.9333	949.6505	787.5852	2.6
a	–0.0543	73.16	–0.9296	91.67	4459.1045	1045.1593	858.3164	4.3
π	–0.0478	72.28	–0.9240	93.99	2789.4701	1206.0832	1183.3384	3.0
$TS_{\pi\Rightarrow\mathbf{a}}$	–0.0458	71.83	–0.9230	91.87	2529.7982	1343.5307	1186.4277	3.1
HCl								
a	–0.4006	70.87	–0.2791	95.84	4113.7630	638.0771	566.8563	3.7
π	–0.3969	70.28	–0.2758	98.40	2290.6818	826.3923	773.0280	2.5
$TS_{\pi\Rightarrow\mathbf{a}}$	–0.3966	70.17	–0.2765	92.71	1951.5337	957.8612	794.8972	2.0

5. Conclusions

In the present work, we have focused on the PESs of the interaction of phenol with the molecules HCN, HOCN, and HF (touching HCl as well), chosen as not somewhat precarious molecules rather the common ones, traditionally betaken to analyze a hydrogen bonding ability of an either molecule [22,23]. We have shown that, in principle, all these complexes can be partly realized throughout a π form with a rather typical π hydrogen bond between these molecules, as proton donors, and a π cloud of the phenolic ring essentially localized in the vicinity of the para carbon atom. In the sense of the discussed bonding abilities, what fundamentally matters in the present work is that this reconciles the practically abandoned phenolic ring with the OH group. We have also shown that the demonstrated π forms are not the single energetic minima on the corresponding PES rather than they are indeed well separated from the other, even global, ones so their experimental detection would be likely possible. We think that this short essay has given the satisfactory answers on the questions **(i)**–**(iv)** posed in Foreground and we believe that it will open a rather rich avenue in the chemistry of phenolic compounds containing π hydrogen bonds, whose lifetimes could be increased using particular phenol substituted derivatives, despite the fact that the firm conclusions will be certainly reached after performing highly demanding MP2 calculations. As wise "phenolic" people say, phenol is inexhaustible as the electron.

Acknowledgments

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17. However, the thorough analysis of the potential energy surface of the phenol-water$_4$ complex, conducted in [18] and juxtaposing it with the PESs of the phenol–water$_{1-3}$ complexes, demonstrates that four different structures, having either 2D or 3D patterns of water molecules, resides at the very bottom of this PES. A *3D* pattern originates when the terminated water molecule becomes contiguous to the π cloud of the phenol ring. This can be explained by that the ability of the phenolic OH-group to accept a hydrogen bond becomes almost exhausted when three water molecules form a 2D ring nearby it (similarly to the ring or book structures of water hexamer which are no longer energetically favorable [19]) and, therefore, competes with the ability of the π cloud of the phenol ring to form the subtle π one with a water molecule.
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