

Supporting information for the article:

## Hydrogen bond donating ability of meta and para hydroxy phenoxy radicals

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### $\alpha_2^H$ values for radical **1** from $K_{HB}$ measured in benzene.

Hunter and co-workers have recently proposed two “universal” donor and acceptor scales referred to H-bond formation in a ideally apolar solvent. Binding free energies in real solvents between a donor ( $\alpha$ ) and an acceptor ( $\beta$ ) can be calculated within reasonable accuracy by using equation 1, if  $\alpha_s$  and  $\beta_s$  values of the employed solvent (or solvent mixtures) are known. Hunter’s  $\alpha$  and  $\beta$  parameters can be derived from the widely known Abraham  $\alpha_2^H$  and  $\beta_2^H$  values, which refer to  $CCl_4$ , by using equations 2 and 3.<sup>1</sup>

$$\Delta G^\circ (\text{kJ mol}^{-1}) = -(\alpha - \alpha_s) (\beta - \beta_s) + 6 \quad (1)$$

$$\alpha = 4.1(\alpha_2^H + 0.33) \quad (2)$$

$$\beta = 10.3(\beta_2^H + 0.06) \quad (3)$$

In the present work, the  $\alpha$  value of **1** was obtained by equation 1, from the  $\alpha_s$  and  $\beta_s$  of benzene (1.0 and 2.2, respectively), the  $\Delta G^\circ$  measured by EPR in benzene, and the  $\beta$  of the co-solvents used for the experiment.

For instance, in the case of DMSO,  $K_{HB}$  was  $810 \pm 50 \text{ M}^{-1}$ , so  $\Delta G^\circ = -16.6 \text{ kJ/mol}$ . Equation 1 can be therefore re-written as equations 4, from which  $\alpha = 4.5$ .

$$-16.6 = -(\alpha - 1.0) (8.7 - 2.2) + 6 \quad (4)$$

1) Hunter, C. A. *Angew. Chem., Int. Ed.* 2004, **43**, 5310–5324. Cook, J. L.; Hunter, C. A.; Low, C. M. R.; Perez-Velasco, A.; Vinter J. G. *Angew. Chem. Int. Ed.* 2008, **47**, 1-4.

### Estimation of solvent effects not related to H-bonds formation

The dielectric effects of some solvents employed in the present work were estimated by studying the EPR spectrum of a radical in which the para OH group of **1** is replaced by a methoxyl group, that is, the 2,6-di-tert-butyl-4-methoxyphenoxy radical (**7**). It is expected that the variations of the **7** spectrum in different solvent mixtures should reflect only dielectric effects. The hyperfine splitting constants for **7** measured in different solvents mixtures are reported in Table S1, where it can be evidenced that the HBA solvents possess dielectric effects only at large concentrations. Thus, corrections to keep into account dielectric effects were performed only in the cases of EtCN and EtOAc at concentrations larger than 1 M.

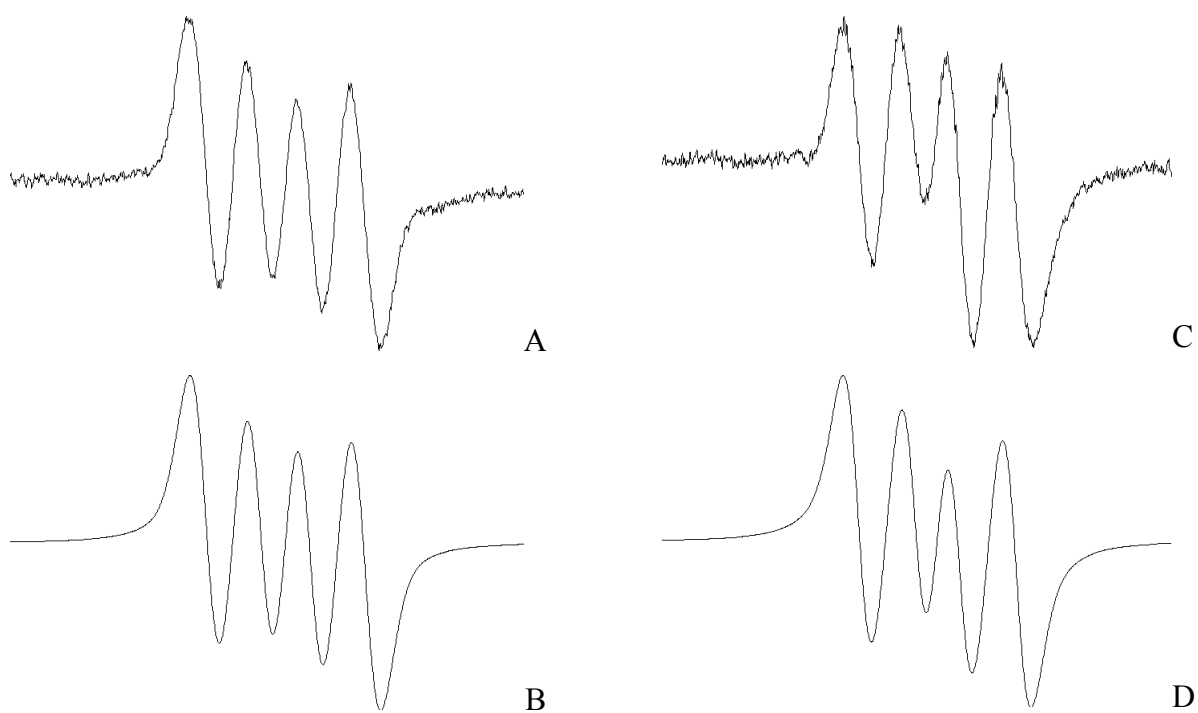
**Table S1.** Solvent effect on EPR spectrum of **7**.

solvent <sup>a</sup>	$a(2\text{H}_{\text{meta}}) / \text{G}$	$a(3\text{H}_{\text{para}}) / \text{G}$
benzene	0.94	1.56
DMSO 0.34 M	0.92	1.57
DMSO 0.67 M	0.92	1.59
DMSO 1.74 M	0.90	1.59
EtOAc 2.6 M	0.92	1.57
EtCN 0.7 M	0.92	1.57
EtCN 1.4 M	0.90	1.59

a) main solvent is benzene.

## Experiments with 4,6-di-tert-butyl-3-hydroxyphenoxyl radical

The 4,6-di-tert-butyl-3-hydroxyphenoxyl radical was generated by photolysis of an oxygen-free 0.015 M solution of the parent phenol in benzene, containing 10% v/v of tert-butylperoxide as radical initiator (see Figure S1). In the absence of the initiator, no spectrum was visible. The coupling constants were measured as 4.04 G ( $1H_{ortho}$ ) and 2.13 G ( $1H_{meta}$ ), typical of neutral phenoxyl radicals. The coupling with the  $H_{OH}$  was too small to be detected. Even after the addition of relatively large amounts of HBA solvents, the spectrum did not change significantly (see Figure S1).



**Figure S1.** Spectrum obtained by irradiating 4,6-di-tert-butyl-3-hydroxyphenol in benzene with 10% of  $t\text{BuOO}t\text{Bu}$  (A) or with HMPA 0.14 M.

In the following section, the detailed results of EPR experiments are reported. In the first table, the experimental hyperfine splitting constants for **1** measured at each co-solvent concentration are shown. The concentrations of the co-solvents are corrected keeping into account that the parent phenol of **1** also act as H-bond donor by the two OH groups. These concentrations were calculated using the chemical kinetic and equilibrium simulator Gepasi<sup>2</sup> (version 3.30, <http://www.gepasi.org>) and the equilibrium constants were estimated by using the  $\alpha_2^H$  values of 4-OMe-phenol (0.57)<sup>3</sup> and of 2,6-di-tert-butyl-4-methylphenol (0.17).<sup>4</sup>

2) P. Mendes, *Trends Biochem. Sci.* 1997, 22, 361-363.

3) see reference 5 in the main article

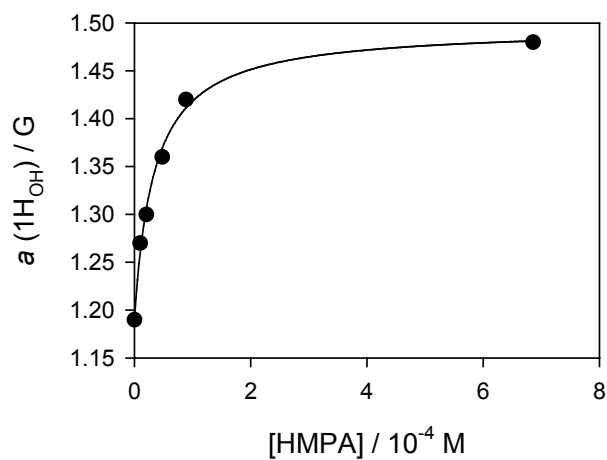
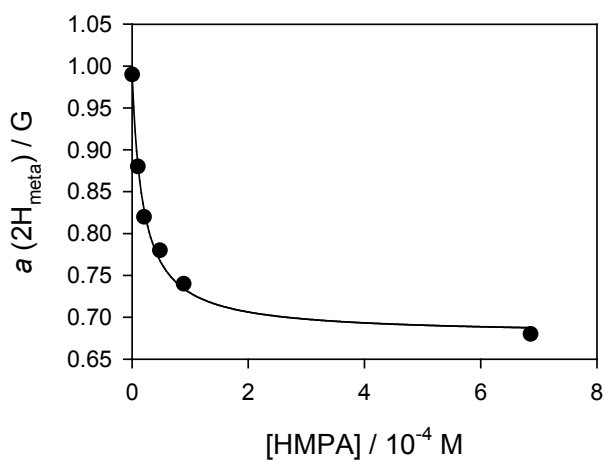
4) G. Litwinienko, E. Megiel, and M. Wojnicz *Org. Lett.*, 2002, 4, 2425–2428

### HBA (hydrogen bond accepting) solvent: hexamethylphosphoramide (HMPA)

[HMPA] / M	[HMPA] <sub>corr</sub> / M	<i>a</i> (2H <sub>meta</sub> ) / G	<i>a</i> (1OH) / G
0	0	0.99	1.19
3.6e-4	1.0e-5	0.88	1.27
7.2e-4	2.1e-5	0.82	1.30
1.4e-3	4.1e-5	0.78	1.36
2.9e-3	8.9e-5	0.74	1.42
0.014	6.9e-4	0.68	1.48

### Fitting results, solvent HMPA: $K_{HB} = (4 \pm 1) \times 10^4 \text{ M}^{-1}$

constant	$K_{HB} / \text{M}^{-1}$	<i>a</i> / G
meta (2H)	3.0e4	0.68
para (1OH)	5.2e4	1.50



$$\Delta G = -6.27 \text{ kcal/mol}$$

$$\alpha = 4.7; \alpha_2^H = 0.82$$

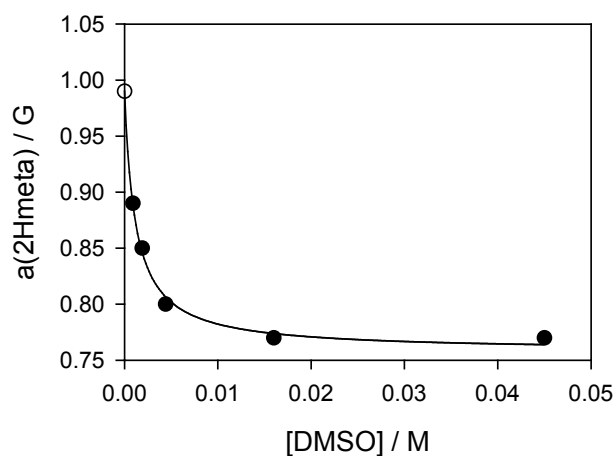
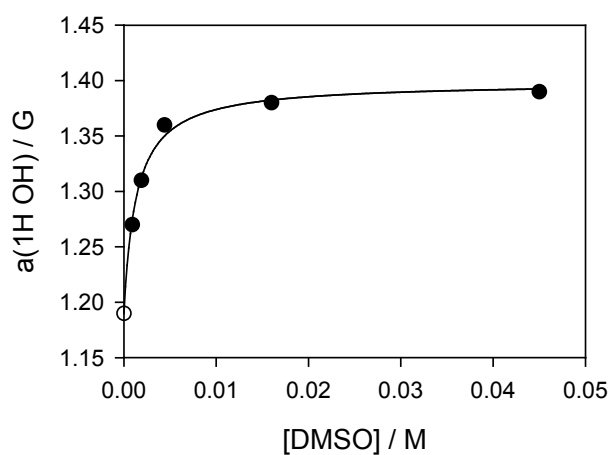
### HBA solvent: dimethylsulfoxide (DMSO)

[DMSO] / M	[DMSO] <sub>corr</sub> / M	<i>a</i> (2Hmeta) / G	<i>a</i> (1OH) / G
0	0	0.99	1.19
5.3e-3	9.0e-4	0.89	1.27
7e-3	1.9e-3	0.85	1.31
0.014	4.4e-3	0.80	1.36
0.035	0.016	0.77	1.38
0.07	0.045	0.77	1.39
0.35 <sup>a</sup>	0.32	0.74	1.43
0.7 <sup>a</sup>	0.67	0.72	1.43

a) not included in H-bond analysis

### Fitting results, solvent DMSO: $K_{\text{HB}} = 810 \pm 50$

constant	$K_{\text{HB}} / \text{M}^{-1}$	<i>a</i> / G
meta (2H)	860	0.76
para (1OH)	750	1.40



$$\Delta G = -3.97 \text{ kcal/mol}$$

$$\alpha = 4.5; \alpha_2^{\text{H}} = 0.76$$

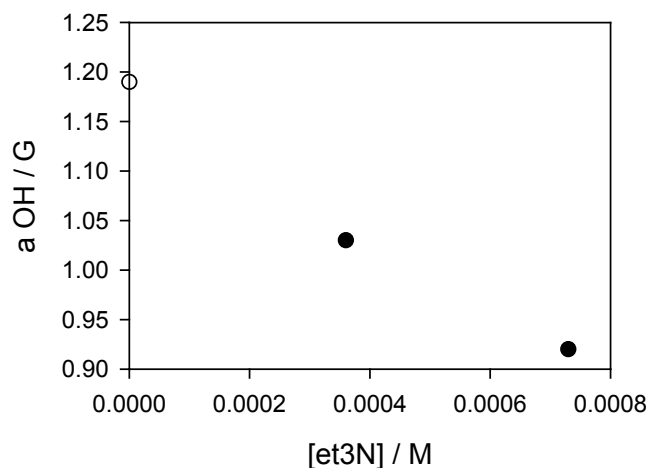
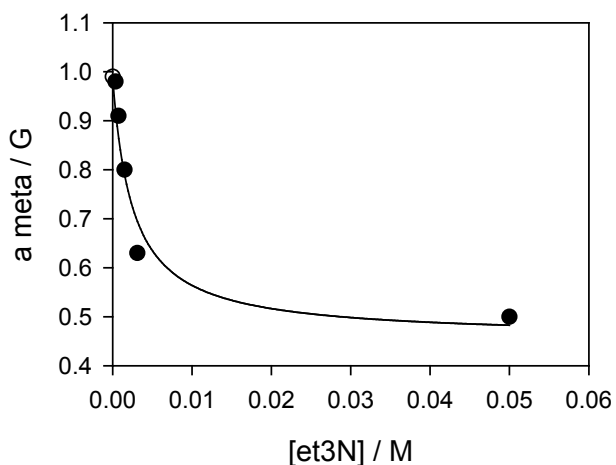
**HBA solvent: triethylamine (TEA)**

[TEA] / M	[TEA] <sub>corr</sub> / M	<i>a</i> (2Hmeta) / G	<i>a</i> (1OH) / G
0	0	0.99	1.19
9e-4	4.9e-4	0.98	1.03
1.8e-3	9.8e-4	0.91	0.92
3.6e-3	2.0e-3	0.8	- b
7.2e-3	4.1e-3	0.63	- b
0.072	5.4e-2	0.50	- b
0.36 <sup>a</sup>	0.33	0.50	0.88
1.1 <sup>a</sup>	1.1	0.53	0.93
1.8 <sup>a</sup>	1.8	0.55	0.95

a) not included in H-bond analysis. b) this constant could not be detected because of the broadening of the outer lines of the triplets.

**Fitting results, solvent TEA:  $K_{\text{HB}} = 292 \pm 30 \text{ M}^{-1}$  (estimated error)**

constant	$K_{\text{HB}} / \text{M}^{-1}$	<i>a</i> / G
meta (2H)	292	0.45
para (1OH)	nd	≈ 0.88



$$\Delta G = -3.36 \text{ kcal/mol}$$

$$\alpha = 4.78; \alpha_2^{\text{H}} = 0.84$$



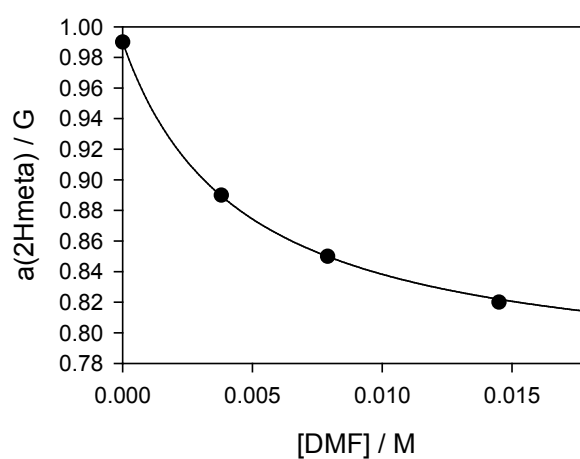
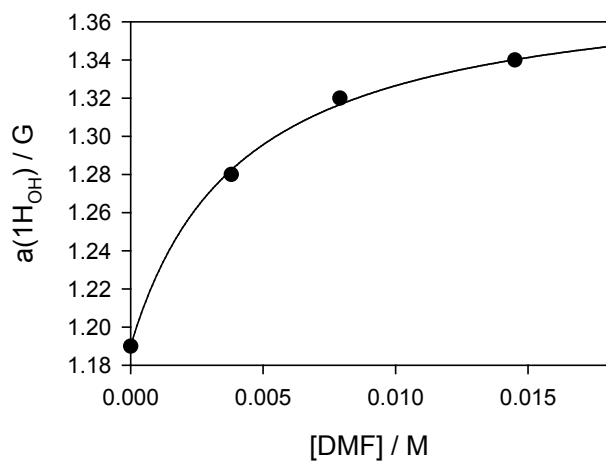
### HBA solvent: dimethylformamide (DMF)

[DMF] / M	[DMF] <sub>corr</sub> / M	<i>a</i> (2Hmeta) / G	<i>a</i> (1OH) / G
0	0	0.99	1.19
6.4e-3	2.9e-3	0.89	1.28
0.013	6.3e-3	0.85	1.32
0.022	0.012	0.82	1.34
0.032	0.018	0.81	1.35
0.6 <sup>a</sup>	0.57	0.76	1.42
2.15 <sup>a</sup>	2.1	0.71	1.43

a) not included in H-bond analysis

### Fitting results, solvent DMF: $K_{HB} = 230 \pm 10 \text{ M}^{-1}$

constant	$K_{HB} / \text{M}^{-1}$	<i>a</i> / G
meta (2H)	241	0.77
para (1OH)	220	1.38



$$\Delta G = -3.22 \text{ kcal/mol}$$

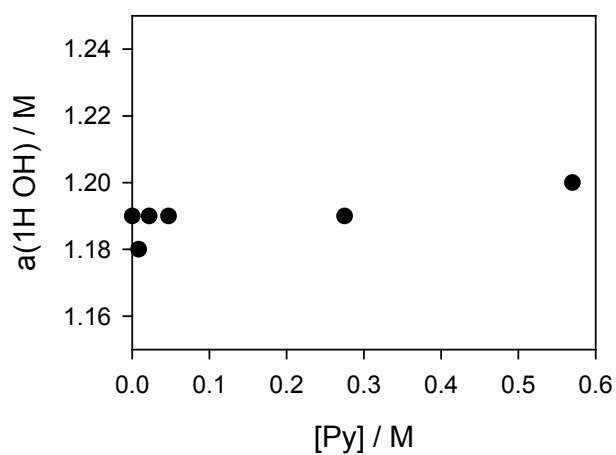
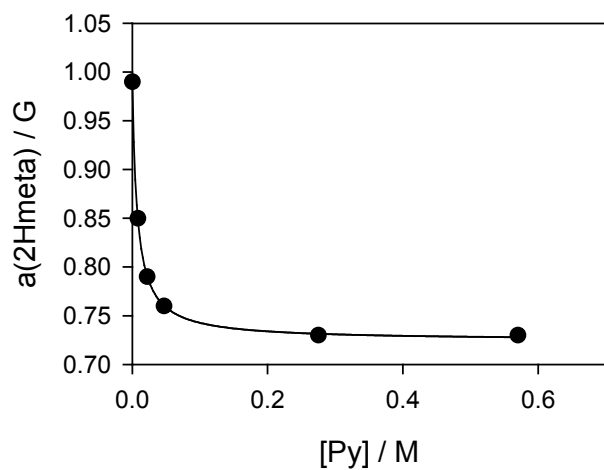
$$\alpha = 4.74; \alpha_2^H = 0.83$$

### HBA solvent: pyridine (Py)

[Py] / M	[Py] <sub>corr</sub> / M	<i>a</i> (2Hmeta) / G	<i>a</i> (1OH) / G
0	0	0.99	1.19
1.2e-2	8.3e-3	0.85	1.18
0.03	0.022	0.79	1.19
0.06	0.047	0.76	1.19
0.3	0.28	0.73	1.19
0.6	0.57	0.73	1.20

### Fitting results, solvent pyridine: $K_{\text{HB}} = 136 \pm 14 \text{ M}^{-1}$ (estimated error)

constant	$K_{\text{HB}} / \text{M}^{-1}$	<i>a</i> / G
meta (2H)	136	0.72
para (1OH)	nd	1.19



$$\Delta G = -2.9 \text{ kcal/mol}$$

$$\alpha = 4.78; \alpha_2^{\text{H}} = 0.84$$

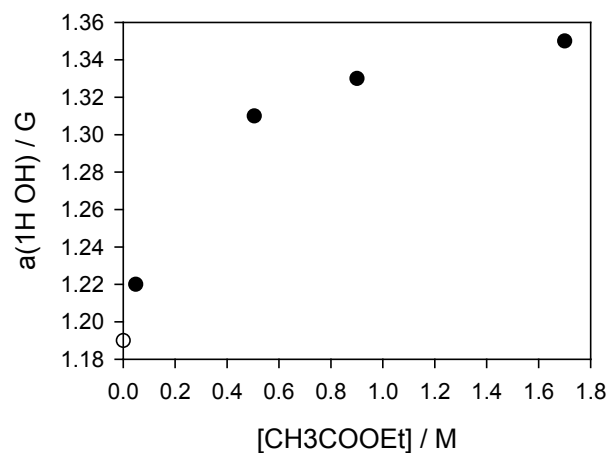
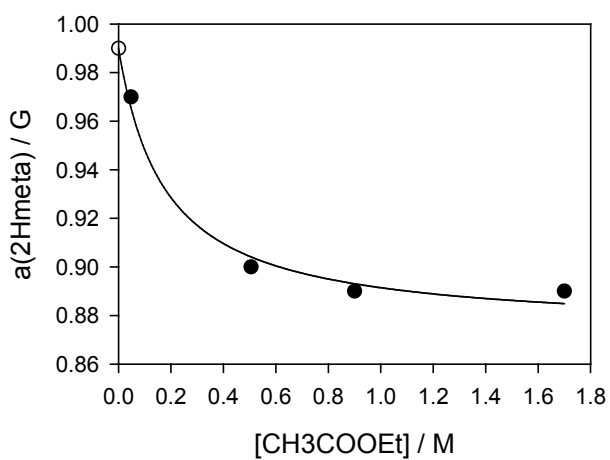
**HBA solvent: ethyl acetate (EtOAc)**

[EtOAc] / M	[EtAc] <sub>corr</sub> / M	<i>a</i> (2Hmeta) / G	<i>a</i> (1OH) / G
0	0	0.99	1.19
0.051	0.048	0.97	1.22
0.52	0.51	0.90	1.31
0.93	0.91	0.89 <sup>a</sup>	1.33
1.7	1.7	0.885 <sup>a</sup>	1.35

a) corrected for *a* variation due to dielectric effects

**Fitting results, solvent EtOAc:  $K_{HB} = 5.7 \pm 0.5 \text{ M}^{-1}$  (estimated error)**

constant	$K_{HB} / \text{M}^{-1}$	<i>a</i> / G
meta (2H)	5.6	0.87
para (1OH)	nd	≈1.32



$$\Delta G = -1.0 \text{ kcal/mol}$$

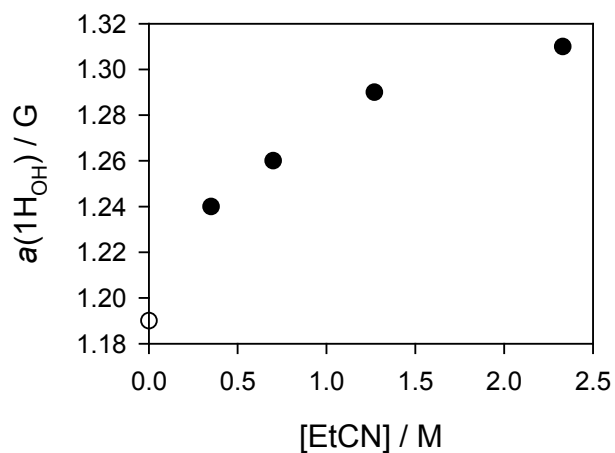
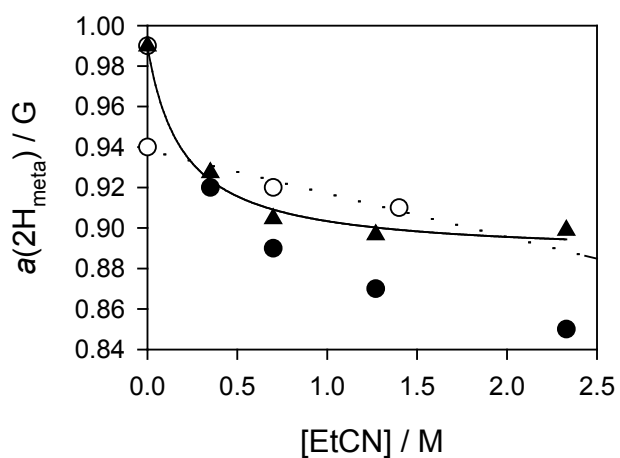
$$\alpha = 4.4; \alpha_2^H = 0.74$$

### HBA solvent: propionitrile (EtCN)

[EtCN] / M	[EtCN] <sub>corr</sub> / M	<i>a</i> (2H <sub>meta</sub> ) / G	<i>a</i> (1OH) / G
0	0	0.99	1.19
0.35	0.35	0.92	1.24
0.70	0.70	0.89	1.26
1.27	1.27	0.87	1.29
2.33	2.33	0.85	1.31

### Fitting results, solvent EtCN: $K_{HB} = 5.1 \pm 0.5 \text{ M}^{-1}$ (estimated error)

constant	$K_{HB} / \text{M}^{-1}$	<i>a</i> / G
meta (2H)	5.1	0.89
para (1OH)	nd	≈ 1.26



(●) Experimental points,

(○)  $H_{\text{meta}}$  of 2,6-tBu-4OMephenoxyl radical (dielectric effect)

▲ corrected values.

$$\Delta G = -0.96 \text{ kcal/mol}$$

$$\alpha = 4.35; \alpha_2^H = 0.73$$

### Data used for determining the $\alpha$ value of 3-OH and 4-OH phenoxy radicals

**Table S2.** Calculated (B3LYP/6-31+g(d,p), gas phase) enthalpy change for the formation of the H-bond between some phenol and three H-bond acceptors.

	$\Delta H_{\text{calc}} / \text{kcal/mol}$		
	Me <sub>2</sub> SO	Me <sub>3</sub> P=O	Me <sub>2</sub> NCHO
4-OMe phenol	-9.11	-9.60	-7.07
phenol	-9.41	-9.95	-7.38
4-F phenol	-9.94	-10.74	-8.04
4-CN phenol	-11.41	-12.79	-9.76
4-NO <sub>2</sub> phenol	-11.95	-13.53	-10.37
3-NO <sub>2</sub> Phenol	-10.93	-13.13	-9.93
3-F phenol	-10.21	-10.98	-8.27

### Treatment of solvent effects by PCM method

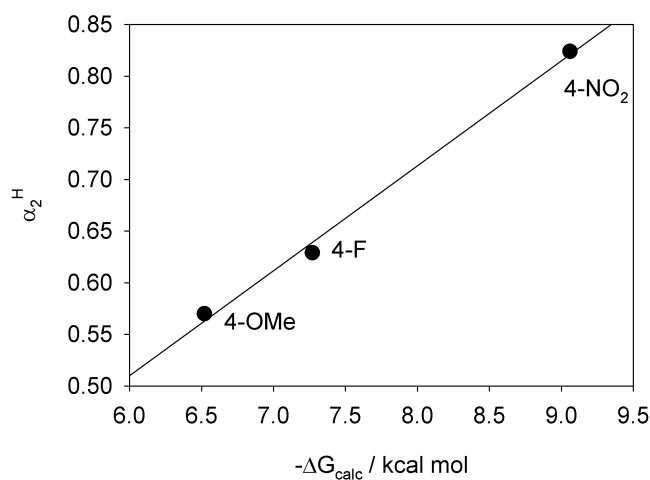
The energies of the interaction with DMSO for some reference phenols and for **4** were calculated using the PCM method and choosing benzene as solvent. The geometries were calculated in the gas phase. The H-bond strength has been calculated from the total free energies in solution.

**Table S3.** H-bond strength calculated at the B3LYP/6-31+g(d,p), solvent benzene.

	$-\Delta G_{\text{calc}} \text{ (PCM)} / \text{kcal mol}^{-1}$
4-OMe PhOH	6.52
4-F PhOH	7.27
4-NO <sub>2</sub> PhOH	9.06
4-OH PhO•	9.39

$$\alpha_2^{\text{H}} = -0.1016 \Delta G_{\text{calc}} \text{ (PCM)} - 0.0997$$

$$\alpha_2^{\text{H}} \text{ (4-OH PhO}\bullet\text{)} = 0.85$$



**Figure S2.** Relation between literature  $\alpha_2^{\text{H}}$  and  $\Delta G_{\text{calc}}$ .

## Cartesian coordinates and electronic energy for the investigated compounds.

### pOmePhOH---DMSO

```
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```

### pOmePhOH---DMF

```
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```

### pOmePhOH---Me3PO

```
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```

```
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,-0.0284591916,1.5034152085\C,2.5157949093,0.0050338068,0.1121652354\C
,1.3798682498,0.032186748,-0.7062238048\O,3.5326945913,-0.0540992626,2
.2544800078\O,-1.0770189394,0.0512385031,-0.8428771891\O,3.1584118615,
-0.0834579223,4.9446527688\P,4.3309063047,0.0218496696,5.9008310496\C,
5.4022353621,-1.4589762414,5.8899371025\C,5.432353375,1.433732331,5.53
49345237\C,3.7923048298,0.2373807498,7.6333121102\H,1.5107136983,0.057
4561744,-1.781885048\H,-1.0148503641,-0.012117279,1.6974276252\H,3.319
0961607,-0.0743808319,3.217067821\H,3.5079118411,0.0091720572,-0.32866
33054\H,1.0061514649,-0.0610110842,3.1556407845\H,4.6443109155,0.30871
06395,8.3163577713\H,3.1903573426,1.1472085644,7.7085786971\H,3.168372
3503,-0.6137298306,7.9199662055\H,6.2373457822,-1.3589461269,6.5900992
488\H,4.8045636961,-2.3337960411,6.1609657423\H,5.7923851631,-1.608178
3176,4.8791219977\H,6.2732808669,1.4828176325,6.2335966748\H,5.8128023
962,1.3317591513,4.5145415734\H,4.8560510274,2.361217584,5.5952653253\
C,-1.0036916419,0.083062501,-2.2577177183\H,-2.0357268632,0.0978516478
,-2.6125588249\H,-0.4852013048,0.9830308461,-2.6157680699\H,-0.4967775
668,-0.8063243335,-2.6564362873\Version=AM64L-G03RevD.02\State=1-A\HF
=-958.4153698\RMSD=5.262e-09\RMSF=5.300e-06\Thermal=0.\Dipole=1.691580
1,0.133922,2.0211245\PG=C01 [X(C10H17O3P1)]\@
```

#### pOmePhOH (most stable conformer)

```
1\1\GINC-RICKWORK\FOpt\RB3LYP\6-31+G(d,p)\C7H8O2\RICKY\09-Aug-2010\0\
#p B3LYP/6-31+g(d,p) opt(readFC) freq Geom=Check scale=0.9806\pOMefen
olo\0,1\C,0.1105803262,0.,-0.0560890559\C,0.0465376091,0.,1.343277662
9\C,1.2141828186,0.,2.1023810819\C,2.4647405648,0.,1.4720194063\C,2.53
19486524,0.,0.0799060231\C,1.3611742832,0.,-0.685872656\O,3.6512076182
,0.,2.1691056439\H,3.4748170697,0.,3.1184488179\H,3.5042159049,0.,-0.4
020825549\H,1.4438754381,0.,-1.7661899379\O,-1.0953155169,0.,-0.711052
5752\H,-0.9271501834,0.,1.8223094644\H,1.148659422,0.,3.1884114533\C,-
1.0905290311,0.,-2.1303896602\H,-2.1386422338,0.,-2.4329959951\H,-0.59
77164228,0.8955338491,-2.5312878153\H,-0.5977164228,-0.8955338491,-2.5
312878153\Version=AM64L-G03RevD.02\State=1-A\HF=-422.020128\RMSD=6.3
29e-09\RMSF=9.311e-05\Thermal=0.\Dipole=-0.2305717,0.,-0.0832586\PG=CS
[SG(C7H6O2),X(H2)]\@
```

#### PhOH

```
1\1\GINC-RICKWORK\FOpt\RB3LYP\6-31+G(d,p)\C6H6O1\RICKY\08-Apr-2009\0\
#p B3lyp/6-31+g(d,p) opt freq geom=check\fenolo\0,1\O,-0.0708272751,
0.,-0.0369615304\C,-0.0042525132,0.,1.3335184651\C,1.2106164061,0.,2.0
277109132\C,-1.2159150227,0.,2.0334123882\C,1.2090835467,0.,3.42567268
85\C,-1.2038822274,0.,3.4280922303\C,0.0051335135,0.,4.1334334272\H,0.
8200847883,0.,-0.4104385198\H,-2.146347912,0.,1.474992277\H,-2.1468676
501,0.,3.9673749519\H,0.0074014247,0.,5.2188656525\H,2.1558225119,0.,3
.9583392424\H,2.1512788848,0.,1.4807760517\Version=AM64L-G03RevD.02\S
tate=1-A\HF=-307.493995\RMSD=8.913e-09\RMSF=4.297e-05\Thermal=0.\Dipo
le=0.5472496,0.,0.0397686\PG=CS [SG(C6H6O1)]\@
```

#### PhOH---DMSO



1\1\GINC-RICKWORK\FOpt\RB3LYP\6-31+G(d,p)\C8H12O2S1\RICKY\28-Apr-2009\  
0\#p B3lyp/6-31+g(d,p) opt freq\fenolo dmso finale\0,1\C,0.02465136  
85,0.2567821254,0.2438962625\C,-0.0439594639,-0.1535422825,1.575578802  
6\C,1.1077537192,-0.5611429593,2.2578678267\C,2.334151481,-0.553490191  
8,1.5873844085\C,2.4174047455,-0.1449516848,0.2539650017\C,1.257862003  
,0.2620903324,-0.4228187939\H,1.0492776522,-0.8803640085,3.2938906866\  
O,1.2803280239,0.6703136852,-1.7226796266\O,3.5857742926,0.9067164529,  
-3.0978358396\S,3.3177598621,1.8433259753,-4.2851384621\C,1.8285226688  
,1.1920320172,-5.1285110701\C,2.5544599013,3.3543807489,-3.5872487777\  
H,2.1948309611,0.6372321109,-2.1005894387\H,-0.8638584235,0.572346831,  
-0.2943672401\H,-1.0050248828,-0.1552785728,2.082882658\H,3.2378189955  
,-0.8681756506,2.1024965557\H,3.3718791738,-0.1405516283,-0.2654304543  
\H,2.2387735119,4.0075227956,-4.4054059533\H,1.7117221886,3.0708791639  
, -2.9519613773\H,3.3243398906,3.8494411087,-2.9924617974\H,2.110028768  
2,0.2322752121,-5.5657861075\H,1.0291127656,1.0521839157,-4.3965335389  
\H,1.531224222,1.8874894893,-5.9182087586\Version=AM64L-G03RevD.02\St  
ate=1-A\HF=-860.7199065\RMSD=4.627e-09\RMSF=4.165e-05\Thermal=0.\Dipol  
e=-0.1847868,1.1991548,-1.5899172\PG=C01 [X(C8H12O2S1)]\@

### PhOH---Me3PO

1\1\GINC-RICKWORK\FOpt\RB3LYP\6-31+G(d,p)\C9H15O2P1\RICKY\14-Aug-2010\  
0\#p B3lyp/6-31+g(d,p) opt freq scale=0.9806\phenol-Me3PO\0,1\C,0.0  
831983339,0.0821950184,-0.151590364\C,-0.0236562185,0.0331919619,1.241  
4675099\C,1.1173508797,-0.0067462455,2.0466448343\C,2.3903128359,0.002  
2077419,1.4536159809\C,2.5032059492,0.0510945148,0.0558929988\C,1.3551  
425565,0.0905433676,-0.7355503696\O,3.53534763,-0.0349225944,2.1846340  
409\H,-0.807602021,0.1130474516,-0.7716825854\O,3.1883834115,-0.084032  
7528,4.8702914302\P,4.3283721113,0.013334605,5.8658699196\C,5.39376059  
9,-1.4714817329,5.8855917888\C,5.4461740293,1.4229620217,5.5445045247\  
C,3.7307231898,0.2240730447,7.5793831677\H,1.4556757229,0.1281323904,-  
1.8171799655\H,-1.0038893402,0.025573562,1.711279022\H,3.3396192057,-0  
.0626470905,3.1519284003\H,3.4939618516,0.0569647083,-0.3881272653\H,1  
.0337980194,-0.0453631674,3.1290212238\H,4.5586525048,0.2884158752,8.2  
920768611\H,3.1308312108,1.1365088691,7.6376679619\H,3.0931938452,-0.6  
251858386,7.8404690841\H,6.2025011,-1.3788543387,6.6170142743\H,4.7830  
378923,-2.3454217163,6.1289200621\H,5.8211057283,-1.6165790143,4.88932  
79337\H,6.2605892767,1.4674358318,6.2741803979\H,5.8645416282,1.323343  
0707,4.5388468646\H,4.8705350871,2.3518538881,5.5864574957\Version=AM  
64L-G03RevD.02\State=1-A\HF=-843.889796\RMSD=6.593e-09\RMSF=5.176e-06\  
Thermal=0.\Dipole=1.5183891,0.105041,2.5638062\PG=C01 [X(C9H15O2P1)]\@

### PhOH---DMF

#p B3lyp/6-31+g(d,p)  
C,0,0.0897646044,0.1452362855,-0.0690319545  
C,0,0.0796229751,0.3909489643,1.3089703975  
C,0,1.2758023175,0.29257601,2.0249653432  
C,0,2.4693380688,-0.0451149609,1.3814018112  
C,0,2.4718836116,-0.2883908988,-0.0011155431  
C,0,1.27383862,-0.1918660659,-0.7243924811  
H,0,-0.8448597384,0.6524026943,1.8147202667  
O,0,3.5997814774,-0.621111742,-0.6851896054

O,0,5.9496813328,-0.4784359483,0.7495490721  
C,0,6.7934825677,0.2105713968,0.1671391816  
N,0,8.0456907625,0.445375759,0.6153617225  
C,0,8.9785384634,1.277875194,-0.1295120025  
C,0,8.5067051119,-0.125980535,1.8752703945  
H,0,1.2851580559,0.4773819774,3.0960169255  
H,0,3.3968827966,-0.1241854696,1.9414938298  
H,0,1.2920540592,-0.3851966924,-1.7924601591  
H,0,-0.832377668,0.2160717946,-0.639822807  
H,0,4.3849127529,-0.6319891952,-0.0931173048  
H,0,6.5741120634,0.6994871409,-0.7959568506  
H,0,7.7027941019,-0.7258549635,2.3006981952  
H,0,9.3850072204,-0.7586494134,1.7036741933  
H,0,8.7788493436,0.6716561192,2.5761833239  
H,0,8.5066360858,1.6312547942,-1.0490754605  
H,0,9.2798554324,2.1478336355,0.4658465748  
H,0,9.8770684829,0.7082092391,-0.3939790147  
HF=-556,041862

### pF-PhOH---DMSO

1\1\GINC-RICKWORK\FOpt\RB3LYP\6-31+G(d,p)\C8H11F1O2S1\RICKY\29-May-200  
9\0\#p B3lyp/6-31+g(d,p) opt freq\dmso - parafluorofenolo\0,1\C,0.0  
299917682,0.0076215514,-0.0315499241\C,-0.0712302694,0.0158377041,1.36  
25729977\C,1.0869475434,0.0032069993,2.1543506393\C,2.3467750326,-0.01  
77470048,1.5395553199\C,2.4522715731,-0.0259700811,0.1477710692\C,1.28  
99047809,-0.0130334862,-0.6134409349\O,1.0386701711,0.0108989695,3.516  
1807926\F,1.3912807898,-0.0211402765,-1.9766399741\O,-1.3077425451,0.0  
484697837,4.8210698183\S,-1.0324834475,0.127612189,6.3303442279\C,0.06  
81705778,1.5697066714,6.5765784427\C,0.1971221083,-1.1782962599,6.6977  
285935\H,0.1047176471,0.0151711678,3.8476730762\H,3.2357865376,-0.0283  
362167,2.1618141592\H,3.4194019637,-0.0427332869,-0.3435507538\H,-0.85  
549678,0.0170251312,-0.6582925\H,-1.0481667477,0.0317522341,1.83706518  
62\H,0.3851952906,1.6047140949,7.6224706711\H,0.9242640916,1.491729254  
8,5.9017718938\H,-0.5195494079,2.4578495316,6.3370144576\H,-0.30492241  
79,-2.1351216519,6.5428322643\H,1.0429095286,-1.0820957836,6.012336542  
3\H,0.5136850587,-1.0888699075,7.740486796\Version=AM64L-G03RevD.02\S  
tate=1-A\HF=-959.959345\RMSD=7.077e-09\RMSF=2.560e-05\Thermal=0.\Dipol  
e=0.1335785,0.1373451,2.7694205\PG=C01 [X(C8H11F1O2S1)]\@

### pF-PhOH---DMF

1\1\GINC-RICKWORK\FOpt\RB3LYP\6-31+G(d,p)\C9H12F1N1O2\RICKY\13-Aug-201  
0\0\#p B3lyp/6-31+g(d,p) opt freq scale=0.9806\PFp dmf\0,1\C,-0.016  
8001445,0.0624473763,0.0400369668\C,-0.0227007136,-0.0786638868,1.4282  
284429\C,1.1909154494,-0.1748766099,2.0985237091\C,2.4053799856,-0.135  
4071887,1.4284307153\C,2.4070375012,0.0053804318,0.0373200541\C,1.1955  
901083,0.1062396709,-0.6642196769\O,1.138239384,0.243869572,-2.0168300  
353\O,3.5636957907,0.5403571575,-3.2767881157\C,3.532685267,1.34270875  
54,-4.2161138545\N,4.577258045,1.6368432803,-5.0188645712\C,5.87308381  
84,0.996611316,-4.8241053504\C,4.4567596487,2.599513419,-6.1042357326\  
F,1.187646527,-0.3123441182,3.4594853088\H,3.3330213241,-0.2154497187,  
1.985459474\H,3.3471719296,0.0360430996,-0.5052487921\H,-0.9469400141,

0.1395967576,-0.5134347779\H,-0.9523030155,-0.114375644,1.9864804327\H  
,2.0398119457,0.2869681271,-2.4083537303\H,2.6141208067,1.8944976794,-  
4.4735001819\H,5.7983271857,0.3054472663,-3.9852460542\H,6.1620642456,  
0.4466660698,-5.7269692104\H,6.6393872618,1.7505739033,-4.6106042044\H  
,3.4405878199,2.999064824,-6.1334834553\H,5.1561458565,3.4313090556,-5  
.9605470749\H,4.673974912,2.1233186909,-7.0674469425\\Version=AM64L-G0  
3RevD.02\State=1-A\HF=-655.281513\RMSD=5.433e-09\RMSF=7.904e-07\Therma  
l=0.\Dipole=1.6220487,1.2199707,-2.793722\PG=C01 [X(C9H12F1N1O2)]\@

### pF-PhOH---Me3PO

1\1\GINC-RICKWORK\FOpt\RB3LYP\6-31+G(d,p)\C9H14F1O2P1\RICKY\14-Aug-201  
0\0\#p B3lyp/6-31+g(d,p) opt freq scale=0.9806\PFp me3po\0,1\C,0.12167283  
36,0.0738183085,-0.1133156166\C,-0.0112840331,0.0248182711,1.267303379  
2\C,1.1407788343,-0.0088225292,2.0584987216\C,2.4106155081,0.007004165  
3,1.4591275557\C,2.5136530572,0.05665062,0.0607316204\C,1.3655165129,0  
.0902581934,-0.7323107601\O,3.5611299126,-0.0242624511,2.1825123906\F,  
-1.0058079127,0.1067660591,-0.8887038819\O,3.2012130075,-0.0788074298,  
4.8584865155\P,4.3329882082,0.0148390179,5.8648930616\C,5.3915425518,-  
1.4745879867,5.8932759931\C,5.459051467,1.4193289397,5.5504250973\C,3.  
7204804029,0.2296111879,7.5718560426\H,1.4298282804,0.1286280315,-1.81  
47243714\H,-0.9996833844,0.0129168039,1.7148489282\H,3.3710327678,-0.0  
539437759,3.1515700926\H,3.4998648157,0.0679621017,-0.3919678061\H,1.0  
607069603,-0.0478429844,3.1406602644\H,4.5426978627,0.2925731661,8.291  
1776984\H,3.1230310059,1.1440102534,7.6234035553\H,3.0783324589,-0.617  
4257648,7.8286541493\H,6.1960410983,-1.3844709079,6.629640805\H,4.7759  
551204,-2.3459150653,6.133648504\H,5.8247743953,-1.6222044301,4.899958  
8236\H,6.2694736777,1.4598276469,6.2847520795\H,5.8833031469,1.3177432  
954,4.5474121137\H,4.8879584632,2.351170695,5.5891402716\\Version=AM64  
L-G03RevD.02\State=1-A\HF=-943.1297148\RMSD=6.587e-09\RMSF=3.502e-06\T  
hermal=0.\Dipole=2.1014304,0.0822558,3.008446\PG=C01 [X(C9H14F1O2P1)]\

### pF-PhOH

1\1\GINC-RICKWORK\FOpt\RB3LYP\6-31+G(d,p)\C6H5F1O1\RICKY\09-Aug-2010\0  
\#p B3lyp/6-31+g(d,p) opt freq scale=0.9806\PFp\0,1\C,0.0031697056,  
-0.000007005,-0.0145940673\C,0.0052939943,-0.000054742,1.3840890213\C,  
1.2163223337,-0.000042373,2.0844273341\C,2.4301741635,0.000045082,1.38  
76865874\C,2.4341944018,0.0001213895,-0.0073697041\C,1.218995426,0.000  
089225,-0.6828326178\O,1.281121685,-0.0000476494,3.4552573346\F,1.2223  
984641,0.0001480656,-2.0461014468\H,0.3913137985,-0.0006631588,3.83091  
4885\H,3.3593080643,0.0000490715,1.9475510711\H,3.3628926814,0.0001910  
074,-0.567393616\H,-0.924394677,-0.0000247249,-0.5763356779\H,-0.93879  
54983,-0.0000923765,1.9238773181\\Version=AM64L-G03RevD.02\State=1-A\H  
F=-406.7325691\RMSD=5.111e-09\RMSF=1.460e-04\Thermal=0.\Dipole=-0.5486  
086,-0.0004118,0.6484583\PG=C01 [X(C6H5F1O1)]\@

### pCN-PhOH---Me3PO

1\1\GINC-RICKWORK\FOpt\RB3LYP\6-31+G(d,p)\C10H14N1O2P1\RICKY\14-Aug-20  
10\0\#p B3lyp/6-31+g(d,p) opt freq scale=0.9806\p CN phenol Me3PO\0  
,1\C,0.0275727102,0.0126907502,-0.0676076618\C,-0.0183164567,0.0195470  
36,1.3390121262\C,1.1542217864,0.0289599998,2.0855841802\C,2.402866276  
5,0.0316785399,1.4353941637\C,2.4532948655,0.0250003216,0.0298530634\C

,1.2804695079,0.0155994873,-0.7122732059\O,3.570405643,0.0404876868,2.1080035909\C,-1.1821753903,0.0028994798,-0.8322944713\O,3.2855483728,0.0540075482,4.7585022043\P,4.3603936741,0.0575733764,5.8314711062\C,5.3654775078,-1.4679718417,5.8389595384\C,5.5441608891,1.4373889792,5.6534044857\C,3.6530296968,0.2093196925,7.5067650909\H,1.3235124042,0.0104265831,-1.7966934152\H,-0.9800550223,0.0174300168,1.8421307559\H,3.4269705352,0.0447405249,3.0902079877\H,3.4226550675,0.0273281054,-0.4575505901\H,1.1188807696,0.0343501206,3.1705194161\H,4.4327220991,0.2079701756,8.2744234633\H,3.0836442367,1.1406865717,7.5702266711\H,2.969881906,-0.6261607991,7.6828675243\H,6.1277720607,-1.4459807257,6.6237632945\H,4.7083625165,-2.3278153003,5.9963517227\H,5.8520390275,-1.5793030683,4.8658241096\H,6.2997448895,1.4242331285,6.444847858\H,6.0380182736,1.362546291,4.6804079121\H,4.9975790246,2.3838828725,5.6904851743\N,-2.167823189,-0.005086582,-1.4543572523\\Version=AM64L-G03RevD.02\State=1-A\HF=-936.140344\RMSD=8.526e-09\RMSF=7.412e-06\Thermal=0.\Dipole=3.3857894,0.02774,3.9958016\PG=C01 [X(C10H14N1O2P1)]\@

### pCN-PhOH---DMF

1\1\GINC-RICKWORK\FOpt\RB3LYP\6-31+G(d,p)\C10H12N2O2\RICKY\13-Aug-2010  
0\0\#p B3lyp/6-31+g(d,p) opt freq scale=0.9806\p CN phenol dmf\0,1\C,0.0032405915,0.0067949561,0.0006847781\C,-0.0053420935,0.0031073966,1.3886052893\C,1.204893011,-0.0033274567,2.1100818072\C,2.4223141079,-0.0072730065,1.4050081137\C,2.4343407173,-0.0044327392,0.0147041563\C,1.2222650152,0.0040341718,-0.6995921504\C,1.1969344876,-0.0066528145,3.5414762671\O,1.1719671779,0.0083067981,-2.0480632489\O,3.6073236812,0.0708386308,-3.2529893455\C,3.6983240996,0.502925523,-4.4087180701\N,4.8349180317,0.5401326151,-5.1321017745\C,6.0919592998,0.0485562651,-4.5777420822\C,4.8580777017,1.0688690444,-6.4890306685\H,3.3582832255,-0.0137579627,1.9543949319\H,3.3753474295,-0.0088285449,-0.526422318\H,-0.9230414489,0.0116602366,-0.5641113142\H,-0.9480876926,0.0051464025,1.9260968665\H,2.0760527354,0.0136678964,-2.4458784766\H,2.8230141096,0.9014202906,-4.9459659465\H,5.908763146,-0.3213794454,-3.5696812105\H,6.4856420422,-0.7629049135,-5.1999434235\H,6.8310844845,0.856792417,-4.5430756767\H,3.8572598497,1.3996217836,-6.7750921221\H,5.5421949669,1.9224247908,-6.5571722993\H,5.1883694559,0.2988070601,-7.1955163341\N,1.1915842265,-0.0090660752,4.7068623355\\Version=AM64L-G03RevD.02\State=1-A\HF=-648.2916585\RMSD=9.055e-09\RMSF=1.459e-06\Thermal=0.\Dipole=1.921681,0.5250425,-4.537698\PG=C01 [X(C10H12N2O2)]\@

### pCN-PhOH---DMSO

1\1\GINC-RICKWORK\FOpt\RB3LYP\6-31+G(d,p)\C9H11N1O2S1\RICKY\13-Aug-2010\0\0\#p B3lyp/6-31+g(d,p) opt freq scale=0.9806\p CN phenol dmsol\0,1\C,0.0027679606,0.0114366899,-0.0037079923\C,-0.0201889379,-0.0042539348,1.3863031348\C,1.1864163465,-0.0185022001,2.1090276526\C,2.4110264113,-0.0173378697,1.4197804869\C,2.4305814046,-0.0017139974,0.031599047\C,1.2261796953,0.0131815024,-0.6987454715\O,1.2185307582,-0.0332223451,3.4594736223\C,1.24704054,0.0299481604,-2.1301031183\O,-1.1194577987,-0.0009392,4.7312904142\S,-1.0493379539,0.1324959266,6.2605295233\C,0.0286542423,1.5711424708,6.6011764467\C,0.0945556516,-1.1740961438,6.8363443954\H,0.3026572742,-0.0316524486,3.8480739535\H,3.333498685,-0.029301991,1.9908434709\H,3.377442423,-0.001000542,-0.498592243\H,-0.92886381

97,0.0223105505,-0.5602120402\H,-0.9654643024,-0.0058315167,1.92074903  
86\H,0.1949779227,1.6470833555,7.6791891473\H,0.9718019023,1.458480914  
2,6.0606298893\H,-0.504452839,2.4545988183,6.2451137727\H,-0.394051237  
4,-2.1296363023,6.6372358019\H,1.0335953185,-1.1097259577,6.2809396833  
\H,0.2598695893,-1.058097571,7.9109510061\N,1.2650175286,0.0440389964,  
-3.2951677963\\Version=AM64L-G03RevD.02\State=1-A\HF=-952.9690123\RMSD  
=4.209e-09\RMSF=7.707e-06\Thermal=0.\Dipole=-0.1373232,0.1621328,4.551  
4043\PG=C01 [X(C9H11N1O2S1)]\@

### pCN-PhOH

1\1\GINC-RICKWORK\FOpt\RB3LYP\6-31+G(d,p)\C7H5N1O1\RICKY\13-Aug-2010\0  
\#p B3lyp/6-31+g(d,p) opt freq scale=0.9806\p CN phenol\0,1\C,0.004  
5455941,-0.0000322392,-0.0012931594\C,0.0024590385,-0.0000876288,1.390  
4445875\C,1.2163462789,-0.0000642601,2.0904565393\C,2.4329472636,0.000  
0310317,1.3947498341\C,2.4332609075,0.00010093,0.0060201499\C,1.219226  
1129,0.0000678747,-0.7080417118\O,1.2803888383,-0.0000913304,3.4523217  
399\C,1.2212909877,0.0001310166,-2.140744299\H,0.3921177047,-0.0004829  
4,3.8336670661\H,3.3608374798,0.0000438319,1.9562482783\H,3.3729317743  
,0.0001731099,-0.5361180645\H,-0.9340786582,-0.0000545573,-0.545195989  
9\H,-0.9406280856,-0.0001429617,1.9314429222\N,1.2225770591,0.00018182  
89,-3.3053342573\\Version=AM64L-G03RevD.02\State=1-A\HF=-399.7399779\R  
MSD=4.958e-09\RMSF=3.210e-05\Thermal=0.\Dipole=-0.5570042,-0.0003296,1  
.9832493\PG=C01 [X(C7H5N1O1)]\@

### pNO<sub>2</sub>-PhOH---DMF

1\1\GINC-RICKWORK\FOpt\RB3LYP\6-31+G(d,p)\C9H12N2O4\RICKY\15-Jun-2009\  
0\#p B3lyp/6-31+g(d,p) opt freq\pNO2phenol-DMF\0,1\C,-0.0035634374,  
-0.0191938974,0.0298927046\C,0.0742825969,0.0259068776,1.4270933717\C,  
1.3091210925,0.0344559972,2.0827309098\C,2.4797214261,-0.0018794058,1.  
3359578807\C,2.4176936133,-0.0451862287,-0.071295664\C,1.1655128926,-0  
.054648281,-0.715193693\N,-1.1527045219,0.0643622962,2.2121241353\O,3.  
5184982743,-0.0799059694,-0.8443568093\O,5.8374476162,0.0063425542,0.5  
435709972\C,6.8710589139,0.4162537702,-0.0003999668\N,8.0838817881,0.4  
625043008,0.5836818536\C,9.2532955778,0.9639999364,-0.125629611\C,8.27  
18889006,0.009647084,1.958289754\H,1.3367655607,0.0682409385,3.1650073  
681\H,3.446253747,0.0026686869,1.82946739\H,1.1365698019,-0.0898933501  
,-1.7989193597\H,-0.9748698274,-0.0255731366,-0.4492040415\H,4.3473053  
735,-0.0621602708,-0.3040405461\H,6.8688201646,0.7845453389,-1.0384732  
558\H,7.3162942464,-0.3419858904,2.3451974013\H,9.0021667354,-0.806574  
0196,1.9883236105\H,8.6383293515,0.834046048,2.5801226966\H,8.97212163  
67,1.2678643766,-1.1362721873\H,9.6761888213,1.8299324007,0.3962187682  
\H,10.0228859092,0.1867740936,-0.1941879679\O,-2.2314038204,0.05297295  
88,1.6078329616\O,-1.055523771,0.1067169403,3.4443973225\\Version=AM64  
L-G03RevD.02\State=1-A\HF=-760.5582293\RMSD=7.445e-09\RMSF=4.887e-06\T  
hermal=0.\Dipole=5.0735401,0.4539078,-0.9301331\PG=C01 [X(C9H12N2O4)]\

### pNO<sub>2</sub>-PhOH---DMSO

1\1\GINC-RICKWORK\FOpt\RB3LYP\6-31+G(d,p)\C8H11N1O4S1\RICKY\20-May-200  
9\0\#p B3lyp/6-31+g(d,p) opt freq\pnitro fenolo+ dmsol\0,1\C,0.04883  
85764,0.0459385238,0.0859753198\C,0.1738962248,0.1688118531,1.48392372  
72\C,1.4508275141,0.1606325849,2.0759128995\C,2.5849714253,0.032500824



8,1.2874351661\C,2.4450729965,-0.0882430718,-0.0999851594\C,1.18407697  
71,-0.0824107254,-0.7040907901\O,-0.8957099225,0.2961336413,2.29268029  
04\N,3.6358807202,-0.2224068466,-0.9303183271\O,-3.2690596367,0.329161  
2193,1.1045835256\S,-4.5130893312,0.5811894425,1.9710691484\C,-4.43089  
98585,-0.6225738374,3.3459671764\C,-4.162765288,2.0911194458,2.9426989  
501\H,-1.7491709307,0.292528159,1.7788761445\H,1.5285369892,0.25565520  
07,3.1537215662\H,3.5753877698,0.0242197233,1.7256828636\H,1.108471452  
,-0.1781389092,-1.7803551883\H,-0.9381758047,0.052232996,-0.3661924384  
\H,-4.9763689308,2.2566163839,3.6541275703\H,-3.2035769318,1.982379063  
5,3.4549448721\H,-4.1169896731,2.9186525922,2.2324081601\H,-4.56398842  
87,-1.6125099368,2.905828469\H,-3.4548318634,-0.5561334433,3.832988496  
\H,-5.2409553072,-0.4174918736,4.051126874\O,3.4848766821,-0.326886490  
9,-2.1529437202\O,4.7383750174,-0.2249123492,-0.3706907168\\Version=AM  
64L-G03RevD.02\State=1-A\HF=-1065.2354292\RMSD=6.734e-09\RMSF=3.041e-0  
6\Thermal=0.\Dipole=-4.0668933,0.5954577,2.5796621\PG=C01 [X(C8H11N1O4  
S1)]\@

### pNO<sub>2</sub>-PhOH---Me<sub>3</sub>PO

1\1\GINC-RICKWORK\FOpt\RB3LYP\6-31+G(d,p)\C9H14N1O4P1\RICKY\14-Aug-201  
0\0\#p B3lyp/6-31+g(d,p) opt freq scale=0.9806\pnitro fenolo Me3PO\\  
0,1\C,0.0351087161,-0.0169835213,-0.0244075244\C,-0.0112158868,0.03306  
83761,1.3727125779\C,1.1735017938,0.0738216251,2.0958772558\C,2.412288  
8239,0.0643525945,1.4219280601\C,2.4402394143,0.0143278943,0.014235369  
3\C,1.2572597608,-0.0262148497,-0.7079272351\O,3.587645547,0.101592894  
4,2.0714273302\N,-1.2085468525,-0.0602561489,-0.7802614274\O,-1.140044  
7509,-0.103361371,-2.0146069499\O,-2.2744524355,-0.0520598965,-0.15217  
86985\O,3.3324535107,0.1719108538,4.7108448848\P,4.3723409419,0.092287  
6717,5.8154606029\C,5.3287065489,-1.4635999327,5.7834901693\C,5.602565  
1028,1.439793624,5.7357413137\C,3.6137427225,0.1919696952,7.4716210076  
\H,1.2612583236,-0.0649033936,-1.7903378713\H,-0.9720706691,0.03953725  
39,1.8727129746\H,3.4639883044,0.132353035,3.0576904129\H,3.4016100075  
,0.008482058,-0.4882272102\H,1.1585138848,0.1136464137,3.1802919584\H,  
4.3660412316,0.1297183066,8.2637148501\H,3.072853864,1.1382442196,7.55  
92805834\H,2.8983168049,-0.6270128963,7.5862292246\H,6.0666657343,-1.5  
001684677,6.59064339\H,4.6413229428,-2.3082983519,5.8828478765\H,5.841  
8019207,-1.5478124448,4.821288328\H,6.3356003783,1.3645684875,6.544729  
95\H,6.1207261801,1.3945965203,4.7736214988\H,5.0853164705,2.400890811  
3,5.8039552646\\Version=AM64L-G03RevD.02\State=1-A\HF=-1048.407098\RMS  
D=2.715e-09\RMSF=3.246e-06\Thermal=0.\Dipole=3.5755643,-0.0019885,4.16  
17656\PG=C01 [X(C9H14N1O4P1)]\@

### pNO<sub>2</sub>-PhOH

1\1\GINC-RICKWORK\FOpt\RB3LYP\6-31+G(d,p)\C6H5N1O3\RICKY\20-May-2009\0  
\#p B3lyp/6-31+g(d,p) opt freq\p nitro fenolo\0,1\C,-0.0224228364,-  
0.0009597056,-0.0101318992\C,0.0035836863,-0.0011728676,1.3927248734\C  
,1.2265082503,-0.0006741144,2.0805261919\C,2.4182081514,-0.0000004512,  
1.3686814316\C,2.3799314226,0.0001552591,-0.0293327877\C,1.1702998546,  
-0.0003288612,-0.7256080747\O,-1.1286745816,-0.0017309869,2.1464695097  
\N,3.6357234677,0.0008300806,-0.7807197238\H,-1.9136858722,-0.00298580  
23,1.5818906531\H,1.2210857183,-0.0008503353,3.1649207988\H,3.37496848  
77,0.000379407,1.876152362\H,1.1757515021,-0.0001706719,-1.8085408397\

H,-0.9720241382,-0.0012638289,-0.5392420512\O,3.5713820717,0.001158001  
6,-2.0134320013\O,4.69056847,0.0016029094,-0.1405269084\\Version=AM64L  
-G03RevD.02\State=1-A\HF=-512.0055777\RMSD=6.462e-09\RMSF=5.673e-05\Th  
ermal=0.\Dipole=-2.1130678,-0.0019481,0.6186646\PG=C01 [X(C6H5N1O3)]\\

### **mNO<sub>2</sub>-PhOH (more stable conformation)**

1\1\GINC-RICKWORK\FOpt\RB3LYP\6-31+G(d,p)\C6H5N1O3\RICKY\03-Sep-2010\0  
\\#p B3lyp/6-31+g(d,p) opt freq scale=0.9806\\3NO2 phenol t\\0,1\C,0.0  
007656914,0,-0.0130401029\C,0.0279914769,0.,1.379012939\C,1.214908656  
7,0.,2.112671773\C,2.4236674033,0.,1.4146386224\C,2.429726688,0.,0.012  
5283437\C,1.2245327698,0.,-0.6875686869\O,3.6359388858,0.,2.0429033914  
\H,3.5208283818,0.,3.0026611043\H,3.3824713331,0.,-0.5062329815\H,1.23  
7167087,0.,-1.7727498431\H,-0.9456825717,0.,-0.5374795725\N,-1.2474663  
845,0.,2.1201399252\H,1.1754205051,0.,3.1962834272\O,-2.2916460164,0.,  
1.4674044056\O,-1.1958506279,0.,3.3520666738\\Version=AM64L-G03RevD.02  
\State=1-A\HF=-512.0032442\RMSD=8.099e-09\RMSF=8.280e-05\Thermal=0.\D  
ipole=1.4152295,0.,-0.50916\PG=CS [SG(C6H5N1O3)]\\@

### **mNO<sub>2</sub>-PhOH---DMF**

1\1\GINC-RICKWORK\FOpt\RB3LYP\6-31+G(d,p)\C9H12N2O4\RICKY\03-Sep-2010\  
0\\#p B3lyp/6-31+g(d,p) opt freq scale=0.9806\\3NO2 phenol t dmf\\0,1\  
C,-0.1503928245,0.0997591225,0.1801775253\C,0.0912486426,-0.0815724017  
,1.5528024998\C,1.3937320631,-0.242146627,2.0236903869\C,2.4828246442,  
-0.2264510273,1.1492998069\C,2.2163758856,-0.0455077185,-0.2073294273\  
C,0.9280124173,0.1172659968,-0.7150045021\H,3.5010520356,-0.3485175599  
,1.4938815163\O,-1.4326861951,0.2510360483,-0.2217521418\O,-1.46027156  
4,0.5823018834,-2.9289244229\C,-2.2945711979,1.0341736092,-3.721298932  
7\N,-2.0923611781,1.1973247542,-5.0437963661\C,-3.1284578576,1.7394307  
604,-5.9115904146\C,-0.8171678059,0.8390276835,-5.6581627879\N,3.34478  
97268,-0.0234303321,-1.15564146\H,0.771112431,0.2533284054,-1.77724540  
15\H,-0.7559223605,-0.0934680733,2.2308701743\H,1.5642402529,-0.381337  
4686,3.0868127173\H,-1.4868093621,0.371530312,-1.1983528186\H,-3.29793  
64806,1.3455563095,-3.3891620648\H,-0.152172537,0.4482459762,-4.889201  
9117\H,-0.9733928725,0.0766108104,-6.4293394487\H,-0.3610767681,1.7213  
742858,-6.1205978654\H,-4.023730192,1.9620173936,-5.3266433686\H,-2.78  
38265942,2.6630761414,-6.390541775\H,-3.3910374357,1.0175318156,-6.693  
3593099\O,3.093445191,0.1376081679,-2.3530487593\O,4.4831501748,-0.166  
6032077,-0.703814758\\Version=AM64L-G03RevD.02\State=1-A\HF=-760.55519  
83\RMSD=6.849e-09\RMSF=1.862e-06\Thermal=0.\Dipole=-2.5650084,0.742488  
1,-1.6663997\PG=C01 [X(C9H12N2O4)]\\@

### **mNO<sub>2</sub>-PhOH---Me3PO**

1\1\GINC-RICKWORK\FOpt\RB3LYP\6-31+G(d,p)\C9H14N1O4P1\RICKY\04-Sep-201  
0\0\\#p B3lyp/6-31+g(d,p) opt freq scale=0.9806\\3NO2 phenol t Me3PO\\  
0,1\C,0.0702504044,-0.1307934773,0.2332859111\C,0.448713577,0.68454709  
11,1.3029338224\C,1.8033072627,0.7189045614,1.6338273604\C,2.769089370  
4,-0.0209116666,0.9552496013\C,2.3721218837,-0.8266969049,-0.121072767  
2\C,1.0117529532,-0.8776193536,-0.4749475209\H,-0.2667946221,1.2748575  
919,1.8597974854\O,3.2497414313,-1.5588320686,-0.8359724009\O,5.706814  
2164,-1.1031744302,0.1592189046\O,6.931878086,-0.2188147316,0.29742955  
25\C,7.9076005636,-0.6277669855,1.7851284361\C,8.0783756762,-0.3731958

587,-1.1173405885\C,6.5324685412,1.5582264165,0.4330488405\H,-0.975626  
3317,-0.1818159495,-0.0536246493\N,2.2468246004,1.5793112079,2.7429744  
756\H,4.172899544,-1.4201739805,-0.5076645054\H,0.71541617,-1.50833138  
04,-1.3068703188\H,3.8063455072,0.015293066,1.2555521289\H,8.799819614  
1,0.0003782727,1.8662631781\H,7.2824630676,-0.4828700899,2.6705938156\  
H,8.2062040442,-1.678711116,1.738980041\H,8.9620185187,0.2596086296,-0  
.9902001079\H,8.3907713471,-1.4170443092,-1.2107348363\H,7.5564949104,  
-0.0850282437,-2.0341356589\H,7.4386973366,2.1599592885,0.5533560804\H  
,6.0054604921,1.880570255,-0.4696497837\H,5.8753149325,1.718363856,1.2  
930967582\O,3.4615487444,1.6749222461,2.9556667971\O,1.3879022455,2.16  
73897276,3.4021052195\\Version=AM64L-G03RevD.02\State=1-A\HF=-1048.404  
23\RMSD=8.038e-09\RMSF=1.955e-05\Thermal=0.\Dipole=2.2821368,0.074461,  
-1.0696837\PG=C01 [X(C9H14N1O4P1)]\@

### **mNO<sub>2</sub>-PhOH---DMSO**

1\1\GINC-RICKWORK\Freq\RB3LYP\6-31+G(d,p)\C8H11N1O4S1\RICKY\08-Sep-201  
0\0\#p B3lyp/6-31+g(d,p) freq scale=0.9806 geom=check\3NO2 phenol t  
dmsol\0,1\C,3.259403289,-1.517011088,0.3518522981\C,3.1983254376,-0.12  
20013727,0.2929374537\C,1.9709328096,0.4522993883,-0.0351675607\C,0.83  
10754292,-0.3001965056,-0.3108144798\C,0.9084613288,-1.696837493,-0.23  
28968373\C,2.1345247458,-2.3012014089,0.0971093584\N,1.8559919187,1.91  
90698333,-0.0819612164\O,0.7291312643,2.4084439268,-0.2298429381\O,-0.  
1577374027,-2.4926478194,-0.4626456936\O,2.8832164539,2.5871726972,0.0  
378480715\O,-2.3197544046,-0.8790258678,-0.8753971942\S,-3.3505789486,  
-0.0986051846,-0.0491587538\C,-3.0156446092,1.6699027593,-0.3742967545  
\C,-2.7762662046,-0.1396602331,1.6892294156\H,4.0584901672,0.502098912  
,0.4962367406\H,-0.9666555941,-1.9533231131,-0.6295243503\H,2.18288105  
49,-3.3840761913,0.1477728662\H,4.1986413314,-1.9987581621,0.605397199  
4\H,-0.0942562956,0.1797316985,-0.5961837605\H,-3.6684879721,2.2771608  
296,0.2589576899\H,-1.9623439419,1.8938054116,-0.1864621979\H,-3.25387  
36388,1.844234932,-1.4251839501\H,-2.8377906865,-1.1781826042,2.019889  
5514\H,-1.7444597511,0.2148106997,1.7454084125\H,-3.4385455697,0.48338  
39358,2.2965450476\\Version=AM64L-G03RevD.02\State=1-A\HF=-1065.231911  
1\RMSD=7.561e-09\RMSF=2.212e-05\ZeroPoint=0.1844889\Thermal=0.1991425\  
Dipole=-1.386028,-0.1430814,1.1781409

### **mF-PhOH (more stable conformer)**

1\1\GINC-RICKWORK\FOpt\RB3LYP\6-31+G(d,p)\C6H5F1O1\RICKY\09-Sep-2010\0  
\#p B3lyp/6-31+g(d,p) opt freq scale=0.9806\3F phenol a\0,1\C,0.021  
6198696,0.,0.0133493828\C,0.0188166175,0.,1.404552384\C,1.2563242496,0  
,.20516603571\C,2.4502954473,0.,1.3258356041\C,2.4072287261,0.,-0.073  
9571336\C,1.1809262523,0.,-0.7479265719\O,3.5357060283,0.,-0.848109977  
5\F,-1.1710985798,0.,-0.639011412\H,4.3223559975,0.,-0.287071391\H,1.1  
410713927,0.,-1.8306887178\H,-0.9185261412,0.,1.9483070701\H,1.2928114  
951,0.,3.1367156701\H,3.4065416558,0.,1.8429429048\\Version=AM64L-G03R  
evD.02\State=1-A\HF=-406.734599\RMSD=9.794e-09\RMSF=4.325e-05\Thermal  
=0.\Dipole=0.8730061,0.,0.8026781\PG=CS [SG(C6H5F1O1)]\@

### **mF-PhOH---DMF**

1\1\GINC-RICKWORK\FOpt\RB3LYP\6-31+G(d,p)\C9H12F1N1O2\RICKY\09-Sep-201  
0\0\#p B3lyp/6-31+g(d,p) opt freq scale=0.9806\3F phenol a dmf\0,1\



C,0.0098778848,0.0382253216,0.0098717495\C,0.001870225,0.0062061139,1.4126261554\C,1.2178355914,-0.0399780004,2.0765471344\C,2.4469864701,-0.0559876099,1.4262856691\C,2.4314763003,-0.0242136735,0.0285958621\C,1.2318975337,0.0219706279,-0.6842931697\H,3.3679977803,-0.093044111,1.9962908324\O,-1.1904048506,0.0823529308,-0.619390635\O,-1.0964139504,0.30651544,-3.3487663753\C,-2.0157341547,0.9684383427,-3.8428913024\N,-2.2037606654,1.1657566373,-5.1646954608\C,-3.3147120305,1.961674229,-5.6661933375\C,-1.2952532373,0.5806810702,-6.1442347568\H,3.372065059,-0.0372061056,-0.5146222302\H,1.2325510613,0.0440792586,-1.769581076\H,-0.9334610245,0.0165573761,1.9599471158\F,1.2025642322,-0.070892843,3.4402921138\H,-1.0800630756,0.1183568929,-1.5975341804\H,-2.7744568908,1.461691964,-3.2140848291\H,-0.5328256003,0.0096432829,-5.6155353561\H,-1.8463317481,-0.0823174949,-6.8208420288\H,-0.8175651749,1.3698800962,-6.7360392037\H,-3.9071230707,2.3391660119,-4.8297868653\H,-2.9456946647,2.8148377926,-6.2471874936\H,-3.9633133689,1.355759223,-6.3095871917\\Version=AM64L-G03RevD.02\State=1-A\HF=-655.2838749\RMSD=6.634e-09\RMSF=2.231e-06\Thermal=0.\Dipole=-1.1529031,0.9293295,-3.2541131\PG=C01 [X(C9H12F1N1O2)]\@

### mF-PhOH---DMSO

1\1\GINC-RICKWORK\FOpt\RB3LYP\6-31+G(d,p)\C8H11F1O2S1\RICKY\09-Sep-2010\0\#p B3lyp/6-31+g(d,p) opt freq scale=0.9806\3F phenol a dmso\0,1\C,-0.0324848906,-0.0370202801,-0.0234513818\C,0.0021295569,-0.0580172661,1.374248077\C,1.2108586869,-0.0204240273,2.0717511616\C,2.4210025777,0.0397991827,1.3609694175\C,2.4108974899,0.0618584672,-0.0412272224\C,1.1860593518,0.0228317219,-0.6901506751\O,3.6282386268,0.0785668474,1.9813384477\H,-0.9612144927,-0.0655523387,-0.581299632\O,3.848016306,0.0438698258,4.6468835195\S,5.33802155,0.0956797127,5.0186913355\C,6.1531827306,-1.2344330025,4.0604454228\C,6.0462441386,1.5157620439,4.105620596\H,3.5365008933,0.0591000668,2.9694091857\H,3.3372171099,0.1082431171,-0.6019375811\F,1.1832836827,0.0445729659,-2.0536820476\H,-0.9301769806,-0.1045302264,1.929475681\H,1.2257542517,-0.0372162942,3.1573211316\H,7.13012831,1.5298166324,4.2492689414\H,5.7841764847,1.4329464149,3.0479119721\H,5.6035206872,2.4172001608,4.5333720721\H,5.7823746191,-2.1810619944,4.4578887074\H,5.8840652274,-1.1376147309,3.0057001715\H,7.2350740914,-1.1689587887,4.2048810187\\Version=AM64L-G03RevD.02\State=1-A\HF=-959.961743\RMSD=3.685e-09\RMSF=1.658e-06\Thermal=0.\Dipole=2.006346,0.0555156,1.4079155\PG=C01 [X(C8H11F1O2S1)]\@

### mF-PhOH---Me3PO

1\1\GINC-RICKWORK\FOpt\RB3LYP\6-31+G(d,p)\C9H14F1O2P1\RICKY\09-Sep-2010\0\#p B3lyp/6-31+g(d,p) opt freq scale=0.9806\3F phenol a me3po\0,1\C,0.0133442458,-0.0050665756,0.0576844337\C,-0.0259591674,0.0034962162,1.4474688956\C,1.1996507206,0.0082171398,2.1213939781\C,2.4113873847,0.0047772917,1.4285118229\C,2.4090711107,-0.0038649302,0.0223123439\C,1.1904973243,-0.0087326535,-0.6744184081\H,-0.9760079721,0.0060239617,1.9690506516\O,3.5487793702,-0.0079224141,-0.7095696455\O,5.8010904001,0.0396589523,0.7648021747\P,7.2242447382,0.1756439109,0.2567989358\C,8.4148628946,0.442404871,1.6158954818\C,7.8095033119,-1.3035808901,-0.6421275488\C,7.4469160784,1.5782209205,-0.8928879598\F,-1.1676499746,-0.0099257193,-0.627228484\H,1.2091140315,0.0144760671,3.2077181499\H,

4.3478884594,-0.0002766025,-0.1269325472\H,1.173846657,-0.0157371965,-  
1.7580761643\H,3.3578828472,0.0077551116,1.9596451891\H,9.4398017305,0.  
.5348943349,1.2438655642\H,8.1415541912,1.3537645493,2.154886793\H,8.3  
563273394,-0.4001315074,2.3105354027\H,8.8402405664,-1.1830474798,-0.9  
894247888\H,7.7493908223,-2.1712013629,0.0208492813\H,7.1564329485,-1.  
4806246976,-1.5013916926\H,8.481128956,1.6525700342,-1.2428854292\H,6.  
7824679075,1.4451573729,-1.7514296034\H,7.1690508962,2.5052535015,-0.3  
836414616\Version=AM64L-G03RevD.02\State=1-A\HF=-943.1320536\RMSD=6.6  
21e-09\RMSF=5.990e-06\Thermal=0.\Dipole=3.7229557,0.2077803,0.1862229\  
PG=C01 [X(C9H14F1O2P1)]\@

## 2,6-di-methyl-4-hydroxyphenoxy radical

1\1\GINC-RICKWORK\FOpt\UB3LYP\6-31+G(d,p)\C8H9O2(2)\RICKY\17-Jun-2009\  
0\#p uB3lyp/6-31+g(d,p) opt freq\2,6 dimetil semichinone1\0,2\C,0.0  
248157895,0.0003631626,0.0147560366\C,0.0206329583,0.0088075544,1.4800  
200697\C,1.2201248511,0.0078205474,2.1636396124\C,2.4451919264,-0.0012  
060996,1.4643346523\C,2.4842595178,-0.0094331981,0.0538157298\C,1.3166  
876809,-0.0088649564,-0.6783026982\C,-1.3056545547,0.0181248003,2.1806  
764165\O,3.6420672493,-0.0024162041,2.1087813617\C,1.3079154962,-0.017  
5541346,-2.17854908\O,-1.0545204051,0.0010320648,-0.6299714326\H,1.227  
6855763,0.014055847,3.2529003344\H,3.4552837825,-0.0161547699,-0.43271  
35132\H,3.5096668456,0.0036926666,3.0670271761\H,-1.8940197778,0.89249  
15206,1.8818153446\H,-1.8995138641,-0.8568608255,1.8946580597\H,-1.183  
3627938,0.0256192475,3.2672243603\H,0.769504035,-0.8935601765,-2.55659  
10943\H,0.7730093479,0.8561078858,-2.5667558088\H,2.3239338249,-0.0220  
649323,-2.5817041827\Version=AM64L-G03RevD.02\State=2-A\HF=-460.72993  
97\S2=0.77351\S2-1=0.\S2A=0.750384\RMSD=4.641e-09\RMSF=2.794e-06\Therm  
al=0.\Dipole=0.9447902,0.0029334,1.2128864\PG=C01 [X(C8H9O2)]\@

## 2,6-di-methyl-4-hydroxyphenoxy radical---DMF

1\1\GINC-RICKWORK\FOpt\UB3LYP\6-31+G(d,p)\C11H16N1O3(2)\RICKY\24-Jun-2  
009\0\#p uB3lyp/6-31+g(d,p) opt freq\QH dmf\0,2\C,0.0005774761,0.00  
24890272,-0.0355306821\C,-0.0091530926,-0.0087882971,1.4293118988\C,1.  
2774404892,-0.0066509621,2.1283093404\C,2.4526006383,0.0059131633,1.40  
57673017\C,2.4303751367,0.0182637444,-0.0100384684\C,1.2006808813,0.01  
59676782,-0.7108910091\O,-1.0930812428,-0.0204207977,2.0702120352\O,3.  
5579617837,0.031281493,-0.743689295\O,5.8796717986,0.0820758691,0.6428  
373604\C,6.9006283323,0.4217498836,0.0319267973\N,8.1399449935,0.45921  
89574,0.5600281652\C,9.291603906,0.8758927661,-0.228217962\C,8.3736605  
76,0.0835120475,1.9504885198\C,1.2586678375,-0.0196604133,3.6294765563  
\H,3.413409677,0.0062600473,1.9148091154\H,1.2346984597,0.0249417319,-  
1.7969301871\C,-1.3222725071,-0.0015941245,-0.7455646817\H,4.369713515  
8,0.0360409463,-0.1771281262\H,6.8648168226,0.7279814846,-1.0256504765  
\H,7.4237872508,-0.2036303844,2.3998462154\H,9.0722995447,-0.759154831  
9,2.0003863748\H,8.7999511059,0.9285026364,2.5027708706\H,8.9749317996  
,1.1267722024,-1.2429798591\H,9.7646598083,1.757287869,0.21961414\H,10  
.0326113612,0.0701127708,-0.2811083619\H,-1.1895798972,0.0114973116,-1  
.8309503335\H,-1.9081958084,-0.8851529198,-0.4687549824\H,-1.924457625  
7,0.8644360563,-0.4491104308\H,2.2726278557,-0.0193875036,4.039418727\  
H,0.7165503101,0.8497175548,4.0179240205\H,0.7232273008,-0.8997069402,  
4.0027583848\Version=AM64L-G03RevD.02\State=2-A\HF=-709.2814056\S2=0.

770234\S2-1=0.\S2A=0.75028\RMSD=6.329e-09\RMSF=2.560e-06\Thermal=0.\Di  
pole=4.465645,0.4312866,-0.5945616\PG=C01 [X(C11H16N1O3)]\@

### 2,6-di-methyl-4-hydroxyphenoxy radical---DMSO

1\1\GINC-RICKWORK\FOpt\UB3LYP\6-31+G(d,p)\C10H15O3S1(2)\RICKY\07-Jul-2  
009\0\#p uB3lyp/6-31+g(d,p) opt=tight int=ultrafine freq geom=check\  
2,6 dimetil semichinone + dmso\0,2\C,-0.0066581658,0.0771890759,-0.06  
34036654\C,-0.0378727968,0.2222564926,1.3444544987\C,1.1588134709,0.20  
08273194,2.098893266\C,2.3803115754,0.0386600853,1.4830718897\C,2.4457  
245946,-0.1140451579,0.0273735743\C,1.1911039891,-0.0879385386,-0.7276  
270855\O,-1.1941279324,0.3847097747,2.0157723311\O,3.5500321007,-0.263  
591977,-0.5583867332\O,-3.4813028919,0.4362364438,0.6774736552\S,-4.71  
73526173,0.6279375895,1.5710009662\C,-4.5993038294,-0.6377883988,2.887  
228613\C,-4.3756880043,2.0947512066,2.6103151526\H,-1.9853408028,0.387  
9017904,1.40850382\H,1.0846706033,0.3160158275,3.1769420684\C,3.670917  
9369,0.0107745211,2.2495539059\C,1.2660841507,-0.2450088574,-2.2187075  
735\H,-0.9450004942,0.0982446738,-0.6129669323\H,-5.1815172926,2.21249  
40887,3.3398804277\H,-3.4074996896,1.9756162555,3.1028984439\H,-4.3526  
36798,2.9563206764,1.940527465\H,-4.7261341453,-1.6078061648,2.4030505  
057\H,-3.6166621079,-0.5802737981,3.3619152143\H,-5.4015741464,-0.4765  
168973,3.6123792465\H,3.4979829768,0.1335067796,3.3223922501\H,4.20254  
92011,-0.9320481878,2.0794660654\H,4.3443359896,0.8029041429,1.9038439  
072\H,0.2716876424,-0.2096324735,-2.6721099631\H,1.8880191764,0.541585  
5036,-2.6602739141\H,1.7462218924,-1.1933003483,-2.4846510596\Version  
=AM64L-G03RevD.02\State=2-A\HF=-1013.9587372\S2=0.77071\S2-1=0.\S2A=0.  
750294\RMSD=7.176e-09\RMSF=1.631e-07\Thermal=0.\Dipole=-3.4559876,0.47  
65099,1.9138954\PG=C01 [X(C10H15O3S1)]\@

### 2,6-di-methyl-4-hydroxyphenoxy radical---Me3PO

1\1\GINC-RICKWORK\FOpt\UB3LYP\6-31+G(d,p)\C11H18O3P1(2)\RICKY\30-Aug-2  
010\0\#p B3lyp/6-31+g(d,p) opt freq scale=0.9806\MQH Me3PO\0,2\C,0.  
0056356468,0.0244015589,-0.0091841932\C,-0.0215551169,0.0201356646,1.3  
698813262\C,1.1822371039,0.0132072816,2.1169955876\C,2.4361610656,0.01  
00973524,1.4591482963\C,2.515555927,0.0139906608,0.0842968223\C,1.2881  
37777,0.0217003156,-0.7153087344\O,1.1877919896,0.0092944904,3.4603426  
645\C,3.8276761808,0.0103395476,-0.6459545164\O,1.3343984386,0.0257096  
012,-1.9741132312\C,-1.2486252674,0.0314237438,-0.8348928392\O,-1.2148  
917116,0.0320962947,4.5881187579\P,-1.5764002368,0.1239680822,6.060327  
7041\C,-0.7693665457,1.5252888767,6.9103281573\C,-3.3706249729,0.34401  
90527,6.3093276179\C,-1.1113544519,-1.3694856191,7.0041008293\H,0.2671  
546449,0.0145765359,3.8375926118\H,3.332569013,0.0043691227,2.07346506  
63\H,-0.9668159728,0.0214428407,1.9068384279\H,-2.1399870295,0.0331024  
06,-0.2011503142\H,-1.2760831219,0.9080342909,-1.4917787422\H,-1.28282  
20843,-0.8415100844,-1.4963459954\H,4.669702921,0.0052202642,0.0519444  
804\H,3.9034674788,-0.8634355462,-1.3027193911\H,3.9107957203,0.886340  
9572,-1.2988666025\H,-1.3887297245,-1.2823521971,8.059079981\H,-1.6126  
699979,-2.2381542384,6.5682412495\H,-0.030858848,-1.5194226544,6.92584  
50295\H,-3.6245729855,0.4074008173,7.3717535931\H,-3.690790156,1.25971  
28995,5.8047231923\H,-3.8992028063,-0.5011974952,5.8599938198\H,-1.050  
1146297,1.5704562804,7.9670541602\H,0.3159488322,1.4169117902,6.829126  
217\H,-1.0603014946,2.4575891088,6.4182614274\Version=AM64L-G03RevD.0

2\State=2-A\HF=-997.1300571\S2=0.769693\S2-1=0.\S2A=0.750264\RMSD=7.01  
4e-09\RMSF=1.251e-05\Thermal=0.\Dipole=-1.7024408,0.1339603,4.466366\P  
G=C01 [X(C11H18O3P1)]\@

#### 4-hydroxyphenoxyl radical---DMSO

1\GINC-RICKWORK\FOpt\UB3LYP\6-31+G(d,p)\C8H11O3S1(2)\RICKY\12-Aug-20  
10\0\#p ub3lyp/6-31+g(d,p) opt freq scale=0.9806\hydroquinone rad dms  
o\0,2\C,-0.015730649,0.0103154213,-0.0020133805\C,-0.0232907869,0.002  
6242628,1.37359996\C,1.2022494567,-0.0075469522,2.0895273607\C,2.43705  
37772,-0.0105536308,1.3916291811\C,2.455470129,-0.0030535514,0.0179978  
119\C,1.2256857195,0.0081851672,-0.7580468767\O,1.2440999367,-0.014524  
062,3.4329015489\O,1.2355122377,0.0156681004,-2.017738615\O,-1.0702757  
824,0.0169236412,4.7092272785\S,-1.0464939537,0.1329887759,6.241785661  
9\C,0.017102701,1.5695582598,6.6309163414\C,0.0804690808,-1.1789835032  
,6.8372525718\H,0.3311050093,-0.0103187689,3.8372634414\H,3.3541145164  
, -0.0192304096,1.9733334355\H,3.389280185,-0.0053526122,-0.5356291831\  
H,-0.9405267424,0.0180957288,-0.5706461109\H,-0.9570193038,0.004117125  
3,1.9298804106\H,0.1486948922,1.6345798729,7.7144123881\H,0.9777013227  
,1.4642555774,6.1205116593\H,-0.5059655094,2.4558102031,6.267068238\H,  
-0.3995398951,-2.1326717591,6.6103619052\H,1.0374549147,-1.1063624688,  
6.3145044765\H,0.2103515912,-1.0762730903,7.9180433564\Version=AM64L-  
G03RevD.02\State=2-A\HF=-935.3113586\S2=0.773909\S2-1=0.\S2A=0.750382\  
RMSD=6.343e-09\RMSF=2.295e-06\Thermal=0.\Dipole=-0.2038484,0.1606278,4  
.5252013\PG=C01 [X(C8H11O3S1)]\@

#### 4-hydroxyphenoxyl radical---Me3PO

1\GINC-RICKWORK\FOpt\UB3LYP\6-31+G(d,p)\C9H14O3P1(2)\RICKY\31-Aug-20  
10\0\#p ub3lyp/6-31+g(d,p) opt freq scale=0.9806\semichinone Me3PO\  
0,2\C,-0.0206162211,-0.15247114,0.0687467267\C,-0.0052344782,-0.139115  
3877,1.5228612351\C,1.2990648619,-0.0172634572,2.1523594653\C,2.454046  
026,0.0791138161,1.4114471152\C,2.3917216877,0.0603527754,-0.007448326  
3\C,1.137903689,-0.0558112893,-0.662700327\O,-1.0641725941,-0.2285023,  
2.2002134819\O,3.48786165,0.1496493876,-0.7745318288\O,5.7355365945,0.  
3208411393,0.6061470064\P,7.2006185923,0.2636705391,0.2089772396\C,8.3  
004976875,0.4101037611,1.6572043229\C,7.6543968769,-1.2974423998,-0.62  
3345729\C,7.6829698171,1.6030627687,-0.9350122888\H,-0.9887854532,-0.2  
422659739,-0.4142912327\H,1.3234795562,-0.0050649564,3.2378297496\H,4.  
3197729349,0.2215191873,-0.2311531155\H,1.1284877638,-0.0653745702,-1.  
7486549191\H,3.4251147675,0.1707808469,1.88975873\H,9.3551177083,0.366  
7974335,1.368992036\H,8.1011295765,1.3601566438,2.1605169337\H,8.08170  
09999,-0.4030453935,2.3547886563\H,8.7156082768,-1.3186103739,-0.88937  
71356\H,7.4312739356,-2.1356526315,0.0426071791\H,7.0528006139,-1.4075  
952649,-1.5300448718\H,8.7450507012,1.5492329124,-1.1930291383\H,7.085  
3695246,1.5276736694,-1.8478906057\H,7.4731037675,2.5674838871,-0.4641  
03753\Version=AM64L-G03RevD.02\State=2-A\HF=-918.4830573\S2=0.77279\S  
2-1=0.\S2A=0.750344\RMSD=6.674e-09\RMSF=9.350e-06\Thermal=0.\Dipole=5.  
063495,0.1614226,-1.118142\PG=C01 [X(C9H14O3P1)]\@

#### 4-hydroxyphenoxyl radical---DMF

uB3lyp/6-31+g(d,p)  
C,0,1.0109590227,1.030102159,-0.530780226

C,0,1.1905372714,1.5912738676,0.7977518373  
C,0,1.5383656884,0.8062382268,1.8727027016  
C,0,1.7327812801,-0.5891542334,1.6995956274  
C,0,1.5659850244,-1.1784717172,0.4197180279  
C,0,1.2182670366,-0.4035257586,-0.6595590294  
O,0,2.0741399363,-1.3994786931,2.714545054  
O,0,0.6930540093,1.7475158376,-1.5164787674  
O,0,2.4149623114,-0.1663898917,5.084153028  
C,0,3.0570578561,-0.7323660658,5.9786356919  
N,0,3.2694425899,-0.2312565236,7.2105015785  
C,0,2.7324475185,1.0705510638,7.5937271547  
C,0,4.0418787393,-0.9612310495,8.206831801  
H,0,1.0368113419,2.6604917925,0.9068445837  
H,0,1.6688532223,1.236697553,2.8617302608  
H,0,1.7216135855,-2.2491264725,0.3264646445  
H,0,1.0862223014,-0.8352856766,-1.646819111  
H,0,2.1756683274,-0.9051781623,3.5680021254  
H,0,3.5150970338,-1.721576317,5.8214357548  
H,0,2.1797915207,1.4836570465,6.750870487  
H,0,2.0624668027,0.962136187,8.4538199487  
H,0,3.5485114713,1.7494727317,7.8651989338  
H,0,4.381105615,-1.9118111198,7.7894498871  
H,0,4.918800637,-0.3799301351,8.5136090023  
H,0,3.4299259844,-1.1655177045,9.092707781  
HF=-630,634180

#### 4-hydroxyphenoxy radical

uB3lyp/6-31+g(d,p)

C,0,-0.0010301266,0.,-0.0175895015  
C,0,-0.0070435123,0.,1.3964043588  
C,0,1.2034623951,0.,2.1278046217  
C,0,2.4045820697,0.,1.4598797892  
C,0,2.4659612906,0.,0.0071538448  
C,0,1.1952046678,0.,-0.6987053084  
O,0,3.5625359491,0.,-0.6106486418  
H,0,1.229247373,0.,-1.7834001132  
H,0,-0.9461724165,0.,-0.5574054642  
O,0,-1.157017495,0.,2.1162657877  
H,0,1.1521683806,0.,3.2119716544  
H,0,3.3487045778,0.,1.9950770079  
H,0,-1.9272990699,0.,1.5303243729  
HF=-382,081279

#### 3-hydroxyphenoxy radical---Me3PO

1\1\GINC-RICKWORK\FOpt\UB3LYP\6-31+G(d,p)\C9H14O3P1(2)\RICKY\02-Sep-20  
10\0\#p B3lyp/6-31+g(d,p) opt Freq scale=0.9806\resorcinolo rad me3p  
o\0,2\C,0.0799600388,0.0207121343,0.0754414499\C,0.2247164334,0.74777  
51802,1.2414893618\C,1.5331069946,0.8671141217,1.8741741916\C,2.652949  
3681,0.2005291548,1.2458679008\C,2.4822950601,-0.5159764614,0.07550927  
75\C,1.1882706939,-0.6095148676,-0.5147396084\H,-0.6091715587,1.248370  
0207,1.7223357976\O,3.4798752827,-1.154007479,-0.5744393015\O,5.833578



8721,-0.7532539573,0.6274474512\P,7.1331622872,-0.059157267,0.26568334  
57\C,8.2832927453,0.0185685766,1.6807439083\C,8.0399635502,-0.90152653  
03,-1.0785637502\C,6.8994885152,1.6656218289,-0.2906631205\H,-0.893905  
3131,-0.0707219579,-0.3973063547\O,1.6716921354,1.5367330664,2.9339262  
088\H,4.3473860999,-1.0291502652,-0.1104286811\H,1.0849819359,-1.18363  
43239,-1.4300848883\H,3.6251572509,0.2745652097,1.7210248349\H,9.21940  
38095,0.5179540225,1.4131845829\H,7.8033974762,0.5618260744,2.49947070  
52\H,8.4984560671,-0.9981206515,2.0209169212\H,8.9778038267,-0.3904896  
501,-1.3167692892\H,8.2550865194,-1.9292553617,-0.772714394\H,7.408320  
0207,-0.9323560261,-1.9709053112\H,7.8540743736,2.1436483806,-0.531264  
8801\H,6.2583757094,1.6736359978,-1.1766859774\H,6.4003425855,2.232245  
1741,0.500442703\Version=AM64L-G03RevD.02\State=2-A\HF=-918.475612\S2  
=0.785755\S2-1=0.\S2A=0.750867\RMSD=5.831e-09\RMSF=3.342e-05\Thermal=0  
\Dipole=2.7502445,0.129005,-1.5338106\PG=C01 [X(C9H14O3P1)]\@

### 3-hydroxyphenoxy radical---DMF

1\1\GINC-RICKWORK\Freq\UB3LYP\6-31+G(d,p)\C9H12N1O3(2)\RICKY\03-Sep-20  
10\0\#p B3lyp/6-31+g(d,p) Freq scale=0.9806 geom=check\resorcinolo r  
ad dmf aw\0,2\C,1.65951219,-0.9338313231,-0.1780661338\C,2.9364078453  
, -1.5206452598,0.0579648947\C,4.0647360608,-0.7179457852,0.293911177\C  
,3.9562304685,0.6596920489,0.3036390414\C,2.6665011122,1.2962753493,0.  
0658753379\C,1.5242938124,0.4414247741,-0.1792497803\H,3.010173604,-2.  
6034281372,0.048021479\H,4.8065935201,1.3088630029,0.4840115038\O,2.56  
08991557,2.5523208671,0.0774432996\O,0.6412601127,-1.7987293152,-0.390  
7249902\O,-1.7464032893,-0.5231000342,-0.6702808639\C,-2.6141808341,-0.  
.5469195131,0.210327174\N,-3.7900468359,0.1101463224,0.1525062703\C,-4  
.7574789587,0.0393471283,1.2383917995\C,-4.1293482468,0.935661167,-1.0  
019746844\H,5.0250536575,-1.1944627996,0.4693258336\H,0.567422763,0.91  
70366389,-0.3664924433\H,-0.2137056077,-1.322247344,-0.5238310204\H,-2  
.4821404334,-1.1286596716,1.1368415688\H,-3.3159710113,0.8777715099,-1  
.7243503547\H,-5.0560173232,0.5750667962,-1.4622352057\H,-4.2704838858  
,1.9773756475,-0.6926028613\H,-4.3782800732,-0.6096350065,2.0309420163  
\H,-4.938633913,1.0356104541,1.6580904501\H,-5.7097719756,-0.366599007  
7,0.8783226209\Version=AM64L-G03RevD.02\State=2-A\HF=-630.6272766\S2=  
0.785937\S2-1=0.\S2A=0.750876\RMSD=7.204e-09\RMSF=2.474e-05\ZeroPoint=  
0.195883\Thermal=0.2103552\Dipole=-2.5951067,-0.862175,0.7652567\

### 3-hydroxyphenoxy radical---DMSO

1\1\GINC-RICKWORK\Freq\UB3LYP\6-31+G(d,p)\C8H11O3S1(2)\RICKY\31-Aug-20  
10\0\#p B3lyp/6-31+g(d,p) Freq scale=0.9806 geom=check\resorcinolo r  
ad dmso tow\0,2\C,-2.7944707784,-1.0188689924,-0.0884709423\C,-1.4610  
330803,-0.539341826,-0.3870541733\C,-1.151461559,0.8016829469,-0.26064  
15206\C,-2.1515954395,1.7260975854,0.1560131808\C,-3.4559645011,1.2921  
561411,0.4460011534\C,-3.7918640552,-0.0435351628,0.3343280735\O,0.074  
3708693,1.3216979223,-0.5089578442\H,-4.7885601806,-0.4128129426,0.551  
668967\O,1.9490147255,-0.5083142512,-1.0593352392\S,3.1777504603,-0.59  
93515684,-0.1435587422\C,2.5409113017,-0.754648367,1.565426144\C,3.837  
645861,1.1016134331,-0.0028083249\H,0.7172153661,0.6169302932,-0.78697  
76591\H,-1.8782184686,2.7732912524,0.2380128048\H,-4.1982711134,2.0208  
899152,0.7589863651\O,-3.0934816977,-2.2394716176,-0.1832811461\H,-0.7  
218537059,-1.2629591549,-0.7153360037\H,3.381489267,-0.7305901444,2.26

43337853\H,1.834765795,0.0542669878,1.76774158\H,2.0342034988,-1.71945  
42686,1.6269613487\H,4.2177679933,1.3742364048,-0.9890172988\H,3.03276  
09138,1.7803867564,0.2901376887\H,4.6524555972,1.113209016,0.726260590  
3\\Version=AM64L-G03RevD.02\State=2-A\HF=-935.3039866\S2=0.786348\S2-1  
=0.\S2A=0.750898\RMSD=8.724e-09\RMSF=1.552e-05\ZeroPoint=0.1730422\The  
rma=0.187013\Dipole=2.3612387,1.4418118,1.4371531\

### 3-hydroxyphenoxy radical (most stable conformer)

uB3lyp/6-31+g(d,p)

C,0,-0.0332898436,0.,-0.0561866773  
C,0,-0.0083966662,0.,1.40007287  
C,0,1.1955418693,0.,2.0791182286  
C,0,2.4120840909,0.,1.377216591  
C,0,2.4204073018,0.,-0.0436327428  
C,0,1.2396925211,0.,-0.7514751233  
H,0,-0.9642680877,0.,1.9129086057  
H,0,1.2134205991,0.,3.1648285732  
H,0,3.363364405,0.,1.8989737642  
O,0,3.6574714157,0.,-0.6240306911  
H,0,1.2149295962,0.,-1.8377532228  
O,0,-1.1230992108,0.,-0.6844903557  
H,0,3.5739548077,0.,-1.5873672951  
HF=382,076763

### 4,6-di-methyl-3-hydroxyphenoxy radical---DMF

1\1\GINC-RICKWORK\FOpt\UB3LYP\6-31+G(d,p)\C11H16N1O3(2)\RICKY\13-Aug-2  
010\0\#p B3lyp/6-31+g(d,p) opt freq scale=0.9806\2,4 metil resorcino  
lo rad tow dmf\0,2\C,-0.0625867233,-0.2431127005,-0.0441945037\C,0.12  
1718322,0.0509601552,1.3194312391\C,1.3682538708,0.2858357111,1.878608  
6614\C,2.552860353,0.2239785125,1.0092181942\C,2.3501665445,-0.0847047  
241,-0.3895711188\C,1.0907864101,-0.305226385,-0.8983982087\H,-0.76031  
23219,0.0931400563,1.9554632879\C,1.5607759073,0.5985203417,3.33215512  
91\O,3.7005583139,0.4357750984,1.4778214188\O,0.8402114486,-0.59029035  
36,-2.2004131959\O,3.1055829248,-0.569726821,-3.722440906\C,3.37661122  
7,0.3439724418,-4.5094473843\N,4.5146892916,0.4314020066,-5.2280686936  
\C,5.5525007727,-0.5874788184,-5.1107071395\C,4.7649300443,1.548193496  
1,-6.1278021074\H,3.2303754297,-0.1399141412,-1.0214931832\C,-1.423629  
6634,-0.4957264913,-0.6220327265\H,1.6733919917,-0.608108438,-2.729033  
4757\H,2.6822458446,1.1815239254,-4.6855078907\H,5.2150268076,-1.35099  
30287,-4.4107195971\H,5.7439143689,-1.043877673,-6.0883627437\H,6.4818  
541773,-0.1387665146,-4.7421349526\H,3.9118981182,2.2304163495,-6.1180  
357275\H,5.6589541846,2.1007164792,-5.8163117475\H,4.9152957445,1.1897  
5255,-7.1526919833\H,0.6046953753,0.6204908394,3.8628457551\H,2.213165  
6526,-0.1429248588,3.8073833694\H,2.0609306016,1.5651010321,3.46060807  
61\H,-2.1980284752,-0.4252959986,0.1461568193\H,-1.6512001459,0.221664  
2172,-1.4197807914\H,-1.474260254,-1.4880764173,-1.0857733797\\Version  
=AM64L-G03RevD.02\State=2-A\HF=-709.2749536\S2=0.779928\S2-1=0.\S2A=0.  
750601\RMSD=6.760e-09\RMSF=3.234e-06\Thermal=0.\Dipole=0.1820414,0.717  
3357,-2.5997349\PG=C01 [X(C11H16N1O3)]\@

### 4,6-di-methyl-3-hydroxyphenoxy radical---DMSO

1\1\GINC-RICKWORK\FOpt\UB3LYP\6-31+G(d,p)\C10H15O3S1(2)\RICKY\12-Aug-2010\0\#p B3lyp/6-31+g(d,p) opt freq scale=0.9806\2,4 metil resorcino  
lo rad tow dmsol\0,2\C,-0.0150096747,0.3154440227,0.4607146161\C,0.1045284919,-0.2781477533,1.7749258311\C,1.3224932117,-0.6919967853,2.2647165786\C,2.5118581193,-0.5610261496,1.4696498424\C,2.4067225626,0.0048217324,0.1856504997\C,1.2057712268,0.4453190107,-0.349030143\O,1.4936400585,-1.2373452685,3.4951876408\C,1.0978883676,1.0463174576,-1.718122297\O,-0.7511333748,-1.2080933797,4.9825158869\S,-0.9730926503,-0.1810644312,6.1002708264\C,-0.7148796558,1.4697225587,5.3529552985\C,0.5348638986,-0.2181490812,7.136656135\H,0.6358542223,-1.2790421521,3.9915529181\C,3.8251834878,-1.033596583,2.0196774707\H,3.3146700502,0.0954894179,-0.4073473303\O,-1.1213567923,0.7156369182,0.0170288209\H,-0.8033968956,-0.394967337,2.3575392374\H,-0.7700677731,2.229292428,6.1376130518\H,0.2511751139,1.4963868797,4.8433440305\H,-1.5203334763,1.6210110659,4.6320664552\H,0.5556143435,-1.1930952748,7.6270531428\H,1.4154146575,-0.1001167067,6.5003756663\H,0.4775636215,0.5750262802,7.8871290789\H,2.0743587454,1.0939715124,-2.2083342696\H,0.4140541594,0.4638120189,-2.3460413453\H,0.6744046507,2.0558631196,-1.6695792865\H,4.6348034965,-0.8693709491,1.3040010512\H,4.0707251133,-0.5151924458,2.9544446395\H,3.7846765707,-2.1008632847,2.2682708163\Version=AM64L-G03RevD.02\State=2-A\HF=-1013.951605\S2=0.780048\S2-1=0.\S2A=0.750606\RMSD=6.294e-09\RM SF=1.724e-05\Thermal=0.\Dipole=1.2560586,0.9652483,2.3172473\PG=C01 [X(C10H15O3S1)]\@

#### 4,6-di-methyl-3-hydroxyphenoxy radical---Me3PO

1\1\GINC-RICKWORK\FOpt\UB3LYP\6-31+G(d,p)\C11H18O3P1(2)\RICKY\01-Sep-2010\0\#p B3lyp/6-31+g(d,p) opt freq scale=0.9806\2,4 metil resorcino  
lo rad tow me3po\0,2\C,0.2182878354,0.0541654478,0.0126344451\C,0.454309533,0.6034363265,1.2638074622\C,1.8098049534,0.5114500712,1.8280572566\C,2.8229361997,-0.1580614904,1.0447819225\C,2.5461903935,-0.6735411728,-0.201635227\C,1.217941044,-0.5822573635,-0.7458774002\C,-0.6126667181,1.2863304571,2.0655696423\O,3.4622996501,-1.2847219366,-0.9859007973\O,5.9170501727,-1.1041396837,0.0804512678\P,7.0167708511,-0.0679428778,0.2148097919\C,8.0377115538,-0.3397677581,1.704004602\C,8.1757275334,-0.0777222418,-1.1984865602\C,6.3927314662,1.6450330208,0.3363242476\H,-0.7820796677,0.1151563961,-0.4115331982\O,2.0684820076,1.0083325714,2.9550225382\H,4.3643580349,-1.2495093058,-0.5761682633\C,0.934104845,-1.1665604871,-2.0977720796\H,3.8135266203,-0.2507068665,1.4751778016\H,8.8382412011,0.4017099155,1.7857116255\H,7.3984488722,-0.2811799379,2.5892457259\H,8.4739092676,-1.3414629944,1.6579019204\H,8.9690843797,0.6658439988,-1.0751681648\H,8.6213774452,-1.0724348583,-1.2872276879\H,7.6202515592,0.1351773699,-2.116143895\H,7.2125606312,2.3626619972,0.4391287587\H,5.8167369805,1.8825605447,-0.562562566\H,5.7286422272,1.7294848725,1.2010500626\H,-0.1123440152,-1.022772359,-2.3789625087\H,1.5728803048,-0.711129952,-2.8640477619\H,1.1616167813,-2.239178132,-2.1159888538\H,-1.5663553033,1.2952337308,1.5302034231\H,-0.753393063,0.7885857098,3.0318916831\H,-0.3258254257,2.3181318457,2.2982213598\Version=AM64L-G03RevD.02\State=2-A\HF=-997.1233803\S2=0.779313\S2-1=0.\S2A=0.750573\RMSD=9.530e-09\RM SF=4.161e-06\Thermal=0.\Dipole=2.1194734,0.7011041,-1.1558492\PG=C01 [X(C11H18O3P1)]\@



#### 4,6-di-methyl-3-hydroxy phenoxy radical

uB3lyp/6-31+g(d,p)

C,0,-0.0109919211,0.,-0.0087864167  
C,0,-0.0245276868,0.,1.4405553089  
C,0,1.2699044139,0.,2.1354498538  
C,0,2.4315770802,0.,1.3782938519  
C,0,2.4320256511,0.,-0.0288672768  
C,0,1.1703413569,0.,-0.705560772  
O,0,-1.1023271237,0.,2.0843643047  
O,0,1.2406102951,0.,-2.0737804179  
C,0,1.277249741,0.,3.6339891469  
H,0,3.3936100635,0.,1.8860293471  
C,0,3.7048365957,0.,-0.8228797109  
H,0,-0.9749511501,0.,-0.5107330489  
H,0,0.3490527,0.,-2.4476170893  
H,0,2.29824508,0.,4.0251598343  
H,0,0.7464878951,0.8750076497,4.0255725709  
H,0,0.7464878951,-0.8750076497,4.0255725709  
H,0,4.577356916,0.,-0.1652060459  
H,0,3.7594752293,-0.8766693432,-1.4792556005  
H,0,3.7594752293,0.8766693432,-1.4792556005  
HF=460,725330

#### 2-methoxy-4-hydroxyphenoxy radical

1\1\GINC-RICKWORK\FOpt\UB3LYP\6-31+G(d,p)\C7H7O3(2)\RICKY\22-Sep-2010\  
0\#\#p uB3lyp/6-31+g(d,p) opt Freq scale=0.9806\oMeQH a\0,2\C,-0.0045  
208421,0.,-0.0158727766\C,-0.0078158356,0.,1.4324266105\C,1.1543145647  
,0.,2.1702800247\C,2.4008285087,0.,1.5049421043\C,2.4870848832,0.,0.10  
14270115\C,1.3264526033,0.,-0.6576849834\H,-0.981727667,0.,1.910791816  
6\H,1.1233878786,0.,3.257782142\O,3.5805242016,0.,2.1832956594\H,3.473  
0930574,0.,-0.3466010852\O,1.2900032182,0.,-1.9986878284\O,-1.06080586  
16,0.,-0.688427277\C,2.517776613,0.,-2.7240640258\H,2.2362790585,0.,-3  
.776914208\H,3.1075040059,0.8966259285,-2.4995930076\H,3.1075040059,-0  
.8966259285,-2.4995930076\H,3.4197982914,0.,3.1368817553\Version=AM64  
L-G03RevD.02\State=2-A"\HF=-496.6114308\S2=0.771853\S2-1=0.\S2A=0.7503  
24\RMSD=8.421e-09\RMSF=8.894e-05\Thermal=0.\Dipole=1.7490273,0.,0.9508  
747\PG=CS [SG(C7H5O3),X(H2)]\@

#### 2-methoxy-4-hydroxyphenoxy radical---DMF

1\1\GINC-RICKWORK\FOpt\UB3LYP\6-31+G(d,p)\C10H14N1O4(2)\RICKY\24-Sep-2  
010\0\#\#p uB3lyp/6-31+g(d,p) opt Freq scale=0.9806\oMeQH t dmf\0,2\C,-0.  
061614665,0.0979480691,-0.009683381\C,-0.0645856212,0.0409160854,1.400  
5472661\C,1.1303663956,-0.0445159256,2.0950802259\C,2.4243529117,-0.07  
66657136,1.3872513772\C,2.3499997887,-0.0164468614,-0.0573535933\C,1.1  
558199844,0.0666089836,-0.7360054177\O,3.514222927,-0.1516952905,2.003  
3937382\O,-1.2589911047,0.1808523697,-0.6195621764\O,-1.1711898886,0.3  
925205832,-3.312706736\C,-2.0823286724,1.0090117085,-3.879286527\N,-2.  
194587994,1.166669361,-5.2127166419\C,-3.2992745706,1.9108486845,-5.80  
18759674\C,-1.2066886403,0.5930966969,-6.1208188952\H,3.2977688397,-0.  
0423201261,-0.5859626357\H,1.1261862251,0.1084769145,-1.820783268\H,-1  
.0248233421,0.0665005945,1.9012748837\O,1.2333261743,-0.1044482257,3.4

368176598\H,-1.1685619776,0.2290980646,-1.6041609229\H,-2.8946161438,1.4886225217,-3.3103219699\H,-0.459991389,0.0593015549,-5.5342148672\H,-1.6931402109,-0.1013434832,-6.8148070052\H,-0.7199354066,1.3866494532,-6.6988511905\H,-3.9552426183,2.2868040379,-5.0136662048\H,-2.923260226,2.762184856,-6.3806668811\H,-3.884761859,1.2667018764,-6.4678943005\C,0.0430065095,-0.0831490588,4.2163300369\H,0.3695370668,-0.1426208636,5.2549167339\H,-0.5169042306,0.8470301342,4.0592415494\H,-0.5991416689,-0.9412586792,3.9825760913\\Version=AM64L-G03RevD.02\State=2-A\HF=-745.163094\S2=0.769434\S2-1=0.\S2A=0.750251\RMSD=2.477e-10\RMSF=8.795e-06\Thermal=0.\Dipole=-3.3055518,0.9928741,-3.2964162\PG=C01 [X(C10H14N1O4)]\@

### 2-methoxy-4-hydroxyphenoxy radical---DMSO

1\1\GINC-RICKWORK\FOpt\UB3LYP\6-31+G(d,p)\C9H13O4S1(2)\RICKY\22-Sep-2010\0\#p uB3lyp/6-31+g(d,p) opt Freq scale=0.9806\oMeQH t dmsO\0,2\C,0.0852756288,0.2542407391,0.0393343288\C,0.0711772576,0.1985993303,1.486062522\C,1.2097126601,-0.0047625934,2.2313240669\C,2.4556034746,-0.1678858349,1.5747581582\C,2.5444804017,-0.1283806039,0.1670954413\C,1.4054502422,0.0746840416,-0.5946400907\O,3.6001778079,-0.3650966289,2.2587109801\O,-0.9530095682,0.4423277006,-0.6380823951\O,3.4819846414,-0.2893397839,4.9092696943\S,4.7947854505,0.0723430767,5.6216441713\C,6.0676735949,-1.0597060527,4.9537408274\C,5.3984532667,1.610798551,4.8361997746\H,3.4487517406,-0.3673061957,3.2438734908\H,3.5222573223,-0.262829449,-0.2795458509\O,1.3834105297,0.1284367099,-1.9401602581\H,-0.8968294062,0.3264928309,1.9601601099\H,1.1739542437,-0.0438584989,3.3163802994\H,6.3861657145,1.8543776426,5.2368766962\H,5.4305400613,1.4780652245,3.752041819\H,4.6877595856,2.3971283133,5.097092692\H,5.8054500561,-2.0633849461,5.293227998\H,6.0573041696,-1.0175559135,3.8617477324\H,7.0450482045,-0.7754738732,5.3530328376\C,2.6040769408,-0.0349179241,-2.6528304433\H,2.3420498038,0.0422865748,-3.7083520832\H,3.3225066986,0.7526273819,-2.3935611593\H,3.0500225854,-1.0175053574,-2.4552845309\\Version=AM64L-G03RevD.02\State=2-A\HF=-1049.8401351\S2=0.769817\S2-1=0.\S2A=0.750262\RMSD=7.138e-09\RMSF=7.781e-06\Thermal=0.\Dipole=4.0519678,0.1568055,1.9737956\PG=C01 [X(C9H13O4S1)]\@

### 2-methoxy-4-hydroxyphenoxy radical---Me3PO

1\1\GINC-RICKWORK\FOpt\UB3LYP\6-31+G(d,p)\C10H16O4P1(2)\RICKY\23-Sep-2010\0\#p uB3lyp/6-31+g(d,p) opt Freq scale=0.9806\oMeQH t Me3PO\0,2\C,-0.0107755549,-0.0317429298,-0.0699261946\C,-0.028066067,0.0645352608,1.3111572852\C,1.2235578833,0.0871423433,2.0913604287\C,2.4444572629,0.0013704172,1.3182236\C,2.4496251754,-0.0945978284,-0.054220455\C,1.2189287292,-0.1114186802,-0.7599802711\O,1.2220170802,0.1750007502,3.3428896484\O,1.1644742547,-0.2028370679,-2.1001373356\O,3.5565626003,-0.3173020105,-3.246291636\O,4.0138389374,-0.304439832,-4.6939852911\C,3.2867615299,1.0625876682,-5.663428005\C,5.8240840741,-0.1210423012,-4.8341777407\C,3.5877555209,-1.8374345602,-5.5913044996\O,-1.1465443277,0.1446382535,2.0596289097\H,3.3702428967,0.0164466393,1.8850387839\H,2.0718872622,-0.2504283437,-2.5035943944\H,-0.9188752939,-0.0496048174,-0.6603884647\H,3.3774047894,-0.1586273982,-0.6145791025\H,6.1493022527,-0.1156534635,-5.8789221925\H,6.1255141986,0.8148761832,-4.3557756418\H,6.3073421248,-0.9490433468,-4.3082691802\H,3.9367426135,-1.807390786,-6

.6280226608\H,4.0443500527,-2.6893673452,-5.0798393362\H,2.502135128,-  
1.9691726022,-5.5791503173\H,3.634926473,1.0503263062,-6.7008213128\H,  
2.1968221237,0.9730702089,-5.647311475\H,3.5612126104,2.0146318389,-5.  
2006156497\C,-2.4093427686,0.1286712263,1.4052974819\H,-3.1539205461,0.  
.201793783,2.1985880207\H,-2.513915421,0.9815232965,0.7230970831\H,-2.  
5559217218,-0.8050334826,0.8481843129\\Version=AM64L-G03RevD.02\State=  
2-A\HF=-1033.0117174\S2=0.769002\S2-1=0.\S2A=0.750238\RMSD=9.113e-09\R  
MSF=5.169e-06\Thermal=0.\Dipole=1.1919956,-0.1906841,-4.9818565\PG=C01  
[X(C10H16O4P1)]\@

### DMF

B3lyp/6-31+g(d,p)

C,0,-0.0855563346,0.1755404303,0.0834962134  
O,0,-0.0906415769,0.0047337632,1.2960421805  
H,0,0.650469525,0.8346117164,-0.4137576991  
N,0,-0.9499557699,-0.3952995779,-0.8032217789  
C,0,-0.8640540224,-0.13503059,-2.2291700154  
C,0,-1.9927493224,-1.2987577769,-0.3407010217  
H,0,-2.9834204711,-0.9108549323,-0.6081367806  
H,0,-1.871466221,-2.28993459,-0.7949280691  
H,0,-1.9174319234,-1.3848555866,0.7434609091  
H,0,-1.7923100661,0.3166171993,-2.601449104  
H,0,-0.0395676979,0.5541556481,-2.4288607016  
H,0,-0.6838508999,-1.0631107862,-2.7863666742  
HF=-248,533389

### DMSO

B3lyp/6-31+g(d,p)

S,0,-0.1037575597,0.179713365,0.060937893  
O,0,-0.0142614492,0.0247015546,1.5694148113  
C,0,1.5982460409,-0.028419701,-0.5970451355  
C,0,-0.7745108374,-1.3983315234,-0.5970451355  
H,0,-0.761160197,-1.3790760762,-1.6905555788  
H,0,-0.1817372632,-2.2301535359,-0.2074160928  
H,0,-1.8024667037,-1.4769171839,-0.2381595451  
H,0,1.5748950142,-0.0303539712,-1.6905555788  
H,0,2.1802811524,0.822523363,-0.2381595451  
H,0,2.022238248,-0.9576876812,-0.2074160928  
HF=-553.208399

### Me3PO

1\1\GINC-RICKWORK\FOpt\RB3LYP\6-31+G(d,p)\C3H9O1P1\RICKY\14-Aug-2010\0  
\#p B3lyp/6-31+g(d,p) opt freq scale=0.9806\\Me3PO\0,1\O,0.042016690  
4,-0.0002301654,0.0811399905\P,0.0119060281,-0.0001066859,1.5865478035  
\C,1.6751376573,-0.0211347018,2.3585204375\C,-0.8236471856,1.464685629  
7,2.3080520638\C,-0.859252135,-1.4435687546,2.3077503161\H,-1.85406881  
82,1.5015120726,1.9430470208\H,-0.8282989661,1.4381908117,3.4023302291  
\H,-0.3083709551,2.3684696069,1.9705758701\H,1.6202738305,-0.019714624  
5,3.4517383182\H,2.2101636368,-0.9146254668,2.0242995726\H,2.233206568  
4,0.857732628,2.0231436701\H,-1.8922289703,-1.4513174082,1.9483481955\  
H,-0.3702124965,-2.3597419002,1.9646069557\H,-0.8567656337,-1.42015104

16,3.4020716503\\Version=AM64L-G03RevD.02\\State=1-A\\HF=-536.377581\\RMS  
D=3.026e-09\\RMSF=5.266e-05\\Thermal=0.\\Dipole=-0.0364835,-0.0001047,1.8  
282761\\PG=C01 [X(C3H9O1P1)]\\@