**Gas phase hydration, bond dissociation enthalpies, and acidity of aldehydes: A CBS-Q//B3,
G4MP2, and G4 theoretical study of substituent effects**

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Abstract. CBS-Q//B3, G4MP2, and G4 composite method calculations were used to estimate gas phase standard state (298.15 K, 1 atm) free energies of hydration ($\Delta_{\text{hydr}}G^\circ_{(\text{g})}$), hydration equilibrium constants ($\log K_{\text{hydr},(\text{g})}$), bond dissociation enthalpies (BDEs), and enthalpies ($\Delta_{\text{d}}H^\circ_{(\text{g})}$) and free energies ($\Delta_{\text{d}}G^\circ_{(\text{g})}$) of aldehydic proton acid dissociation for various substituted aldehydes with electron withdrawing and electron releasing groups. Good quality $\log K_{\text{hydr},(\text{g})}$ correlations with the Swain-Lupton resonance effect parameters R and R^+ were found, allowing extension of the model to predict $\log K_{\text{hydr},(\text{g})}$ values for 487 substituted aldehydes having available R -values and 108 substituted aldehydes having available R^+ -values. Good correlations were also found between experimental aqueous phase hydration equilibrium constants ($\log K_{\text{hydr},(\text{aq})}$) and summative R/R^+ -values for peripheral substituents on a range of carbonyl derivatives (aldehydes, ketones, esters, and amides), suggesting the structure-reactivity modeling approach can be extended to include all possible combinations of $R_1C(O)R_2$ carbonyl substitution in both gas and aqueous systems. Computationally derived BDEs and $\Delta_{\text{d}}H^\circ_{(\text{g})} / \Delta_{\text{d}}G^\circ_{(\text{g})}$ were in good agreement with the limited experimental and theoretical datasets. BDEs did not generally correlate with any of the Hammett substituent constants or Swain-Lupton parameters considered. Gas phase acidities exhibited high correlation coefficients with Hammett inductive substituent constants (σ_{I}) and field effect parameters (F), allowing these to be employed as surrogates for estimating the gas phase aldehydic proton acidities of a larger potential compound range.

Keywords: Aldehydes; Gas phase; Hydration; Bond dissociation enthalpies; Acidity; Composite methods

Introduction

The solution phase hydration of carbonyl compounds plays a fundamental role in organic chemistry and biochemistry owing to the mechanistic importance of tetrahedral intermediates, as well as both thermodynamic and kinetic relevance in synthetic, industrial, medicinal, and environmental chemistry.^{1, 2} Aqueous phase studies have shown hydration equilibria can be substantial for some substituted aldehydes,³⁻⁸ and corresponding structure-reactivity investigations have correlated equilibrium constants with Hammett substituent parameters and applied other linear free energy approaches.⁸⁻¹⁴ Because carbonyl hydration is less favorable in the gas phase, theoretical studies have generally concentrated on aqueous phase reactivity and mechanistic/kinetic modeling and are typically limited to smaller compounds such as formaldehyde, with fewer studies focusing on larger databases of molecules and/or gas phase equilibria.¹⁵⁻²⁹

Among the various classes of carbonyl derivatives, aldehydes play an important role in the chemistry of natural and polluted atmospheres.³⁰⁻³² Recent findings suggest that some hydrated aldehydes may have significant populations in air samples,³³⁻³⁶ warranting their consideration in environmental fate and toxicology modeling efforts, gas-particle and air-water partitioning studies, and our understanding of formation pathways for secondary organic aerosols. Furthermore, given the complexity of atmospheric chemistry, and the ever increasing diversity of anthropogenic compounds being emitted into the troposphere, there is also a need to investigate the potential gas phase hydration behavior for a broad range of substituted aldehydes. An additional goal is the development of reliable structure-reactivity

relationships, as these can be included in environmental models and be applied to systems that are difficult to measure experimentally or model theoretically. In some cases, experimental measurements of gas phase aldehyde hydration may not be possible because of the low value of an equilibrium constant or competitive side reactions for reactants and products.

In the current work, we employ high level theoretical methods and established physical organic substituent constant/structure-property approaches to study equilibria for the gas phase hydration of a wide range of substituted aldehydes. In addition, we have examined the gas phase bond dissociation enthalpies (BDEs) and aldehydic hydrogen acidities for various aldehydes with the intent of benchmarking the composite methods and examining possible structure-activity relationships. Gas phase BDEs are directly relevant for atmospheric chemistry, as they are strongly related to rates of degradation by oxidants such as the hydroxyl, nitrate, and chlorine radicals and ozone. In addition, gas phase BDEs are often correlated with solution phase BDEs, and consequently offer insights into likely condensed phase reactivity trends. Gas phase acidities of these compounds are both of fundamental interest, and often correlate with solution phase acidities in various solvents.

Computational Methods

Calculations were conducted using Gaussian 09.³⁷ All calculations used the same gas phase starting geometries obtained with the PM6³⁸ semiempirical method as implemented in MOPAC 2009 (<http://www.openmopac.net/>; v. 9.281). Complete Basis Set (CBS) calculations used the CBS-Q//B3

method.^{39,40} Gaussian-n calculations used the G4⁴¹ and G4MP2⁴² methods. All molecular enthalpies and free energies include zero point and thermal corrections. For hydrated aldehydes, no a priori assumptions were made regarding molecular conformations. All hydrated compounds were subjected to a molecular mechanics (MM) molecular dynamics (MD) conformational search with an unconstrained MD trajectory via the Verlet velocity algorithm and quasi-Newton gradient (maximum number of iterations=10,000; $\epsilon=10^{-4}$) using the following default parameters in Gabedit v.2.2.12 (<http://gabedit.sourceforge.net/>):⁴³ Amber MM model with inclusion of bond stretch, angle bend, torsion, non-bonded, and electrostatic charge-charge terms; post-processing identical structure removal with an energy tolerance of 0.01 kcal/mol and distance tolerance of 0.01 Å and maximum 10 final lowest energy structures. Additional MM conformational studies were conducted using the MMFF94 force field and a systematic rotor search within Avogadro v.1.0.1 (<http://avogadro.openmolecules.net/>). Depending on the number of conformers generated by each approach, between two and nine lowest energy MM conformations for each hydrated compound were subjected to calculations at each of the CBS-Q//B3, G4MP2, and G4 levels of theory. Only the lowest energy conformation (cartesian coordinates provided in Supporting Information; graphical illustrations of the G4 level lowest energy minima are given in Supporting Information Figure S1) for each compound from each composite method calculation was used for further analysis. Optimized structures were confirmed as true minima by vibrational analysis at the same level. Unless otherwise noted, all Hammett substituent constants and resonance and field parameters are from the compendium of Hansch et al.⁴⁴ Statistical analyses were conducted using KyPlot v.2.0.b.15 (<http://www.kyenslab.com/en/>).

Results and Discussion

Aldehyde substituents were chosen to span a broad range of electron withdrawing (EWG) and electron releasing (ERG) abilities. The resulting gas phase standard state (298.15 K, 1 atm) Gibbs free energies of hydration ($\Delta_{\text{hydr}}G^\circ_{(\text{g})}$; Figure 1) calculated at the CBS-Q//B3, G4MP2, and G4 levels of theory span 28.0 kcal/mol from -6.8 (H(O)CPF₄) to 21.2 (H(O)CN(CH₃)₂) kcal/mol (Table 1). The corresponding equilibrium constants ($\log K_{\text{hydr},(\text{g})}$) range over 20.5 orders of magnitude from +5.0 to -15.5. Good agreement was found among the three theoretical methods, with mean unsigned maximum variations in $\Delta_{\text{hydr}}G^\circ_{(\text{g})}$ and $\log K_{\text{hydr},(\text{g})}$ of 1.3 kcal/mol and 1.0 units, respectively.

Our $\Delta_{\text{hydr}}G^\circ_{(\text{g})}$ for formaldehyde (1.2 to 2.3 kcal/mol) are in good agreement with the HF/6-31G(d,p) and HF/6-31+G(d,p) results of Ventura et al. (0.5 and 2.3 kcal/mol, respectively),^{17,20} but these authors found substantially more favorable $\Delta_{\text{hydr}}G^\circ_{(\text{g})}$ at the other levels of theory they considered (all values in kcal/mol): MNDO (-3.7), AM1 (-13.2), PM3 (-3.1), MNDO/M (-20.6), HF/4-31G (-1.7), MP2/6-31G(d,p) (-0.2), and MP3/6-31G(d,p) (-1.4). In another study, Erion and Reddy²¹ found formaldehyde $\Delta_{\text{hydr}}G^\circ_{(\text{g})}$ using various levels of theory of -0.6 (MP4/6-31G**), -1.0 (QCISD(T)/6-31G**), -1.1 of(HF/6-31G**), -1.8 (MP2/6-31G**), and -3.0 (MP3/6-31G**) kcal/mol. This group also conducted calculations on CCl₃C(O)H, obtaining the following $\Delta_{\text{hydr}}G^\circ_{(\text{g})}$: -0.7 (HF/6-31G**), -1.1 (MP4/6-31G**), -1.9 (QCISD(T)/6-31G**), -2.6 (MP2/6-31G**), and -3.9 (MP3/6-31G**) kcal/mol. By comparison, we obtain $\Delta_{\text{hydr}}G^\circ_{(\text{g})}$ between 0.5 to 2.1 kcal/mol at the CBS-Q//B3, G4MP2, and G4 levels of theory for CCl₃C(O)H.

The calculated $\Delta\Delta_{\text{hydr}}G^\circ_{(\text{g})}$ of about zero between formaldehyde and $\text{CCl}_3\text{C}(\text{O})\text{H}$ is, however, equivalent between our work and that of Erion and Reddy²¹ at all levels of theory in both studies. These authors also found $\Delta\Delta_{\text{hydr}}G^\circ_{(\text{g})}$ between formaldehyde and acetaldehyde at 3 to 4 kcal/mol, in qualitative agreement with our value of 1.5 kcal/mol using each of the CBS-Q//B3, G4MP2, and G4 methods. The comparison suggests a systematic difference in the results between our two investigations, with qualitative agreement but modest quantitative disagreement. There is clearly substantial disagreement (on the order of several kcal/mol) between various levels of theory regarding the $\Delta_{\text{hydr}}G^\circ_{(\text{g})}$ for even simple aldehydes. It is of interest that many of the prior semiempirical, HF, DFT, and MPn calculations predicted a $\Delta_{\text{hydr}}G^\circ_{(\text{g})} < 0$ for formaldehyde. If such was the case, we would expect to see a dominant population of the hydrated form during gas phase studies of this compound, which is not observed experimentally.^{7,45}

More recently, Kent et al.⁴⁶ have conducted a theoretical study of the conversion of gas phase methandiol to formaldehyde. Using the HF, MP2, MP4, CCSD, CCSD(T), and QCI(T) model chemistries with the cc-pVDZ and cc-pVTZ basis sets, these authors obtained $\Delta_{\text{hydr}}G^\circ_{(\text{g})}$ ranging from 1.0 to 3.3 kcal/mol, with the highest level CCSD(T)/cc-pVTZ and QCI(T)/cc-pVTZ methods yielding $\Delta_{\text{hydr}}G^\circ_{(\text{g})}$ of 1.0 and 1.1 kcal/mol, respectively. The values are in excellent agreement with our calculations, particularly our G4 $\Delta_{\text{hydr}}G^\circ_{(\text{g})}$ of 1.2 kcal/mol. Consequently, the similar positive $\Delta_{\text{hydr}}G^\circ_{(\text{g})}$ of 1 to 2 kcal/mol reported herein and by Kent et al.⁴⁶ using high-level methods are likely the most accurate thermodynamic data for the gas phase hydration of formaldehyde.

Increasing EWG strength results in more favorable $\Delta_{\text{hydr}}G^\circ_{(\text{g})}$ at the CBS-Q//B3, G4MP2, and G4 levels of theory, as the electron withdrawing substituents increase the electrophilicity of the carbonyl carbon. To quantify this effect, we applied the Swain-Lupton approach⁴⁷⁻⁴⁹ using field effect (F) and resonance effect (R) parameters⁴⁴ for each of the substituted aldehydes in the following equation, where f and r are coefficients obtained from multiple linear regression and C is a regression constant: $\log K_{\text{hydr, (g)}} = fF + rR + C$. During our initial statistical investigations, we observed that $\text{C}\equiv\text{C}-\text{CH}_3$ ($R=-0.26$) was clustering separate from the other α -sp carbons ($\text{C}\equiv\text{C}-\text{H}$, $\text{C}\equiv\text{C}-\text{CF}_3$, $\text{C}\equiv\text{C}-\text{C}_6\text{H}_5$, and $\text{C}\equiv\text{N}$). The cause of this discrepancy, either an erroneous R -value for $\text{C}\equiv\text{C}-\text{CH}_3$ or an exception to an expected α -sp grouping system for $\Delta_{\text{hydr}}G^\circ_{(\text{g})}$, cannot be unambiguously resolved without new experimental data. R -values are commonly derived from F -values and Hammett substituent constants by way of equations such as $R = \sigma_p - \alpha F$ (where $\alpha=0.921$).⁵⁰ Using this equation and the σ_p and F -values given by Hansch et al.⁴⁴ consistently yields R -values for $\text{C}\equiv\text{C}-\text{H}$ (0.01 vs. 0.03), $\text{C}\equiv\text{N}$ (0.19 vs. 0.15), $\text{C}\equiv\text{C}-\text{CH}_3$ (-0.24 vs. -0.26), $\text{C}\equiv\text{C}-\text{CF}_3$ (0.17 vs. 0.14), and $\text{C}\equiv\text{C}-\text{C}_6\text{H}_5$ (0.03 vs. 0.01) within ± 0.04 units of those provided in ref. (44). If one assumes the contribution of the α - $\text{C}\equiv\text{C}$ moiety to the σ_p of $\text{C}\equiv\text{C}-\text{H}$, $\text{C}\equiv\text{C}-\text{CH}_3$, $\text{C}\equiv\text{C}-\text{CF}_3$, and $\text{C}\equiv\text{C}-\text{C}_6\text{H}_5$ is constant, and that the σ_p are all accurate, linearly regressing the σ_p of H (0.00), CH_3 (-0.17), CF_3 (0.54), and C_6H_5 (-0.01) against the σ_p of $\text{C}\equiv\text{C}-\text{H}$ (0.23), $\text{C}\equiv\text{C}-\text{CH}_3$ (0.03), $\text{C}\equiv\text{C}-\text{CF}_3$ (0.51), and $\text{C}\equiv\text{C}-\text{C}_6\text{H}_5$ (0.16) should give a high correlation coefficient, which is the case ($r=0.981$, $p=0.02$, $m=0.64$, $b=0.17$).

Similarly, assuming the contribution of the α - $\text{C}\equiv\text{C}$ moiety to the F -value of $\text{C}\equiv\text{C}-\text{H}$, $\text{C}\equiv\text{C}-\text{CH}_3$, $\text{C}\equiv\text{C}-\text{CF}_3$, and $\text{C}\equiv\text{C}-\text{C}_6\text{H}_5$ is constant, and that the F -values are all accurate, linearly regressing the F of H (0.03), CH_3 (0.01), CF_3 (0.38), and C_6H_5 (0.12) against the F of $\text{C}\equiv\text{C}-\text{H}$ (0.22), $\text{C}\equiv\text{C}-\text{CH}_3$ (0.29), $\text{C}\equiv\text{C}-\text{CF}_3$ (0.37), and $\text{C}\equiv\text{C}-\text{C}_6\text{H}_5$ (0.15) should also yield a straight line. This is not observed, and the

regression is non-significant ($p=0.40$). Omitting $\text{C}\equiv\text{C}-\text{CH}_3$ does not result in a significant regression ($p=0.36$). F -values can also be estimated from equations of the form $F = a\sigma_m + b\sigma_p + \varepsilon$, where constants of $a=1.369 / b=-0.373 / \varepsilon=-0.009$ ⁵⁰ and $a=1.297\pm 0.147 / b=-0.385\pm 0.089 / \varepsilon=0.033\pm 0.026$ ⁴⁴ have been reported. Use of these constants and the σ_m and σ_p values from ref. (44) yields F -values of 0.27 and 0.29, respectively, in agreement with the original F -value of 0.29. To examine the potential inaccuracy of σ_m for $\text{C}\equiv\text{C}-\text{CH}_3$, σ_m for H (0.00), CH_3 (-0.07), CF_3 (0.43), and C_6H_5 (0.06) were linearly regressed against the σ_m of $\text{C}\equiv\text{C}-\text{H}$ (0.21), $\text{C}\equiv\text{C}-\text{CH}_3$ (0.21), $\text{C}\equiv\text{C}-\text{CF}_3$ (0.41), and $\text{C}\equiv\text{C}-\text{C}_6\text{H}_5$ (0.14). Neither regressions using all four paired compounds ($p=0.13$) or $\text{C}\equiv\text{C}-\text{H}$, $\text{C}\equiv\text{C}-\text{CF}_3$, and $\text{C}\equiv\text{C}-\text{C}_6\text{H}_5$ ($p=0.24$) yield significant relationships.

However, the available substituent constant dataset for α -sp carbons may be insufficient to evaluate the reliability of the $\text{C}\equiv\text{C}-\text{CH}_3$ R -value. Thus, we looked at the correlation between the $\Sigma\sigma_m$ -values ($\sigma_{m,R1} + \sigma_{m,R2}$) for substituents on $\text{CH}=\text{C}(\text{R}_1\text{R}_2)$ functionalities and the σ_m -values for the entire $\text{CH}=\text{C}(\text{R}_1\text{R}_2)$ moieties on the following groups: $\text{CH}=\text{CH}_2$, $\text{CH}=\text{C}(\text{CN})_2$, $\text{CH}=\text{CH}(\text{NO}_2)-t$, $\text{CH}=\text{CH}(\text{CF}_3)-c$, $\text{CH}=\text{CH}(\text{CF}_3)-t$, $\text{CH}=\text{CH}(\text{SO}_2\text{CF}_3)$, $\text{CH}=\text{CH}(\text{CN})$, $\text{CH}=\text{CH}(\text{CHO})$, $\text{CH}=\text{CH}(\text{Me})-t$, $\text{CH}=\text{CH}(\text{COMe})$, $\text{CH}=\text{CH}(\text{COOEt})$, $\text{CH}=\text{CH}(\text{C}_6\text{H}_5)$, and $\text{CH}=\text{CH}(\text{COC}_6\text{H}_5)$. In this larger dataset, we found a significant linear relationship ($r=0.942$, $p<10^{-5}$, $m=0.46$, $b=0.02$), suggesting that an analogous trend should exist for $\text{C}\equiv\text{C}-\text{R}$ groups. Thus, approximating the trend between σ_m for H, CF_3 , and C_6H_5 against the σ_m of $\text{C}\equiv\text{C}-\text{H}$, $\text{C}\equiv\text{C}-\text{CF}_3$, and $\text{C}\equiv\text{C}-\text{C}_6\text{H}_5$ ($m=0.56$, $b=0.16$), and intersecting the σ_m of CH_3 (-0.07), yields a revised $\text{C}\equiv\text{C}-\text{CH}_3$ σ_m of 0.12. With a $\sigma_m=0.12$ for $\text{C}\equiv\text{C}-\text{CH}_3$, F -values of 0.14 and 0.18 are obtained with the equation $F = a\sigma_m + b\sigma_p + \varepsilon$ and the corresponding regression constants from ref. (50) and (44), respectively. Consequently, revised R -values of -0.10 and -0.14 for $\text{C}\equiv\text{C}-\text{CH}_3$ arise from the relationship $R = \sigma_p - 0.921F$. The use of $R=-0.10$ for $\text{C}\equiv\text{C}-\text{CH}_3$ places this substituent substantially closer to other α -

sp carbons in plots of $\Delta_{\text{hydr}}G^\circ_{(\text{g})}$ against R at each level of theory we examined, and we use this revised R -value in subsequent analyses and discussions. However, future experimental clarification on this issue is required.

Using both the field and resonance effect substituent constants, we obtain reasonable correlation coefficients ($n=31$) with corresponding values for f , r , and C at the three levels of theory (error bars are standard errors throughout the manuscript): CBS-Q//B3, $r=0.926$, $SE=1.61$, $CV=-0.51$, $f=2.79\pm1.44$ ($p=0.06$), $r=13.1\pm1.1$ ($p<10^{-11}$), $C=-2.68\pm0.54$ ($p<10^{-4}$); G4MP2, $r=0.918$, $SE=1.61$, $CV=-0.40$, $f=2.24\pm1.44$ ($p=0.13$), $r=12.5\pm1.1$ ($p<10^{-10}$), $C=-3.51\pm0.54$ ($p<10^{-6}$); and G4, $r=0.918$, $SE=1.64$, $CV=-0.50$, $f=2.40\pm1.47$ ($p=0.11$), $r=12.7\pm1.2$ ($p<10^{-10}$), $C=-2.74\pm0.55$ ($p<10^{-4}$). All three levels of theory yield statistically non-significant ($p>0.05$) regression coefficients for the field effect constant F , suggesting a significant probability that $f\approx 0$ (and thus, negligible field effects). Although Hammett substituent constants (σ_m , σ_p , σ_p^+ , σ_p^- , σ_F , σ_I , σ_R , σ_R^+ , σ^*/E_s , and σ_R^-) and R^- values are not available for all substituents under consideration, the available subsets we examined did not provide as good correlations as the F/R values, and were not considered further.

Consequently, we omitted the field effect term from further analysis, and investigated the theoretical gas phase hydration thermodynamics using only the resonance effect parameters R (Figure 2) and R^+ (Figure 3). Using the R parameter, the following two generally separate aldehyde substituent groups emerge from the analysis, with approximately parallel regression lines for R against $\log K_{\text{hydr},(\text{g})}$: (a) α -sp³ carbons and α -saturated and unsaturated heteroatoms; and (b) α -sp and α -sp² carbons. Linearly regressing the CBS-Q//B3, G4MP2, and G4 $\log K_{\text{hydr},(\text{g})}$ against the corresponding R -values gave the regression statistics in Table 2 for each of the two groups of compounds, as well as for all substituents

combined into a single group. Although strong correlations for $\log K_{\text{hydr,(g)}}$ were observed at each level of theory against the R -values within each group ((a), $r>0.954$; (b), $r>0.973$), and for all compounds combined ($r>0.912$), the use of the R^+ resonance effect parameter for positively charged reaction centers substantially improved the quality of fit for all compounds ($r>0.958$) on the subset of 20 substituents having available R^+ -values (Figure 3 and Table 3). By comparison, correlation coefficients of 0.941 (CBS-Q//B3), 0.938 (G4MP2), and 0.937 (G4) were found between the estimated $\log K_{\text{hydr,(g)}}$ and corresponding R -values for this 20 substituent subset, displaying both lower quality regression fits and separate grouping of sp^3 versus sp/sp^2 hybridized α -carbons (Supporting Information Figure S2) compared to the application of R^+ -values (where α -carbon hybridization dependent clustering was not observed). We note our use of a revised R^+ -value of -0.38 for para-bromobenzene (C_6H_4 -4-Br), corrected from the value of +0.38 given in Table V of Hansch et al.^[44] The positive R^+ for C_6H_4 -4-Br in ref. (44) is likely a typographic error, as analogous electron withdrawing substituents on benzene have negative R^+ -values (e.g., C_6H_4 -4-Cl, -0.37; C_6H_4 -3-Cl, -0.34; and C_6H_4 -4-NO₂, -0.22), as do the parent halogen substituents (e.g., F=-0.52, Cl=-0.31, and Br=-0.30). The use of either R or R^+ based resonance parameters for $\log K_{\text{hydr,(g)}}$ correlation analysis is theoretically defensible, since both the neutral and charge separated carbonyl resonance forms ($C=O$ and C^+-O^-) are expected to contribute to the hydration reaction. Multiple linear regressions of the general form $\log K = rR + r^+R^+ + C$ (where r and r^+ potentially represent the relative contributions of the neutral and positively charged resonance forms) are precluded given the multicollinearity between R and R^+ ($r=0.977$ for the 20 substituents we considered).

Application of the R -value based regression equations towards 487 substituted aldehydes (including the 31 compounds in the training set) with available R -values for uncharged substituents yields the estimated $\log K_{\text{hydr,(g)}}$ ranging between -16.0 ($\text{N}(\text{C}_3\text{H}_7)_2$) and +10.6 ($\text{N}=\text{NPO}(\text{OEt})_2$) shown in Supporting Information Table S1. Analogous application of the R^+ -value based regression equations towards 108 substituted aldehydes (including the 20 compounds in the training set) with available R^+ -values for uncharged substituents yields the estimated $\log K_{\text{hydr,(g)}}$ ranging between -17.7 ($\text{N}(\text{C}_2\text{H}_5)_2$) and +2.8 ($\text{P}(\text{C}_6\text{H}_5)_2$) shown in Supporting Information Table S2. Charged substituents (e.g., O^- , CO_2^- , $\text{N}^+(\text{CH}_3)_3$) were not considered in these gas phase $\log K_{\text{hydr}}$ estimates using either the R or R^+ based approaches because these charge side groups are generally considered non-volatile and are not expected to have significant gas phase populations amenable to hydration reactions. Similarly, a number of substituents included in our analysis would also be expected to undergo hydrolysis in the presence of atmospheric water (e.g., acyl halides, transition metal complexes) at rates competitive with, or exceeding, that of corresponding aldehyde hydrolysis reactions, but they are retained in the database for completeness. Regression derived standard errors in the $\log K_{\text{hydr,(g)}}$ estimates are about 1.0 to 1.5 units for most compounds. For the 108 substituents with both R and R^+ values, good agreement was observed between $\log K_{\text{hydr,(g)}}$ obtained using both correlation approaches at each level of theory (Supporting Information Figure S3). The value of such correlations and resulting $\log K_{\text{hydr,(g)}}$ estimates resides in the conformational complexity and large size of many substituents for which R/R^+ -values are available. In many cases, high level calculations on these moieties are either impossible (beyond the basis set limits) or impractical (large numbers of low energy conformers requiring investigation and/or many heavy atoms present).

As a sample application of these results, recent experimental³³ and theoretical³⁴ evidence suggests perfluoroalkyl aldehydes (PFAlDs) are likely present in the atmosphere in the hydrated form. These compounds are both derivatives and precursors of other well known perfluorinated compounds, and are thought to play an important role towards our understandings into the global cycling of these contaminants.⁵¹⁻⁵³ As part of our initial suite of calculations provided in Table 1, we found that the C₁ PFAlD (CF₃C(O)H) is expected to have a log K_{hydr,(g)} ranging from 0.6 (G4MP2) to 1.8 (CBS-Q//B3), consistent with the experimental data.³³ Additional calculations at the CBS-Q//B3 and G4MP2 levels on the C₂ (CF₃CF₂C(O)H), C₃ (CF₃(CF₂)₂C(O)H), and C₄ (CF₃(CF₂)₃C(O)H) PFAlDs gave the following log K_{hydr,(g)}: C₂, 0.9 (CBS-Q//B3) and -0.3 (G4MP2); C₃, 0.7 (CBS-Q//B3) and -0.4 (G4MP2); and C₄, 1.1 (CBS-Q//B3) and -0.1 (G4MP2). Corresponding G4 calculations on the C₂ through C₄ PFAlD derivatives were impractical due to the high computational expense. By comparison, the Swain-Lupton regression-derived log K_{hydr,(g)} for these compounds using correlations with *R*-values are 0.1_{CBS-Q//B3} / -1.0_{G4MP2} (C₂), -0.2_{CBS-Q//B3} / -1.3_{G4MP2} (C₃), and 0.1_{CBS-Q//B3} / -1.0_{G4MP2} (C₄). *R*⁺ substituent constants are not available for CF₃CF₂, CF₃(CF₂)₂, and CF₃(CF₂)₃. The results show that the longer chain (i.e., >C₄) PFAlDs – which are of primary interest to the environmental chemistry community – will likely be present substantially, if not dominantly, as the hydrated form in the atmosphere. Similarly, other aldehydes with α-EWGs such as nitro and variously substituted carbonyl moieties are also expected to have significant hydrated populations in gas phase atmospheric samples. Consequently, ambient atmospheric modeling efforts and associated risk assessments, as well as studies in engineered systems, will need to account for the gas phase hydration of such compounds. In another experimental study, Axson et al.³⁵ have recently provided an experimental log K_{hydr,(g)} of 2.2±0.1 for methylglyoxal (H₃CC(O)C(O)H). Our calculations at the CBS-Q//B3, G4MP2, and G4 levels obtain log K_{hydr,(g)} of -0.6, -1.6, and -0.7, respectively. In their

work, Axson et al.³⁵ noted that their reported $\log K_{\text{hydr,(g)}}$ is “significantly more favorable than theoretical predictions, even ones made in aqueous solution.” Our results are, however, consistent with those of Barsanti and Pankow, who estimated that gas phase hydration of methylglyoxal would not be thermodynamically favorable.⁵⁴ Further clarification is required to better define whether the two theoretical estimates, or the experimental datapoint, accurately reflect the gas phase hydration thermodynamics of this model secondary organic aerosol precursor.

Our calculations were limited to gas phase asymmetric carbonyl substitutions of the general form $R_1C(O)R_2$ where $R_2=H$ (i.e., aldehydes). We sought to examine whether the findings could be extended into the aqueous phase and also towards symmetric and asymmetric carbonyl substitutions where $R_2 \neq H$ and $R_1=R_2$ or $R_1 \neq R_2$ (i.e., ketones and carboxylic acid derivatives). Gomez-Bombarelli et al.²⁶ have recently published a compilation of experimental $\log K_{\text{hydr,(aq)}}$ and conducted corresponding B3LYP/6-31++G(d,p), MP2/6-31++G(d,p), and CBS-Q $\log K_{\text{hydr,(aq)}}$ calculations directly using the IEFPCM implicit solvation model. When the sum of the R -values ($\Sigma R = R_{R1} + R_{R2}$) on either side of the carbonyl moiety from this compilation is plotted against the experimental $\log K_{\text{hydr,(aq)}}$ values, a strong correlation exists ($n=35$, $r=0.975$, $p<10^{-22}$, $SE=1.22$, $CV=-0.29$, $m=14.78 \pm 0.59$, $b=2.13 \pm 0.33$) among all datapoints, although the three thioesters ($H(O)CSC_2H_5$, $H_3CC(O)SC_2H_5$, and $F_3CC(O)SC_2H_5$) are outliers (Figure 4(a)). The use of R^+ ($\Sigma R^+ = R^+_{R1} + R^+_{R2}$) does not substantially change the summary statistics for the correlation ($n=28$, $r=0.972$, $p<10^{-17}$, $SE=1.20$, $CV=-0.28$, $m=8.08 \pm 0.38$, $b=2.31 \pm 0.38$), but removes the outlying nature of various substituent groups (notably the thioesters), thereby allowing greater confidence in applying the regression towards substituent functional group classes not included in the training set. SC_2H_5 does not have a R^+ -value in Hansch et al.,^[44] thus, a value of -0.81 was estimated based on the $R^+=-0.83$ for SCH_3 and the $\Delta R^+=0.02$ between CH_3 ($R^+=-0.32$) and C_2H_5 ($R^+=-0.30$).

The strong agreement for ΣR and ΣR^+ based approaches towards $\log K_{\text{hydr,(aq)}}$ estimation across multiple functional group classes and over a $\log K_{\text{hydr,(aq)}}$ range of about 20 units suggests that not only can the gas phase R/R^+ -value $\log K_{\text{hydr}}$ modeling approaches extend into aqueous systems, but also that a simple summative approach to R/R^+ -values about the carbonyl moiety can likely be used to extend our $\log K_{\text{hydr,(g)}}$ regression equations presented above towards all possible functional group combinations of $R_1C(O)R_2$. A sample application of the ΣR^+ based approaches towards $\log K_{\text{hydr,(aq)}}$ estimation for various aldehydes is provided in Supporting Information Table S3. Using the regression equation shown in Figure 4(b), $\log K_{\text{hydr,(aq)}}$ were estimated for 115 aldehydes having available R^+ substituent constants from ref. (44). Predicted $\log K_{\text{hydr,(aq)}}$ range from -18.4 (S^-) for strongly electron releasing substituents to +7.2 ($P(C_6H_5)_2$) for strongly electron withdrawing groups. The estimated $\log K_{\text{hydr,(aq)}}$ end members are the symmetric ketones $C(O)S_2^{2-}$ ($\log K_{\text{hydr,(aq)}}=-39.0$) and $C(O)(P(C_6H_5)_2)_2$ ($\log K_{\text{hydr,(aq)}}=+12.0$), well outside the current experimental range of -14.2 to +3.4. We note that many of the substituents are susceptible to rapid aqueous phase hydrolysis (e.g., various carboxylic acid derivatives), and would therefore hydrolyze having kinetic parameters competitive with – or exceeding – that of hydration reactions, but we retain these functional groups in the database for completeness.

Gas phase standard state (298.15 K, 1 atm) bond dissociation enthalpies (BDEs) were also calculated at the CBS-Q//B3, G4MP2, and G4 levels of theory on various substituted aldehydes (Table 4). Good agreement was found between the theoretical values and the limited available experimental dataset. The radical species of several α - and β -unsaturated members ($R=C(O)CH_3$, $CH=CH_2$, $C\equiv CH$, NO_2 , $C\equiv CCH_3$, $C\equiv CCF_3$, and $C(CN)_3$), as well as $R=PF_4$, did not readily converge at all three levels of theory, and thus

were omitted from further analysis. We found no high quality general correlations between BDEs at any of the levels of theory and F , R , R^+ , R^- , σ_m , σ_p , σ_p^+ , σ_p^- , σ_F , σ_I , σ_R , σ^*/E_s , σ_R^+ , and σ_R^- substituent constants.

Analogous calculations were conducted to estimate the gas phase standard state (298.15 K, 1 atm) enthalpies ($\Delta_d H^\circ_{(g)}$) and free energies ($\Delta_d G^\circ_{(g)}$) of aldehyde proton acid dissociation for these compounds (Table 5). As with the BDE calculations, good agreement was found between the theoretical values and the available experimental dataset. The deprotonated anionic forms did not converge at all levels of theory for the following aldehyde substituents: NH_2 , $C\equiv N$, $C\equiv CH$, $C\equiv CCH_3$, $C\equiv CCF_3$, NO_2 , CF_3 , Cl , Br , SiH_3 , $Si(CH_3)_3$, SiH_3 , SiF_3 , $SiCl_3$, CCl_3 , CBr_3 , $C(C\equiv N)_3$, PF_4 , and GeH_3 .

Multiple linear regression of the σ_m/σ_p , σ_I/σ_R , and F/R pairs did not yield high quality correlations with statistical significance for both independent variables. Among the univariate correlations, σ_I displayed an excellent quality of fit ($n=9$, $r=-0.966$, $SE=3.1$, $CV=0.008$, $m=-60.3\pm 6.1$, $b=387.1\pm 1.4$) against the G4 $\Delta_d G^\circ_{(g)}$ data, in addition to the CBS-Q//B3 ($n=9$, $r=-0.965$, $SE=3.1$, $CV=0.008$, $m=-59.7\pm 6.1$, $b=387.2\pm 1.4$) and G4MP2 ($n=9$, $r=-0.967$, $SE=3.0$, $CV=0.008$, $m=-59.0\pm 5.9$, $b=386.7\pm 1.4$) datasets. Multiple regression of the general form $\alpha\sigma_I + \beta\sigma_R = \Delta_d G^\circ_{(g)}$ gave insignificant ($p>0.05$) β -coefficients for σ_R , suggesting inductive influences dominate gas phase acidity variations for substituted aldehydes. Similar qualities of fit were obtained between σ_I and the theoretical $\Delta_d H^\circ_{(g)}$ (all $n=9$): CBS-Q//B3, $r=-0.967$, $SE=3.1$, $CV=0.008$, $m=-60.6\pm 6.0$, $b=395.4\pm 1.4$; G4MP2, $r=-0.969$, $SE=2.9$, $CV=0.008$, $m=-59.8\pm 5.7$, $b=394.8\pm 1.3$; and G4, $r=-0.969$, $SE=3.0$, $CV=0.008$, $m=-61.3\pm 5.9$, $b=395.3\pm 1.4$.

Using these correlations and σ_I values for a range of substituents reported by Charton⁵⁵ yields the estimated $\Delta_d H^\circ_{(g)}$ and $\Delta_d G^\circ_{(g)}$ given in Table 6. The predicted $\Delta_d H^\circ_{(g)}$ range within these substituents is

from 351.8 to 396.0 kcal/mol, and a $\Delta_d G^\circ_{(g)}$ range from 344.3 to 387.8 kcal/mol. These boundaries correspond to the currently known experimental data end members for fluorine and dimethylamino substituents, respectively. We also note that the Swain-Lupton F -parameter yields a modestly lower quality of fit as compared to the σ_I substituent constant (e.g., r of -0.924 against the G4 $\Delta_d G^\circ_{(g)}$ data, compared to a corresponding r of -0.966 for σ_I), but a larger parameter database is available for F , thereby substantially extending the range of possible substituents that can be modeled. In addition, σ_I can be estimated from F -values using equations such as $F = 0.888\sigma_I + 0.017$,^[44] further extending the scope of our $\Delta_d H^\circ_{(g)} / \Delta_d G^\circ_{(g)}$ models.

Conclusions

Gas phase standard state (298.15 K, 1 atm) free energies of hydration ($\Delta_{\text{hydr}} G^\circ_{(g)}$) and corresponding equilibrium constants ($\log K_{\text{hydr}(g)}$), bond dissociation enthalpies (BDEs), and enthalpies ($\Delta_d H^\circ_{(g)}$) and free energies ($\Delta_d G^\circ_{(g)}$) of aldehydic proton acid dissociation were calculated using the composite method CBS-Q//B3, G4MP2, and G4 levels of theory on a range of substituted aldehydes with various electron withdrawing and electron releasing groups. More electron withdrawing substituents increasingly favor higher $\log K_{\text{hydr}(g)}$, and two groupings of theoretical values that depend on substituent classification each display excellent correlation with the Swain-Lupton resonance effect parameters R and R^+ , and no significant correlation with the corresponding field effect parameter (F). Using these correlations, $\log K_{\text{hydr}(g)}$ was predicted for 487 substituted aldehydes having available R -values and 108 substituted aldehydes having available R^+ -values. The sum of R and R^+ on substituents attached to members of various carbonyl derivative classes also display strong correlations with aqueous phase hydration equilibrium constants ($\log K_{\text{hydr}(aq)}$), reliably extending the modeling efforts into the condensed phase

and suggesting the gas phase modeling approach can be used to predict $\log K_{\text{hydr,(g)}}$ for all possible symmetric and asymmetric carbonyl derivatives. Both the computationally derived BDEs and $\Delta_d H^\circ_{(\text{g})}$ / $\Delta_d G^\circ_{(\text{g})}$ exhibited good agreement with the limited experimental and theoretical datasets. No predictive univariate or multivariate correlations were found between the theoretical gas phase BDEs and the major Hammett substituent constants or Swain-Lupton parameters, suggesting general structure-activity relationships across different types of functional groups may be absent for this combination of physical property and general compound class. High correlation coefficients were observed between gas phase acidities and the Hammett inductive substituent constant (σ_I), facilitating estimation of $\Delta_d H^\circ_{(\text{g})}$ / $\Delta_d G^\circ_{(\text{g})}$ for other compounds with known σ_I values. Good correlations were also found between $\Delta_d H^\circ_{(\text{g})}$ / $\Delta_d G^\circ_{(\text{g})}$ and the corresponding F -values, allowing this substituent parameter (which is available for a large number of compounds, and can also be used to estimate σ_I values) to also be employed for the estimation of gas phase aldehydic proton acidities.

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Supporting Information. Raw energies and Cartesian coordinates for all optimized structures at the G4 level of theory, graphical images of aldehyde hydrate minimum energy conformations, $\log K_{\text{hydr,(g)}}$ and $\log K_{\text{hydr,(aq)}}$ predictions for a broad suite of substituents having experimental R and R^+ values, and additional statistical analyses.

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Table 1. Estimated gas phase standard state (298.15 K, 1 atm) free energies of hydration ($\Delta_{\text{hydr}}G^\circ_{(\text{g})}$) and corresponding hydration equilibrium constants ($\log K_{\text{hydr},(\text{g})}$) for various aldehydes with electron withdrawing and electron releasing substituents at the CBS-Q//B3, G4MP2, and G4 levels of theory.

substituent	$\Delta_{\text{hydr}}G^\circ_{(\text{g})}$ (kcal/mol)			$\log K_{\text{hydr},(\text{g})}$		
	CBS-Q//B3	G4MP2	G4	CBS-Q//B3	G4MP2	G4
C(O)CH ₃	0.9	2.1	1.0	-0.6	-1.6	-0.7
NH ₂	16.6	17.2	16.5	-12.1	-12.6	-12.1
C(CH ₃) ₃	4.3	5.4	4.4	-3.2	-4.0	-3.2
C≡N	1.1	2.5	1.5	-0.8	-1.9	-1.1
N(CH ₃) ₂	20.7	21.2	20.3	-15.1	-15.5	-14.8
CH=CH ₂	7.1	8.0	7.1	-5.2	-5.9	-5.2
C≡CH	4.6	5.7	4.8	-3.4	-4.2	-3.5
F	6.9	7.8	6.7	-5.0	-5.8	-4.9
H	1.3	2.3	1.2	-0.9	-1.6	-0.9
OH	14.4	15.3	14.3	-10.5	-11.2	-10.5
CH ₃	2.8	3.8	2.7	-2.0	-2.7	-2.0
NO ₂	-1.8	-0.1	-1.3	1.4	0.1	0.9
C ₆ H ₅	7.0	8.0	7.1	-5.1	-5.9	-5.2
CF ₃	-2.4	-0.9	-2.0	1.8	0.6	1.5
Si(CH ₃) ₃	1.7	2.9	1.8	-1.3	-2.2	-1.3
Br	7.7	9.5	8.2	-5.6	-6.9	-6.0
Cl	8.0	9.4	8.3	-5.9	-6.9	-6.1
SiCl ₃	-0.4	1.8	0.5	0.3	-1.3	-0.4
SiF ₃	0.1	1.8	0.4	-0.1	-1.3	-0.3

SiH ₃	3.2	4.4	3.2	-2.4	-3.2	-2.4
CBr ₃	2.3	3.1	1.9	-1.7	-2.3	-1.4
CCl ₃	0.5	2.1	0.9	-0.4	-1.5	-0.7
C≡CCF ₃	2.4	3.6	2.6	-1.7	-2.6	-1.9
C≡CCH ₃	4.4	4.6	3.6	-3.2	-3.3	-2.7
C(C≡N) ₃	-3.2	-1.6	-2.8	2.3	1.2	2.0
C ₆ H ₄ -4-Br	6.5	7.7	6.8	-4.8	-5.7	-5.0
C ₆ H ₄ -4-Cl	6.7	7.8	6.8	-4.9	-5.7	-5.0
C ₆ H ₄ -4-F	7.0	8.1	7.1	-5.1	-5.9	-5.2
C ₆ H ₄ -4-CH ₃	7.7	8.8	7.9	-5.6	-6.4	-5.8
PF ₄	-6.8	-4.3	-5.8	5.0	3.1	4.3
GeH ₃	3.1	4.8	3.6	-2.3	-3.5	-2.6

Table 2. Linear regression statistics for CBS-Q//B3, G4MP2, and G4 estimated gas phase $\log K_{\text{hydr,(g)}}$ against Swain-Lupton resonance effect (R) parameters for the two groups ((a) and (b)) of substituted aldehydes and for the combined sets of substituents.

	n	r	p	SE	CV	m	b
Group (a): α -sp ³ carbons and α -saturated/unsaturated heteroatoms							
CBS-Q//B3	21	0.957	$<10^{-10}$	1.45	-0.50	14.8±1.0	-1.06±0.34
G4MP2	21	0.954	$<10^{-10}$	1.42	-0.37	14.0±1.0	-2.11±0.33
G4	21	0.956	$<10^{-10}$	1.42	-0.47	14.3±1.0	-1.25±0.34
Group (b): α -sp/ α -sp ² carbons							
CBS-Q//B3	10	0.977	$<10^{-5}$	0.44	-0.12	14.6±1.1	-3.41±0.14
G4MP2	10	0.975	$<10^{-5}$	0.44	-0.09	13.9±1.1	-4.29±0.14
G4	10	0.973	$<10^{-5}$	0.47	-0.12	14.3±1.2	-3.56±0.15
Groups (a) and (b)							
CBS-Q//B3	31	0.918	$<10^{-12}$	1.67	-0.53	13.4±1.1	-1.83±0.32
G4MP2	31	0.913	$<10^{-12}$	1.63	-0.40	12.7±1.1	-2.82±0.31
G4	31	0.912	$<10^{-12}$	1.67	-0.51	12.9±1.1	-2.01±0.32

Table 3. Linear regression statistics for CBS-Q//B3, G4MP2, and G4 estimated gas phase $\log K_{\text{hydr,(g)}}$ against Swain-Lupton positive charged resonance effect (R^+) parameters for all substituents.

	n	r	p	SE	CV	m	b
CBS-Q//B3	20	0.960	$<10^{-10}$	1.24	-0.29	7.55 ± 0.52	-1.69 ± 0.32
G4MP2	20	0.958	$<10^{-10}$	1.23	-0.24	7.20 ± 0.51	-2.70 ± 0.32
G4	20	0.959	$<10^{-10}$	1.23	-0.28	7.31 ± 0.51	-1.90 ± 0.32

Table 4. Estimated gas phase standard state (298.15 K, 1 atm) bond dissociation enthalpies (BDEs) of the aldehyde C-H bond for various aldehydes with electron withdrawing and electron releasing substituents at the CBS-Q//B3, G4MP2, and G4 levels of theory. Available experimental BDEs ^{56,57} are shown for comparison. Values are in kcal/mol.

substituent	expt.	CBS-Q//B3	G4MP2	G4
NH ₂	n/a ^a	94.5	93.2	93.5
C(CH ₃) ₃	89.7	89.7	86.7	87.7
C≡N	n/a	91.1	91.1	91.4
N(CH ₃) ₂	n/a	95.0	92.5	93.2
F	101.1	101.9	100.3	100.8
H	88.0±0.2	89.1	87.9	88.2
OH	96.6	100.9	99.1	99.6
CH ₃	89.4±0.3	89.0	87.7	88.0
C ₆ H ₅	88.7±2.6	91.5	88.2	89.3
CF ₃	93.3	93.5	90.0	91.1
Si(CH ₃) ₃	n/a	79.5	76.7	77.6
Br	n/a	86.0	84.7	85.2
Cl	n/a	91.7	90.4	90.9
SiCl ₃	n/a	81.6	78.6	79.7
SiF ₃	n/a	81.9	78.7	79.8
SiH ₃	n/a	79.8	78.5	78.9
CBr ₃	n/a	99.1	90.4	91.5
CCl ₃	n/a	93.9	90.7	91.7
C ₆ H ₄ -4-Br	n/a	91.7	87.8	89.1

$\text{C}_6\text{H}_4\text{-4-Cl}$	n/a	91.7	87.8	89.1
$\text{C}_6\text{H}_4\text{-4-F}$	n/a	91.6	87.7	89.0
$\text{C}_6\text{H}_4\text{-4-CH}_3$	n/a	91.5	87.5	88.9
GeH_3	n/a	79.3	78.0	78.4

^a not available.

Table 5. Estimated gas phase standard state (298.15 K, 1 atm) enthalpies ($\Delta_d H^\circ_{(g)}$) and free energies ($\Delta_d G^\circ_{(g)}$) of aldehyde proton acid dissociation for various aldehydes with electron withdrawing and electron releasing substituents at the CBS-Q//B3, G4MP2, and G4 levels of theory. Available experimental values⁵⁸ are shown for comparison. Values are in kcal/mol.

substituent	$\Delta_d H^\circ_{(g)}$			$\Delta_d G^\circ_{(g)}$				
	expt.	CBS-Q//B3	G4MP2	G4	expt.	CBS-Q//B3	G4MP2	G4
C(O)CH ₃	n/a ^a	376.0	376.2	376.0	n/a	368.9	369.0	368.9
C(CH ₃) ₃	387.4±4.1 ⁵⁹	392.1	391.9	392.6	381.0±4.0 ⁵⁹	383.7	383.7	384.4
N(CH ₃) ₂	399.1±4.1 ⁶⁰	392.4	392.1	392.5	392.0±4.0 ⁶⁰	383.8	384.1	384.5
CH=CH ₂	n/a	392.2	391.8	392.3	n/a	384.1	383.4	383.9
F	349.7±3.3 ⁶¹ 352.6±4.6 ⁶²	362.1	361.6	361.2	n/a	353.8	353.5	353.1
H	394.5±0.1 ⁶³	397.2	395.2	395.2	386.6±0.3 ⁶³ 394.0±4.5 ⁶⁴	389.3	387.6	387.6
OH	n/a ^b	379.2	378.8	378.9	n/a ^b	371.4	370.9	371.1
CH ₃	393.1±0.9 ⁶⁵ 391.0±2.1 ⁶⁶ 387.0±8.0 ⁶⁷ <382.0 ⁶⁸	393.3	393.3	393.4	385.4±1.1 ⁶⁵ 383.3±2.0 ⁶⁶ <374.30±0.6 ⁶⁸	384.4	384.3	384.4
C ₆ H ₅	n/a	388.1	387.6	388.3	n/a	380.6	380.1	380.7
C ₆ H ₄ -4-Br	n/a	382.3	382.0	382.6	n/a	374.7	374.3	374.9
C ₆ H ₄ -4-Cl	n/a	383.0	382.8	383.4	n/a	375.4	375.1	375.7
C ₆ H ₄ -4-F	n/a	384.9	384.5	385.0	n/a	377.4	376.9	377.4
C ₆ H ₄ -4-CH ₃	n/a ^c	389.2	388.8	389.4	n/a ^c	382.1	381.6	382.2

^a not available. ^b experimental $\Delta_d H^\circ_{(g)}$ and $\Delta_d G^\circ_{(g)}$ are available for formic acid, but the values are for the more acidic carboxylic acid moiety ($\Delta_d H^\circ_{(g)} \approx 340$ to 346 kcal/mol;⁶⁹⁻⁷² $\Delta_d G^\circ_{(g)} \approx 338$ to 339 kcal/mol⁶⁹⁻⁷³). ^c experimental $\Delta_d H^\circ_{(g)}$ and $\Delta_d G^\circ_{(g)}$ are available for 4-methylbenzaldehyde, but the values are for the more acidic methyl group ($\Delta_d H^\circ_{(g)} = 359.8 \pm 2.4$ kcal/mol;⁷⁴ $\Delta_d G^\circ_{(g)} = 352.6 \pm 2.3$ kcal/mol⁷⁴).

Table 6. Estimated gas phase standard state (298.15 K, 1 atm) enthalpies ($\Delta_d H^\circ_{(g)}$) and free energies ($\Delta_d G^\circ_{(g)}$) of aldehyde proton acid dissociation for various aldehydes with electron withdrawing and electron releasing substituents using training set correlations developed between the Hammett inductive substituent constants (σ_I) and $\Delta_d H^\circ_{(g)} / \Delta_d G^\circ_{(g)}$ calculated at the CBS-Q//B3, G4MP2, and G4 levels of theory. Values are in kcal/mol. Error bars are standard errors derived from the regression analysis.

substituent	$\Delta_d H^\circ_{(g)}$			$\Delta_d G^\circ_{(g)}$		
	CBS-Q//B3	G4MP2	G4	CBS-Q//B3	G4MP2	G4
NO ₂	354.8±4.5	354.7±4.2	354.2±4.4	347.2±4.5	347.2±4.4	346.7±4.5
H	395.4±3.4	394.8±3.2	395.3±3.3	387.2±3.4	386.7±3.3	387.1±3.4
CH ₃	396.0±3.4	395.4±3.2	395.9±3.3	387.8±3.4	387.3±3.3	387.7±3.4
C ₂ H ₅	396.0±3.4	395.4±3.2	395.9±3.3	387.8±3.4	387.3±3.3	387.7±3.4
CH ₂ OH	388.7±3.3	388.2±3.1	388.5±3.2	380.6±3.3	380.2±3.2	380.5±3.3
OH	380.9±3.3	380.5±3.1	380.6±3.2	372.9±3.3	372.6±3.2	372.7±3.3
OCH ₃	377.2±3.4	376.9±3.2	376.9±3.3	369.3±3.4	369.0±3.3	369.0±3.4
OC ₆ H ₅	371.2±3.6	370.9±3.4	370.8±3.5	363.3±3.6	363.1±3.5	363.0±3.6
CO ₂ C ₂ H ₅	377.2±3.4	376.9±3.2	376.9±3.3	369.3±3.4	369.0±3.3	369.0±3.4
Cl	366.9±3.8	366.7±3.6	366.5±3.7	359.1±3.8	359.0±3.7	358.8±3.8
Br	366.9±3.8	366.7±3.6	366.5±3.7	359.1±3.8	359.0±3.7	358.8±3.8
C≡N	360.9±4.1	360.7±3.9	360.3±4.0	353.2±4.1	353.1±4.0	352.8±4.1
CH(CH ₃) ₂	394.8±3.4	394.2±3.2	394.7±3.3	386.6±3.4	386.1±3.3	386.5±3.4
C(CH ₃) ₃	396.0±3.4	395.4±3.2	395.9±3.3	387.8±3.4	387.3±3.3	387.7±3.4
CH ₂ OCH ₃	388.7±3.3	388.2±3.1	388.5±3.2	380.6±3.3	380.2±3.2	380.5±3.3
CH ₂ OCOCH ₃	386.3±3.2	385.9±3.1	386.1±3.2	378.2±3.3	377.9±3.2	378.1±3.2
tosylmethyl	381.5±3.3	381.1±3.1	381.2±3.2	373.5±3.3	373.1±3.2	373.3±3.3

CH ₂ Cl	385.1±3.2	384.7±3.1	384.9±3.2	377.0±3.3	376.7±3.2	376.9±3.2
CH ₂ Br	383.3±3.3	382.9±3.1	383.0±3.2	375.3±3.3	374.9±3.2	375.1±3.3
CH ₂ I	385.1±3.2	384.7±3.1	384.9±3.2	377.0±3.3	376.7±3.2	376.9±3.2
CH(OH) ₂	382.1±3.3	381.7±3.1	381.8±3.2	374.1±3.3	373.7±3.2	373.9±3.3
CH=CH ₂	388.7±3.3	388.2±3.1	388.5±3.2	380.6±3.3	380.2±3.2	380.5±3.3
C(CH ₃)=CH ₂	389.3±3.3	388.8±3.1	389.1±3.2	381.2±3.3	380.8±3.2	381.1±3.3
C≡CH	377.8±3.3	377.5±3.2	377.5±3.3	369.9±3.4	369.6±3.3	369.6±3.3
C ₆ H ₅	388.1±3.2	387.6±3.1	387.9±3.2	380.0±3.3	379.6±3.2	379.9±3.3
COCH ₃	377.2±3.4	376.9±3.2	376.9±3.3	369.3±3.4	369.0±3.3	369.0±3.4
CONH ₂	378.4±3.3	378.1±3.1	378.1±3.2	370.5±3.4	370.2±3.2	370.3±3.3
NH ₂	385.1±3.2	384.7±3.1	384.9±3.2	377.0±3.3	376.7±3.2	376.9±3.2
NHCH ₃	387.5±3.2	387.1±3.1	387.3±3.2	379.4±3.3	379.0±3.2	379.3±3.3
N(CH ₃) ₂	385.1±3.2	384.7±3.1	384.9±3.2	377.0±3.3	376.7±3.2	376.9±3.2
NHCOCH ₃	378.4±3.3	378.1±3.1	378.1±3.2	370.5±3.4	370.2±3.2	370.3±3.3
OCOCH ₃	372.4±3.5	372.1±3.3	372.0±3.4	364.5±3.6	364.3±3.4	364.2±3.5
SCH ₃	377.2±3.4	376.9±3.2	376.9±3.3	369.3±3.4	369.0±3.3	369.0±3.4
SO ₂ CH ₃	359.6±4.2	359.5±3.9	359.1±4.1	352.0±4.2	351.9±4.1	351.6±4.2
SO ₂ CF ₃	352.4±4.7	352.3±4.4	351.8±4.5	344.8±4.7	344.8±4.5	344.3±4.7
F	362.7±4.0	362.5±3.8	362.2±3.9	355.0±4.0	354.9±3.9	354.6±4.0
I	371.2±3.6	370.9±3.4	370.8±3.5	363.3±3.6	363.1±3.5	363.0±3.6

Figure Captions

Figure 1. General scheme for the gas phase hydration of substituted aldehydes.

Figure 2. Correlations between the Swain-Lupton resonance effect parameter (R) and estimated gas phase standard state (298.15 K, 1 atm) equilibrium hydration constants ($\log K_{\text{hydr,(g)}}$) for various substituted aldehydes at the (a) CBS-Q//B3, (b) G4MP2, and (c) G4 levels of theory. Open (group (a); $n=21$) symbols are for sp^3 -hybridized α -carbon substituents and saturated/unsaturated α -heteroatom moieties. Closed (group (b); $n=10$) symbols refer to sp and sp^2 -hybridized α -carbon substituents. Best fit linear regressions for each group are shown as dash-dot-dot (group (a)) and dashed (group (b)) lines. A best fit regression for all datapoints ($n=31$) is shown as a solid line. Identities of the substituents are given in Table 1 and summaries of the statistical analyses are provided in Table 2.

Figure 3. Correlations between the Swain-Lupton positively charged reaction center resonance effect parameter (R^+) and estimated gas phase standard state (298.15 K, 1 atm) equilibrium hydration constants ($\log K_{\text{hydr,(g)}}$) for various substituted aldehydes ($n=20$) at the (a) CBS-Q//B3, (b) G4MP2, and (c) G4 levels of theory. Open (group (a)) symbols are for sp^3 -hybridized α -carbon substituents and saturated/unsaturated α -heteroatom moieties. Closed (group (b)) symbols refer to sp and sp^2 -hybridized α -carbon substituents. A best fit regression for all datapoints is shown as a solid line. Summaries of the statistical analyses are provided in Table 3. Aldehyde substituents in the analysis include the following: NH_2 ; $\text{C}(\text{CH}_3)_3$; $\text{C}\equiv\text{N}$; $\text{N}(\text{CH}_3)_2$; $\text{CH}=\text{CH}_2$; $\text{C}\equiv\text{CH}$; F; H; OH; CH_3 ; NO_2 ; C_6H_5 ; CF_3 ; $\text{Si}(\text{CH}_3)_3$; Br; Cl; SiCl_3 ; SiH_3 ; $\text{C}_6\text{H}_4\text{-4Br}$; and $\text{C}_6\text{H}_4\text{-4Cl}$.

Figure 4. Correlation between the sum of Swain-Lupton resonance effect parameters (a) R and (b) R^+ on carbonyl substituents with experimental aqueous phase equilibrium hydration constants ($\log K_{\text{hydr,(aq)}}$) for various aldehydes, ketones, esters, thioesters, and amides. Experimental data taken from the compilation in ref. [26]. Best fit linear regressions for each plot that include all datapoints are shown as solid lines with the following statistical descriptors: (a) $n=35$, $r=0.975$, $p<10^{-22}$, $SE=1.22$, $CV=-0.29$, $m=14.8\pm0.6$, $b=2.13\pm0.33$; (b) $n=28$, $r=0.972$, $p<10^{-17}$, $SE=1.20$, $CV=-0.28$, $m=8.08\pm0.38$, $b=2.31\pm0.38$.

Figure 1

Figure 2

Figure 3

Figure 4

Supporting Information

**Gas phase hydration, bond dissociation enthalpies, and acidity of aldehydes:
A CBS-Q//B3, G4MP2, and G4 theoretical study of substituent effects**

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Figure S1. Gas phase standard state (298.15 K, 1 atm) lowest energy conformations of the aldehyde hydrates under consideration optimized at the G4 level of theory.

$\text{H(OH)}_2\text{CC}_6\text{H}_5$

$\text{H(OH)}_2\text{CCF}_3$

$\text{H(OH)}_2\text{CSi(CH}_3)_3$

$\text{H(OH)}_2\text{CBr}$

$\text{H(OH)}_2\text{CCl}$

$\text{H(OH)}_2\text{CSiCl}_3$

$\text{H(OH)}_2\text{CSiF}_3$

$\text{H(OH)}_2\text{CSiH}_3$

$\text{H(OH)}_2\text{CCBr}_3$

$\text{H(OH)}_2\text{CCl}_3$

$\text{H(OH)}_2\text{CC}\equiv\text{CF}_3$

$\text{H(OH)}_2\text{CC}\equiv\text{CCH}_3$

$\text{H}(\text{OH})_2\text{CC}(\text{C}\equiv\text{N})_3$

$\text{H}(\text{OH})_2\text{CC}_6\text{H}_4-4-\text{Br}$

$\text{H}(\text{OH})_2\text{CC}_6\text{H}_4-4-\text{Cl}$

$\text{H}(\text{OH})_2\text{CC}_6\text{H}_4-4-\text{F}$

$\text{H}(\text{OH})_2\text{CC}_6\text{H}_4-4-\text{CH}_3$

$\text{H}(\text{OH})_2\text{CPF}_4$

$\text{H}(\text{OH})_2\text{CGeH}_3$

Figure S2. Correlations between the Swain-Lupton resonance effect parameter (R) and estimated gas phase standard state (298.15 K, 1 atm) equilibrium hydration constants ($\log K_{\text{hydr},(g)}$) for various substituted aldehydes ($n=20$) at the (a) CBS-Q//B3, (b) G4MP2, and (c) G4 levels of theory. Open (group (a)) symbols are for sp^3 -hybridized α -carbon substituents and saturated/unsaturated α -heteroatom moieties. Closed (group (b)) symbols refer to sp and sp^2 -hybridized α -carbon substituents. A best fit regression for all datapoints is shown as a solid line with regression-derived statistical descriptors (including standard errors for slope and y-intercept) shown in each plot. Aldehyde substituents in the analysis include the following: NH_2 ; $\text{C}(\text{CH}_3)_3$; $\text{C}\equiv\text{N}$; $\text{N}(\text{CH}_3)_2$; $\text{CH}=\text{CH}_2$; $\text{C}\equiv\text{CH}$; F ; H ; OH ; CH_3 ; NO_2 ; C_6H_5 ; CF_3 ; $\text{Si}(\text{CH}_3)_3$; Br ; Cl ; SiCl_3 ; SiH_3 ; $\text{C}_6\text{H}_4\text{-4Br}$; and $\text{C}_6\text{H}_4\text{-4Cl}$.

Figure S3. Comparison between estimated gas phase standard state (298.15 K, 1 atm) equilibrium hydration constants ($\log K_{\text{hydr},(g)}$) for various substituted aldehydes ($n=108$) obtained via correlation analyses using the Swain-Lupton resonance effect parameters (R) and positively charged reaction center resonance effect parameters (R^+) at the (a) CBS-Q//B3, (b) G4MP2, and (c) G4 levels of theory. A best fit regression is shown as a solid line with regression-derived statistical descriptors (including standard errors for slope and y-intercept) shown in each plot; 1:1 lines are dashed.

Table S1. Estimated gas phase standard state (298.15 K, 1 atm) hydration equilibrium constants ($\log K_{\text{hydr}, (g)}$) for various aldehydes ($n=487$) with electron withdrawing and electron releasing substituents using training set correlations developed between Swain-Lupton resonance effect (R) parameters and $\log K_{\text{hydr}, (g)}$ calculated at the CBS-Q//B3, G4MP2, and G4 levels of theory. Estimated $\log K_{\text{hydr}, (g)}$ presented in the table below are calculated from Swain-Lupton resonance effect (R) parameters given in ref. (1). Group (a) comprises sp^3 -hybridized α -carbon and saturated/unsaturated α -heteroatom substituents. Group (b) comprises sp and sp^2 -hybridized α -carbon substituents.

substituent	group (a)			group (b)			all data		
	CBS-Q//B3	G4MP2	G4	CBS-Q//B3	G4MP2	G4	CBS-Q//B3	G4MP2	G4
BF ₂	2.2	1.0	1.9	n/a	n/a	n/a	1.2	0.1	0.9
Br	-4.3	-5.2	-4.4	n/a	n/a	n/a	-5.0	-5.8	-5.0
GeBr ₃	0.7	-0.4	0.5	n/a	n/a	n/a	-0.2	-1.3	-0.4
SiBr ₃	0.9	-0.3	0.6	n/a	n/a	n/a	-0.1	-1.1	-0.3
Cl	-3.9	-4.8	-4.0	n/a	n/a	n/a	-4.6	-5.4	-4.6
HgCl	-0.8	-1.8	-1.0	n/a	n/a	n/a	-1.6	-2.6	-1.8
SO ₂ Cl	-1.8	-2.8	-2.0	n/a	n/a	n/a	-2.6	-3.5	-2.7
SCl	-0.2	-1.3	-0.4	n/a	n/a	n/a	-1.0	-2.1	-1.2
ICl ₂	0.1	-1.0	-0.1	n/a	n/a	n/a	-0.8	-1.8	-1.0
P(O)Cl ₂	1.9	0.7	1.6	n/a	n/a	n/a	0.9	-0.2	0.7
PCL ₂	0.6	-0.6	0.3	n/a	n/a	n/a	-0.3	-1.4	-0.6
P(S)Cl ₂	1.5	0.3	1.2	n/a	n/a	n/a	0.5	-0.6	0.2
GeCl ₃	1.0	-0.1	0.7	n/a	n/a	n/a	0.1	-1.0	-0.2
SiCl ₃	0.7	-0.4	0.5	n/a	n/a	n/a	-0.2	-1.3	-0.4
F	-6.8	-7.6	-6.8	n/a	n/a	n/a	-7.4	-8.1	-7.4
HgF	-1.4	-2.4	-1.5	n/a	n/a	n/a	-2.2	-3.1	-2.3
SOF	1.3	0.1	1.0	n/a	n/a	n/a	0.4	-0.7	0.1
SO ₂ F	1.8	0.6	1.5	n/a	n/a	n/a	0.8	-0.3	0.5
IF ₂	-0.9	-2.0	-1.1	n/a	n/a	n/a	-1.7	-2.7	-1.9
POF ₂	1.2	0.0	0.9	n/a	n/a	n/a	0.2	-0.9	0.0
PF ₂	1.2	0.0	0.9	n/a	n/a	n/a	0.2	-0.9	0.0
GeF ₃	2.0	0.8	1.7	n/a	n/a	n/a	1.1	-0.1	0.8
SF ₃	1.5	0.3	1.2	n/a	n/a	n/a	0.5	-0.6	0.2
SiF ₃	2.2	1.0	1.9	n/a	n/a	n/a	1.2	0.1	0.9
IF ₄	1.5	0.3	1.2	n/a	n/a	n/a	0.5	-0.6	0.2
PF ₄	2.8	1.5	2.5	n/a	n/a	n/a	1.8	0.6	1.5
SF ₅	0.7	-0.4	0.5	n/a	n/a	n/a	-0.2	-1.3	-0.4
I	-4.6	-5.5	-4.7	n/a	n/a	n/a	-5.3	-6.1	-5.3
IO	0.0	-1.1	-0.3	n/a	n/a	n/a	-0.9	-1.9	-1.1
IO ₂	1.5	0.3	1.2	n/a	n/a	n/a	0.5	-0.6	0.2
NO	5.2	3.8	4.8	n/a	n/a	n/a	4.0	2.7	3.6
NO ₂	0.9	-0.3	0.6	n/a	n/a	n/a	-0.1	-1.1	-0.3

ONO ₂	2.2	1.0	1.9	n/a	n/a	n/a	1.2	0.1	0.9
N ₃	-7.0	-7.7	-7.0	n/a	n/a	n/a	-7.5	-8.2	-7.5
H	-1.1	-2.1	-1.3	n/a	n/a	n/a	-1.9	-2.9	-2.1
NHNO ₂	-7.3	-8.0	-7.3	n/a	n/a	n/a	-7.8	-8.5	-7.8
OH	-11.4	-11.9	-11.3	n/a	n/a	n/a	-11.7	-12.2	-11.6
S(O)OH	-2.2	-3.2	-2.4	n/a	n/a	n/a	-3.0	-3.9	-3.1
SH	-3.3	-4.2	-3.4	n/a	n/a	n/a	-4.0	-4.9	-4.1
B(OH) ₂	1.2	0.0	0.9	n/a	n/a	n/a	0.2	-0.9	0.0
NH ₂	-12.0	-12.5	-11.8	n/a	n/a	n/a	-12.3	-12.7	-12.1
NHOH	-7.7	-8.4	-7.7	n/a	n/a	n/a	-8.2	-8.9	-8.2
SO ₂ NH ₂	0.6	-0.6	0.3	n/a	n/a	n/a	-0.3	-1.4	-0.6
PO(OH) ₂	0.1	-1.0	-0.1	n/a	n/a	n/a	-0.8	-1.8	-1.0
PH ₂	-1.7	-2.7	-1.8	n/a	n/a	n/a	-2.4	-3.4	-2.6
GeH ₃	-1.4	-2.4	-1.5	n/a	n/a	n/a	-2.2	-3.1	-2.3
NHNH ₂	-12.5	-12.9	-12.3	n/a	n/a	n/a	-12.7	-13.1	-12.5
SiH ₃	-0.5	-1.5	-0.7	n/a	n/a	n/a	-1.3	-2.3	-1.5
CBr ₃	-0.9	-2.0	-1.1	n/a	n/a	n/a	-1.7	-2.7	-1.9
CClF ₂	-0.2	-1.3	-0.4	n/a	n/a	n/a	-1.0	-2.1	-1.2
5-chloro-1-tetrazolyl	-0.6	-1.7	-0.8	n/a	n/a	n/a	-1.5	-2.5	-1.7
C(O)Cl	n/a	n/a	n/a	-1.2	-2.2	-1.4	0.2	-0.9	0.0
N=CCl ₂	-3.0	-3.9	-3.1	n/a	n/a	n/a	-3.7	-4.6	-3.8
CCl ₃	0.3	-0.8	0.0	n/a	n/a	n/a	-0.6	-1.7	-0.8
OCcl ₃	-2.7	-3.6	-2.8	n/a	n/a	n/a	-3.4	-4.3	-3.6
C(O)F	n/a	n/a	n/a	-0.2	-1.2	-0.4	1.2	0.1	0.9
OCF ₂ O	-1.1	-2.1	-1.3	n/a	n/a	n/a	-1.9	-2.9	-2.1
CF ₃	1.3	0.1	1.0	n/a	n/a	n/a	0.4	-0.7	0.1
HgCF ₃	-0.6	-1.7	-0.8	n/a	n/a	n/a	-1.5	-2.5	-1.7
HgSCF ₃	-0.5	-1.5	-0.7	n/a	n/a	n/a	-1.3	-2.3	-1.5
I=NSO ₂ CF ₃	1.2	0.0	0.9	n/a	n/a	n/a	0.2	-0.9	0.0
N=NCF ₃	1.6	0.4	1.3	n/a	n/a	n/a	0.6	-0.5	0.4
OCF ₃	-1.7	-2.7	-1.8	n/a	n/a	n/a	-2.4	-3.4	-2.6
SOCF ₃	0.6	-0.6	0.3	n/a	n/a	n/a	-0.3	-1.4	-0.6
SeOCF ₃	0.0	-1.1	-0.3	n/a	n/a	n/a	-0.9	-1.9	-1.1
SO ₂ CF ₃	2.2	1.0	1.9	n/a	n/a	n/a	1.2	0.1	0.9
SeO ₂ CF ₃	2.5	1.3	2.2	n/a	n/a	n/a	1.5	0.3	1.2
OSO ₂ CF ₃	-1.5	-2.5	-1.7	n/a	n/a	n/a	-2.3	-3.3	-2.5
SCF ₃	1.0	-0.1	0.7	n/a	n/a	n/a	0.1	-1.0	-0.2
SeCF ₃	-0.8	-1.8	-1.0	n/a	n/a	n/a	-1.6	-2.6	-1.8
HgCN	0.1	-1.0	-0.1	n/a	n/a	n/a	-0.8	-1.8	-1.0
CN	n/a	n/a	n/a	-1.2	-2.2	-1.4	0.2	-0.9	0.0
NC	-0.8	-1.8	-1.0	n/a	n/a	n/a	-1.6	-2.6	-1.8

CN (BBr ₃)	-3.4	-4.3	-3.5	n/a	n/a	n/a	-4.1	-5.0	-4.2
CN (BCl ₃)	-1.8	-2.8	-2.0	n/a	n/a	n/a	-2.6	-3.5	-2.7
CN (BF ₃)	-1.8	-2.8	-2.0	n/a	n/a	n/a	-2.6	-3.5	-2.7
N=C=O	-2.8	-3.8	-3.0	n/a	n/a	n/a	-3.6	-4.5	-3.7
OCN	-3.3	-4.2	-3.4	n/a	n/a	n/a	-4.0	-4.9	-4.1
SO ₂ CN	3.2	2.0	2.9	n/a	n/a	n/a	2.2	1.0	1.9
N=C=S	-3.0	-3.9	-3.1	n/a	n/a	n/a	-3.7	-4.6	-3.8
SCN	-0.6	-1.7	-0.8	n/a	n/a	n/a	-1.5	-2.5	-1.7
SeCN	0.3	-0.8	0.0	n/a	n/a	n/a	-0.6	-1.7	-0.8
N=N-C≡N	5.9	4.5	5.5	n/a	n/a	n/a	4.7	3.4	4.3
N(O)=NCN	1.8	0.6	1.5	n/a	n/a	n/a	0.8	-0.3	0.5
C(NO ₂) ₃	1.5	0.3	1.2	n/a	n/a	n/a	0.5	-0.6	0.2
5-azido-1-tetrazolyl	-0.9	-2.0	-1.1	n/a	n/a	n/a	-1.7	-2.7	-1.9
CHBr ₂	-0.9	-2.0	-1.1	n/a	n/a	n/a	-1.7	-2.7	-1.9
CHCl ₂	-0.9	-2.0	-1.1	n/a	n/a	n/a	-1.7	-2.7	-1.9
OCHCl ₂	-3.6	-4.5	-3.7	n/a	n/a	n/a	-4.3	-5.1	-4.4
CHF ₂	-0.6	-1.7	-0.8	n/a	n/a	n/a	-1.5	-2.5	-1.7
OCHF ₂	-3.9	-4.8	-4.0	n/a	n/a	n/a	-4.6	-5.4	-4.6
SOCHF ₂	0.0	-1.1	-0.3	n/a	n/a	n/a	-0.9	-1.9	-1.1
SO ₂ CHF ₂	1.8	0.6	1.5	n/a	n/a	n/a	0.8	-0.3	0.5
SCHF ₂	-0.3	-1.4	-0.5	n/a	n/a	n/a	-1.2	-2.2	-1.4
S(O) (=NH) CF ₃	1.9	0.7	1.6	n/a	n/a	n/a	0.9	-0.2	0.7
NHSO ₂ CF ₃	-1.9	-2.9	-2.1	n/a	n/a	n/a	-2.7	-3.7	-2.9
CHI ₂	-1.2	-2.2	-1.4	n/a	n/a	n/a	-2.0	-3.0	-2.2
NHCN	-4.3	-5.2	-4.4	n/a	n/a	n/a	-5.0	-5.8	-5.0
1-(1H)-tetrazolyl	-1.4	-2.4	-1.5	n/a	n/a	n/a	-2.2	-3.1	-2.3
5-(1H)-tetrazolyl	-2.4	-3.4	-2.5	n/a	n/a	n/a	-3.2	-4.1	-3.3
5-hydroxy-1-tetrazolyl	-2.2	-3.2	-2.4	n/a	n/a	n/a	-3.0	-3.9	-3.1
5-mercapto-1-tetrazolyl	-1.2	-2.2	-1.4	n/a	n/a	n/a	-2.0	-3.0	-2.2
-3.4	-4.3	-3.5	n/a	n/a	n/a	-4.1	-5.0	-4.2
C(O)H	n/a	n/a	n/a	-2.1	-3.0	-2.3	-0.6	-1.7	-0.8
C(O)OH	n/a	n/a	n/a	-1.8	-2.8	-2.0	-0.3	-1.4	-0.6
CH ₂ Br	-1.1	-2.1	-1.3	n/a	n/a	n/a	-1.9	-2.9	-2.1
CH ₂ Cl	-1.2	-2.2	-1.4	n/a	n/a	n/a	-2.0	-3.0	-2.2
OCH ₂ Cl	-4.8	-5.6	-4.8	n/a	n/a	n/a	-5.4	-6.2	-5.5
CH ₂ F	-1.7	-2.7	-1.8	n/a	n/a	n/a	-2.4	-3.4	-2.6
OCH ₂ F	-5.1	-5.9	-5.1	n/a	n/a	n/a	-5.7	-6.5	-5.7
SCH ₂ F	-1.8	-2.8	-2.0	n/a	n/a	n/a	-2.6	-3.5	-2.7

CH ₂ I	-1.2	-2.2	-1.4	n/a	n/a	n/a	-2.0	-3.0	-2.2
NHCHO	-5.2	-6.0	-5.3	n/a	n/a	n/a	-5.8	-6.6	-5.9
C (O) NH ₂	n/a	n/a	n/a	-2.0	-2.9	-2.1	-0.5	-1.5	-0.7
C (S) NH ₂	n/a	n/a	n/a	-2.5	-3.5	-2.7	-1.0	-2.1	-1.2
CH=NOH-t	n/a	n/a	n/a	-6.0	-6.8	-6.1	-4.4	-5.3	-4.5
N (O) =NCONH ₂	0.0	-1.1	-0.3	n/a	n/a	n/a	-0.9	-1.9	-1.1
Me	-3.7	-4.6	-3.8	n/a	n/a	n/a	-4.4	-5.3	-4.5
CH ₂ SO ₂ R	-0.9	-2.0	-1.1	n/a	n/a	n/a	-1.7	-2.7	-1.9
SiMeCl ₂	0.4	-0.7	0.2	n/a	n/a	n/a	-0.5	-1.5	-0.7
SiMeF ₂	-2.4	-3.4	-2.5	n/a	n/a	n/a	-3.2	-4.1	-3.3
HgMe	-7.7	-8.4	-7.7	n/a	n/a	n/a	-8.2	-8.9	-8.2
NHCH ₂ SO ₃	-11.3	-11.8	-11.1	n/a	n/a	n/a	-11.6	-12.1	-11.4
NHCONH ₂	-5.9	-6.7	-6.0	n/a	n/a	n/a	-6.5	-7.3	-6.5
N (Me) NO ₂	1.6	0.4	1.3	n/a	n/a	n/a	0.6	-0.5	0.4
NHCSNH ₂	-2.5	-3.5	-2.7	n/a	n/a	n/a	-3.3	-4.2	-3.4
OMe	-9.3	-9.9	-9.3	n/a	n/a	n/a	-9.8	-10.3	-9.7
CH ₂ OH	-1.5	-2.5	-1.7	n/a	n/a	n/a	-2.3	-3.3	-2.5
SOMe	-1.5	-2.5	-1.7	n/a	n/a	n/a	-2.3	-3.3	-2.5
S (OMe)	-2.1	-3.1	-2.3	n/a	n/a	n/a	-2.9	-3.8	-3.0
OS (=O) CH ₃	-0.8	-1.8	-1.0	n/a	n/a	n/a	-1.6	-2.6	-1.8
S (O) OMe	0.0	-1.1	-0.3	n/a	n/a	n/a	-0.9	-1.9	-1.1
SO ₂ Me	1.8	0.6	1.5	n/a	n/a	n/a	0.8	-0.3	0.5
SSO ₂ Me	1.3	0.1	1.0	n/a	n/a	n/a	0.4	-0.7	0.1
OSO ₂ Me	-1.7	-2.7	-1.8	n/a	n/a	n/a	-2.4	-3.4	-2.6
SMe	-4.5	-5.3	-4.5	n/a	n/a	n/a	-5.1	-5.9	-5.2
SSMe	-3.1	-4.1	-3.3	n/a	n/a	n/a	-3.9	-4.7	-4.0
SeMe	-3.4	-4.3	-3.5	n/a	n/a	n/a	-4.1	-5.0	-4.2
NHMe	-11.9	-12.3	-11.7	n/a	n/a	n/a	-12.1	-12.6	-12.0
CH ₂ NH ₂	-3.3	-4.2	-3.4	n/a	n/a	n/a	-4.0	-4.9	-4.1
NHSO ₂ Me	-4.8	-5.6	-4.8	n/a	n/a	n/a	-5.4	-6.2	-5.5
N (COF) ₂	-1.1	-2.1	-1.3	n/a	n/a	n/a	-1.9	-2.9	-2.1
HgOCOCF ₃	-0.5	-1.5	-0.7	n/a	n/a	n/a	-1.3	-2.3	-1.5
C (O) CF ₃	n/a	n/a	n/a	0.4	-0.7	0.2	1.8	0.6	1.5
SCOCF ₃	-1.4	-2.4	-1.5	n/a	n/a	n/a	-2.2	-3.1	-2.3
OCOCF ₃	-2.8	-3.8	-3.0	n/a	n/a	n/a	-3.6	-4.5	-3.7
N (CF ₃) C=O (F)	-0.9	-2.0	-1.1	n/a	n/a	n/a	-1.7	-2.7	-1.9
CF ₂ CF ₃	0.1	-1.0	-0.1	n/a	n/a	n/a	-0.8	-1.8	-1.0
OCF ₂ CF ₃	-5.1	-5.9	-5.1	n/a	n/a	n/a	-5.7	-6.5	-5.7
SO ₂ CF ₂ CF ₃	2.9	1.7	2.6	n/a	n/a	n/a	1.9	0.7	1.6
SCF ₂ CF ₃	-0.2	-1.3	-0.4	n/a	n/a	n/a	-1.0	-2.1	-1.2
N (CF ₃) ₂	1.6	0.4	1.3	n/a	n/a	n/a	0.6	-0.5	0.4

$S(CF_3)=NSO_2CF_3$	2.0	0.8	1.7	n/a	n/a	n/a	1.1	-0.1	0.8
$SO(CF_3)=NSO_2CF_3$	3.5	2.2	3.2	n/a	n/a	n/a	2.5	1.3	2.1
$N(SO_2CF_3)_2$	3.8	2.5	3.5	n/a	n/a	n/a	2.7	1.5	2.4
$P(CF_3)_2$	1.0	-0.1	0.7	n/a	n/a	n/a	0.1	-1.0	-0.2
$P(CN)_2$	1.2	0.0	0.9	n/a	n/a	n/a	0.2	-0.9	0.0
$C\equiv CH$	n/a	n/a	n/a	-3.3	-4.2	-3.4	-1.7	-2.7	-1.9
OCF_2CHFC1	-2.5	-3.5	-2.7	n/a	n/a	n/a	-3.3	-4.2	-3.4
$NHCOCF_3$	-4.9	-5.7	-5.0	n/a	n/a	n/a	-5.5	-6.3	-5.6
$CH=NSO_2CF_3$	n/a	n/a	n/a	2.0	0.8	1.7	3.3	2.0	3.0
OCF_2CHF_2	-3.0	-3.9	-3.1	n/a	n/a	n/a	-3.7	-4.6	-3.8
SCF_2CHF_2	0.7	-0.4	0.5	n/a	n/a	n/a	-0.2	-1.3	-0.4
-0.5	-1.5	-0.7	n/a	n/a	n/a	-1.3	-2.3	-1.5
$SC\equiv CH$	-2.7	-3.6	-2.8	n/a	n/a	n/a	-3.4	-4.3	-3.6
$SCH=CHCl$	-2.5	-3.5	-2.7	n/a	n/a	n/a	-3.3	-4.2	-3.4
$SeCH=CHCl$	-1.7	-2.7	-1.8	n/a	n/a	n/a	-2.4	-3.4	-2.6
CH_2CF_3	-1.9	-2.9	-2.1	n/a	n/a	n/a	-2.7	-3.7	-2.9
CH_2SOCF_3	-1.5	-2.5	-1.7	n/a	n/a	n/a	-2.3	-3.3	-2.5
$CH_2SO_2CF_3$	-0.8	-1.8	-1.0	n/a	n/a	n/a	-1.6	-2.6	-1.8
CH_2SCF_3	-0.8	-1.8	-1.0	n/a	n/a	n/a	-1.6	-2.6	-1.8
CH_2CN	-0.9	-2.0	-1.1	n/a	n/a	n/a	-1.7	-2.7	-1.9
$CH=CHNO_2-t$	n/a	n/a	n/a	-4.7	-5.5	-4.8	-3.2	-4.1	-3.3
CH_2SCN	-1.1	-2.1	-1.3	n/a	n/a	n/a	-1.9	-2.9	-2.1
$CH=CH_2$	n/a	n/a	n/a	-5.9	-6.6	-6.0	-4.3	-5.1	-4.4
$NHCOCH_2Cl$	-5.5	-6.3	-5.5	n/a	n/a	n/a	-6.1	-6.9	-6.1
$N(Me)SO_2CF_3$	-1.4	-2.4	-1.5	n/a	n/a	n/a	-2.2	-3.1	-2.3
$HgOCOCH_3$	-0.9	-2.0	-1.1	n/a	n/a	n/a	-1.7	-2.7	-1.9
$C(Me)(NO_2)_2$	0.6	-0.6	0.3	n/a	n/a	n/a	-0.3	-1.4	-0.6
oxiranyl	-1.9	-2.9	-2.1	n/a	n/a	n/a	-2.7	-3.7	-2.9
$OCH=CH_2$	-7.4	-8.1	-7.4	n/a	n/a	n/a	-7.9	-8.6	-7.9
$C(O)Me$	n/a	n/a	n/a	-0.9	-1.9	-1.1	0.5	-0.6	0.2
$SCOMe$	0.0	-1.1	-0.3	n/a	n/a	n/a	-0.9	-1.9	-1.1
$OCOMe$	-2.7	-3.6	-2.8	n/a	n/a	n/a	-3.4	-4.3	-3.6
$C(O)OMe$	n/a	n/a	n/a	-1.8	-2.8	-2.0	-0.3	-1.4	-0.6
2-thiacyclopropyl	-2.1	-3.1	-2.3	n/a	n/a	n/a	-2.9	-3.8	-3.0
$SCH=CH_2$	-2.4	-3.4	-2.5	n/a	n/a	n/a	-3.2	-4.1	-3.3
$SeCH=CH_2$	-2.2	-3.2	-2.4	n/a	n/a	n/a	-3.0	-3.9	-3.1
1-aziridinyl	-4.8	-5.6	-4.8	n/a	n/a	n/a	-5.4	-6.2	-5.5
2-aziridinyl	-2.4	-3.4	-2.5	n/a	n/a	n/a	-3.2	-4.1	-3.3

N-methyl-3-oxaziridiny1	-0.8	-1.8	-1.0	n/a	n/a	n/a	-1.6	-2.6	-1.8
NHCOOMe	-4.6	-5.5	-4.7	n/a	n/a	n/a	-5.3	-6.1	-5.3
NHCOMe	-5.6	-6.4	-5.7	n/a	n/a	n/a	-6.2	-7.0	-6.3
CONHMe	-1.2	-2.2	-1.4	n/a	n/a	n/a	-2.0	-3.0	-2.2
CH=NOMe	n/a	n/a	n/a	-2.0	-2.9	-2.1	-0.5	-1.5	-0.7
CH ₂ CONH ₂	-1.2	-2.2	-1.4	n/a	n/a	n/a	-2.0	-3.0	-2.2
NHCSMe	-3.7	-4.6	-3.8	n/a	n/a	n/a	-4.4	-5.3	-4.5
CSNHMe	-0.3	-1.4	-0.5	n/a	n/a	n/a	-1.2	-2.2	-1.4
CH=NNHCSNH ₂	n/a	n/a	n/a	-4.3	-5.1	-4.4	-2.7	-3.7	-2.9
Et	-3.3	-4.2	-3.4	n/a	n/a	n/a	-4.0	-4.9	-4.1
CH=NNHCONHNNH ₂	n/a	n/a	n/a	-4.9	-5.7	-5.0	-3.3	-4.2	-3.4
OCH ₂ CH ₃	-8.5	-9.1	-8.4	n/a	n/a	n/a	-8.9	-9.5	-8.8
CH (OH) Me	-4.5	-5.3	-4.5	n/a	n/a	n/a	-5.1	-5.9	-5.2
CH ₂ OMe	-2.8	-3.8	-3.0	n/a	n/a	n/a	-3.6	-4.5	-3.7
SO ₂ Et	1.6	0.4	1.3	n/a	n/a	n/a	0.6	-0.5	0.4
SEt	-4.5	-5.3	-4.5	n/a	n/a	n/a	-5.1	-5.9	-5.2
P (Cl) NMe ₂	2.6	1.4	2.3	n/a	n/a	n/a	1.6	0.5	1.3
SiClMe ₂	-0.3	-1.4	-0.5	n/a	n/a	n/a	-1.2	-2.2	-1.4
SiFMe ₂	-0.5	-1.5	-0.7	n/a	n/a	n/a	-1.3	-2.3	-1.5
NHEt	-9.5	-10.1	-9.4	n/a	n/a	n/a	-9.9	-10.5	-9.8
N (Me) ₂	-15.6	-15.8	-15.3	n/a	n/a	n/a	-15.7	-15.9	-15.4
N (Me) SO ₂ Me	-0.6	-1.7	-0.8	n/a	n/a	n/a	-1.5	-2.5	-1.7
SO ₂ NMe ₂	2.0	0.8	1.7	n/a	n/a	n/a	1.1	-0.1	0.8
N (SO ₂ Me) ₂	-0.5	-1.5	-0.7	n/a	n/a	n/a	-1.3	-2.3	-1.5
SN (Me) ₂	-1.9	-2.9	-2.1	n/a	n/a	n/a	-2.7	-3.7	-2.9
N=NNMe ₂	-1.2	-2.2	-1.4	n/a	n/a	n/a	-2.0	-3.0	-2.2
P (O) Me ₂	0.4	-0.7	0.2	n/a	n/a	n/a	-0.5	-1.5	-0.7
PO (OMe) ₂	1.3	0.1	1.0	n/a	n/a	n/a	0.4	-0.7	0.1
PMe ₂	-0.9	-2.0	-1.1	n/a	n/a	n/a	-1.7	-2.7	-1.9
SiH (Me) ₂	-0.9	-2.0	-1.1	n/a	n/a	n/a	-1.7	-2.7	-1.9
1- (1, 7 (BH) ₁₀ -C ₂ H)	0.4	-0.7	0.2	n/a	n/a	n/a	-0.5	-1.5	-0.7
2- (1, 7 (BH) ₁₀ -C ₂ H)	-1.2	-2.2	-1.4	n/a	n/a	n/a	-2.0	-3.0	-2.2
4- (1, 7 (BH) ₁₀ -C ₂ H)	-0.8	-1.8	-1.0	n/a	n/a	n/a	-1.6	-2.6	-1.8
1- (1, 2 (BH) ₁₀ -C ₂ H)	-2.1	-3.1	-2.3	n/a	n/a	n/a	-2.9	-3.8	-3.0
3- (1, 2 (BH) ₁₀ -C ₂ H)	-1.5	-2.5	-1.7	n/a	n/a	n/a	-2.3	-3.3	-2.5
C≡CCF ₃	n/a	n/a	n/a	-1.4	-2.3	-1.6	0.1	-1.0	-0.2
CF=CF CF ₃ -t	n/a	n/a	n/a	-2.0	-2.9	-2.1	-0.5	-1.5	-0.7
N=C (CF ₃) ₂	-2.4	-3.4	-2.5	n/a	n/a	n/a	-3.2	-4.1	-3.3
CF ₂ CF ₂ CF ₃	-0.2	-1.3	-0.4	n/a	n/a	n/a	-1.0	-2.1	-1.2
CF (CF ₃) ₂	2.2	1.0	1.9	n/a	n/a	n/a	1.2	0.1	0.9
SO ₂ CF ₂ CF ₂ CF ₃	3.1	1.8	2.7	n/a	n/a	n/a	2.0	0.9	1.7

SO ₂ CF(CF ₃) ₂	3.4	2.1	3.0	n/a	n/a	n/a	2.3	1.1	2.0
SCF ₂ CF ₂ CF ₃	-0.3	-1.4	-0.5	n/a	n/a	n/a	-1.2	-2.2	-1.4
SCF(CF ₃) ₂	-0.6	-1.7	-0.8	n/a	n/a	n/a	-1.5	-2.5	-1.7
TeCF ₂ CF ₂ CF ₃	-0.6	-1.7	-0.8	n/a	n/a	n/a	-1.5	-2.5	-1.7
C(OH)(CF ₃) ₂	-0.9	-2.0	-1.1	n/a	n/a	n/a	-1.7	-2.7	-1.9
CH(SCF ₃) ₂	-0.9	-2.0	-1.1	n/a	n/a	n/a	-1.7	-2.7	-1.9
CH(CN) ₂	-1.1	-2.1	-1.3	n/a	n/a	n/a	-1.9	-2.9	-2.1
CH=CHCF ₃ -c	n/a	n/a	n/a	-3.3	-4.2	-3.4	-1.7	-2.7	-1.9
CH=CHCF ₃ -t	n/a	n/a	n/a	-3.0	-3.9	-3.1	-1.5	-2.5	-1.7
CH=CHSO ₂ CF ₃	n/a	n/a	n/a	1.4	0.3	1.2	2.7	1.5	2.4
CH=CHCN	n/a	n/a	n/a	-5.0	-5.8	-5.1	-3.4	-4.3	-3.6
C≡CMe	n/a	n/a	n/a	-7.2	-7.9	-7.3	-5.5	-6.3	-5.6
N(Me)COCF ₃	-1.4	-2.4	-1.5	n/a	n/a	n/a	-2.2	-3.1	-2.3
CH=CHCHO	n/a	n/a	n/a	-5.8	-6.5	-5.8	-4.1	-5.0	-4.2
cyclopropyl	-4.5	-5.3	-4.5	n/a	n/a	n/a	-5.1	-5.9	-5.2
C(Me)=CH ₂	n/a	n/a	n/a	-4.6	-5.4	-4.7	-3.0	-3.9	-3.1
CH=CHMe-t	n/a	n/a	n/a	-6.0	-6.8	-6.1	-4.4	-5.3	-4.5
CH ₂ CH=CH ₂	-2.2	-3.2	-2.4	n/a	n/a	n/a	-3.0	-3.9	-3.1
C(Et)(NO ₂) ₂	0.9	-0.3	0.6	n/a	n/a	n/a	-0.1	-1.1	-0.3
OCH ₂ CH=CH ₂	-8.5	-9.1	-8.4	n/a	n/a	n/a	-8.9	-9.5	-8.8
C(O)Et	n/a	n/a	n/a	-1.4	-2.3	-1.6	0.1	-1.0	-0.2
C(O)OEt	n/a	n/a	n/a	-1.8	-2.8	-2.0	-0.3	-1.4	-0.6
CH ₂ OCOME	-1.4	-2.4	-1.5	n/a	n/a	n/a	-2.2	-3.1	-2.3
CH ₂ CH ₂ COOH	-2.4	-3.4	-2.5	n/a	n/a	n/a	-3.2	-4.1	-3.3
SCH ₂ CH=CH ₂	-2.7	-3.6	-2.8	n/a	n/a	n/a	-3.4	-4.3	-3.6
SeCH ₂ CH=CH ₂	-3.1	-4.1	-3.3	n/a	n/a	n/a	-3.9	-4.7	-4.0
N(Me)COMe	-2.2	-3.2	-2.4	n/a	n/a	n/a	-3.0	-3.9	-3.1
CH ₂ NHCOMe	-3.6	-4.5	-3.7	n/a	n/a	n/a	-4.3	-5.1	-4.4
NHCOOEt	-6.7	-7.4	-6.7	n/a	n/a	n/a	-7.2	-7.9	-7.2
C(NO ₂)Me ₂	-0.9	-2.0	-1.1	n/a	n/a	n/a	-1.7	-2.7	-1.9
isopropyl	-3.9	-4.8	-4.0	n/a	n/a	n/a	-4.6	-5.4	-4.6
CH ₂ CH ₂ CH ₃	-3.1	-4.1	-3.3	n/a	n/a	n/a	-3.9	-4.7	-4.0
NHCONHEt	-7.7	-8.4	-7.7	n/a	n/a	n/a	-8.2	-8.9	-8.2
NHCSNHEt	-5.9	-6.7	-6.0	n/a	n/a	n/a	-6.5	-7.3	-6.5
OCHMe ₂	-12.8	-13.2	-12.5	n/a	n/a	n/a	-13.0	-13.4	-12.8
OCH ₂ CH ₂ CH ₃	-8.6	-9.2	-8.5	n/a	n/a	n/a	-9.1	-9.7	-9.0
CH ₂ CH(OH)Me	-2.7	-3.6	-2.8	n/a	n/a	n/a	-3.4	-4.3	-3.6
C(OOH)Me ₂	-5.6	-6.4	-5.7	n/a	n/a	n/a	-6.2	-7.0	-6.3
SCHMe ₂	-4.5	-5.3	-4.5	n/a	n/a	n/a	-5.1	-5.9	-5.2
CH ₂ NMe ₂	-1.4	-2.4	-1.5	n/a	n/a	n/a	-2.2	-3.1	-2.3
GeMe ₃	-1.5	-2.5	-1.7	n/a	n/a	n/a	-2.3	-3.3	-2.5

Si (Me) ₂ OMe	-2.7	-3.6	-2.8	n/a	n/a	n/a	-3.4	-4.3	-3.6
OSiMe ₃	-9.6	-10.2	-9.5	n/a	n/a	n/a	-10.0	-10.6	-9.9
SiMe (OMe) ₂	-0.3	-1.4	-0.5	n/a	n/a	n/a	-1.2	-2.2	-1.4
Si (OMe) ₃	-0.6	-1.7	-0.8	n/a	n/a	n/a	-1.5	-2.5	-1.7
SiMe ₃	-2.2	-3.2	-2.4	n/a	n/a	n/a	-3.0	-3.9	-3.1
SnMe ₃	-1.5	-2.5	-1.7	n/a	n/a	n/a	-2.3	-3.3	-2.5
1- (1, 2) - (BH) ₁₀ -C ₂ Me	2.2	1.0	1.9	n/a	n/a	n/a	1.2	0.1	0.9
CH ₂ -1- (1, 7- (BH) ₁₀ -C ₂ H)	-1.4	-2.4	-1.5	n/a	n/a	n/a	-2.2	-3.1	-2.3
CH ₂ -1- (1, 2- (BH) ₁₀ -C ₂ H)	-1.4	-2.4	-1.5	n/a	n/a	n/a	-2.2	-3.1	-2.3
1- (1, 2- (BH) ₁₀ -C ₃ H ₃ HgCH ₃)	-0.6	-1.7	-0.8	n/a	n/a	n/a	-1.5	-2.5	-1.7
2- (hydroxymethyl) carboran-1-yl	1.2	0.0	0.9	n/a	n/a	n/a	0.2	-0.9	0.0
I (OCOCF ₃) ₂	1.3	0.1	1.0	n/a	n/a	n/a	0.4	-0.7	0.1
cyclo-C ₄ F ₇	0.1	-1.0	-0.1	n/a	n/a	n/a	-0.8	-1.8	-1.0
C (O) CF ₂ CF ₂ CF ₃	n/a	n/a	n/a	0.1	-1.0	-0.1	1.5	0.3	1.2
C (CF ₃) ₃	-0.8	-1.8	-1.0	n/a	n/a	n/a	-1.6	-2.6	-1.8
(CF ₂) ₃ CF ₃	0.1	-1.0	-0.1	n/a	n/a	n/a	-0.8	-1.8	-1.0
SO ₂ C (CF ₃) ₃	3.2	2.0	2.9	n/a	n/a	n/a	2.2	1.0	1.9
SC (CF ₃) ₃	0.6	-0.6	0.3	n/a	n/a	n/a	-0.3	-1.4	-0.6
C (SCF ₃) ₃	-0.5	-1.5	-0.7	n/a	n/a	n/a	-1.3	-2.3	-1.5
SeC (CF ₃) ₃	0.1	-1.0	-0.1	n/a	n/a	n/a	-0.8	-1.8	-1.0
C (CN) ₃	-0.5	-1.5	-0.7	n/a	n/a	n/a	-1.3	-2.3	-1.5
cyclo-1- (OH) C ₄ F ₆	-0.9	-2.0	-1.1	n/a	n/a	n/a	-1.7	-2.7	-1.9
CH=C (CN) ₂	n/a	n/a	n/a	0.5	-0.5	0.3	1.9	0.7	1.6
2- (5-bromofuryl)	n/a	n/a	n/a	-6.8	-7.5	-6.8	-5.1	-5.9	-5.2
-2.4	-3.4	-2.5	n/a	n/a	n/a	-3.2	-4.1	-3.3
3-chloro-1-pyrroline-2,5-dione	-1.2	-2.2	-1.4	n/a	n/a	n/a	-2.0	-3.0	-2.2
3-pyridazinyl	n/a	n/a	n/a	0.5	-0.5	0.3	1.9	0.7	1.6
C (Me) (CN) ₂	-1.4	-2.4	-1.5	n/a	n/a	n/a	-2.2	-3.1	-2.3
4-pyrimidinyl	n/a	n/a	n/a	3.2	1.9	2.9	4.4	3.1	4.0
2-pyrimidinyl	n/a	n/a	n/a	2.4	1.3	2.2	3.7	2.4	3.4
5-pyrimidinyl	n/a	n/a	n/a	-1.4	-2.3	-1.6	0.1	-1.0	-0.2
2-furyl	n/a	n/a	n/a	-4.6	-5.4	-4.7	-3.0	-3.9	-3.1
2-thienyl	n/a	n/a	n/a	-4.6	-5.4	-4.7	-3.0	-3.9	-3.1
3-thienyl	n/a	n/a	n/a	-4.9	-5.7	-5.0	-3.3	-4.2	-3.4
2-selenienyl	n/a	n/a	n/a	-4.3	-5.1	-4.4	-2.7	-3.7	-2.9
2-tellurienyl	n/a	n/a	n/a	-4.4	-5.3	-4.6	-2.9	-3.8	-3.0
1-pyrryl	n/a	n/a	n/a	-5.3	-6.1	-5.4	-3.7	-4.6	-3.8
1-pyrroline-2,5-dione	n/a	n/a	n/a	-4.1	-5.0	-4.3	-2.6	-3.5	-2.7

CH=CHCOMe	n/a	n/a	n/a	-8.1	-8.7	-8.1	-6.4	-7.1	-6.4
I (OCOMe) ₂	0.1	-1.0	-0.1	n/a	n/a	n/a	-0.8	-1.8	-1.0
N (COMe) ₂	-1.5	-2.5	-1.7	n/a	n/a	n/a	-2.3	-3.3	-2.5
cyclobutyl	-3.4	-4.3	-3.5	n/a	n/a	n/a	-4.1	-5.0	-4.2
C (O) CHMe ₂	n/a	n/a	n/a	-1.7	-2.6	-1.8	-0.2	-1.3	-0.4
NHCOCH (Me) ₂	-5.6	-6.4	-5.7	n/a	n/a	n/a	-6.2	-7.0	-6.3
C (Me) ₃	-3.7	-4.6	-3.8	n/a	n/a	n/a	-4.4	-5.3	-4.5
CH (Me) Et	-2.5	-3.5	-2.7	n/a	n/a	n/a	-3.3	-4.2	-3.4
CH ₂ CH (Me) ₂	-2.7	-3.6	-2.8	n/a	n/a	n/a	-3.4	-4.3	-3.6
(CH ₂) ₃ CH ₃	-3.3	-4.2	-3.4	n/a	n/a	n/a	-4.0	-4.9	-4.1
O (CH ₂) ₃ CH ₃	-10.1	-10.6	-10.0	n/a	n/a	n/a	-10.5	-11.0	-10.3
CH ₂ C (OH) Me ₂	-1.9	-2.9	-2.1	n/a	n/a	n/a	-2.7	-3.7	-2.9
C (OMe) ₃	-1.8	-2.8	-2.0	n/a	n/a	n/a	-2.6	-3.5	-2.7
AsEt ₂	-5.8	-6.6	-5.8	n/a	n/a	n/a	-6.4	-7.1	-6.4
As (O) Et ₂	-3.4	-4.3	-3.5	n/a	n/a	n/a	-4.1	-5.0	-4.2
As (S) Et ₂	-2.5	-3.5	-2.7	n/a	n/a	n/a	-3.3	-4.2	-3.4
NH (CH ₂) ₃ CH ₃	-5.5	-6.3	-5.5	n/a	n/a	n/a	-6.1	-6.9	-6.1
N (Et) ₂	-11.9	-12.3	-11.7	n/a	n/a	n/a	-12.1	-12.6	-12.0
PO (Et) ₂	1.0	-0.1	0.7	n/a	n/a	n/a	0.1	-1.0	-0.2
N=NPO (OEt) ₂	10.6	9.0	10.0	n/a	n/a	n/a	9.2	7.6	8.7
PO (OEt) ₂	0.1	-1.0	-0.1	n/a	n/a	n/a	-0.8	-1.8	-1.0
P (Et) ₂	-0.8	-1.8	-1.0	n/a	n/a	n/a	-1.6	-2.6	-1.8
P (S) Et ₂	0.4	-0.7	0.2	n/a	n/a	n/a	-0.5	-1.5	-0.7
CH ₂ OSi (CH ₃) ₃	-1.8	-2.8	-2.0	n/a	n/a	n/a	-2.6	-3.5	-2.7
CH ₂ Si (Me) ₃	-2.8	-3.8	-3.0	n/a	n/a	n/a	-3.6	-4.5	-3.7
PO (N (Me) ₂) ₂	0.9	-0.3	0.6	n/a	n/a	n/a	-0.1	-1.1	-0.3
P (N (Me) ₂) ₂	0.1	-1.0	-0.1	n/a	n/a	n/a	-0.8	-1.8	-1.0
2 (methylcarbonyl) carboran-1-yl	3.7	2.4	3.3	n/a	n/a	n/a	2.6	1.4	2.3
2-[(carbonyloxy)methyl] carboran-1-yl	0.1	-1.0	-0.1	n/a	n/a	n/a	-0.8	-1.8	-1.0
CH ₂ -1-(1,2-(BH) ₁₀ -C ₂ Me)	-1.2	-2.2	-1.4	n/a	n/a	n/a	-2.0	-3.0	-2.2
C (CN)=C (CN) ₂	n/a	n/a	n/a	1.4	0.3	1.2	2.7	1.5	2.4
2-(5-cyanofuryl)	n/a	n/a	n/a	-6.6	-7.3	-6.7	-5.0	-5.8	-5.0
2-(5-formylfuryl)	n/a	n/a	n/a	-9.1	-9.7	-9.1	-7.4	-8.1	-7.4
2-pyridyl	n/a	n/a	n/a	-6.8	-7.5	-6.8	-5.1	-5.9	-5.2
3-pyridyl	n/a	n/a	n/a	-3.3	-4.2	-3.4	-1.7	-2.7	-1.9
4-pyridyl	n/a	n/a	n/a	-0.1	-1.1	-0.3	1.3	0.2	1.1
2-(4,6-dimethyl-s-triazinyl)	n/a	n/a	n/a	-0.8	-1.8	-1.0	0.6	-0.5	0.4
1-cyclopentenyl	n/a	n/a	n/a	-3.7	-4.6	-3.8	-2.2	-3.1	-2.3
CH=CHCOOEt	n/a	n/a	n/a	-6.9	-7.6	-7.0	-5.3	-6.1	-5.3
cyclopentyl	-3.4	-4.3	-3.5	n/a	n/a	n/a	-4.1	-5.0	-4.2
C (O) C (Me) ₃	n/a	n/a	n/a	-2.5	-3.5	-2.7	-1.0	-2.1	-1.2

NHCO ₂ (CH ₂) ₃ CH ₃	-3.7	-4.6	-3.8	n/a	n/a	n/a	-4.4	-5.3	-4.5
C (Et) (Me) ₂	-4.2	-5.0	-4.3	n/a	n/a	n/a	-4.8	-5.7	-4.9
CH ₂ C (Me) ₃	-3.1	-4.1	-3.3	n/a	n/a	n/a	-3.9	-4.7	-4.0
(CH ₂) ₄ CH ₃	-3.1	-4.1	-3.3	n/a	n/a	n/a	-3.9	-4.7	-4.0
O (CH ₂) ₄ CH ₃	-10.4	-10.9	-10.3	n/a	n/a	n/a	-10.7	-11.3	-10.6
CH ₂ PO (OEt) ₂	-2.7	-3.6	-2.8	n/a	n/a	n/a	-3.4	-4.3	-3.6
CH ₂ CH ₂ Si (Me) ₃	-1.9	-2.9	-2.1	n/a	n/a	n/a	-2.7	-3.7	-2.9
Si (Me) ₂ OSi (Me) ₃	-1.8	-2.8	-2.0	n/a	n/a	n/a	-2.6	-3.5	-2.7
C ₆ Cl ₅	n/a	n/a	n/a	-3.8	-4.7	-4.0	-2.3	-3.3	-2.5
C ₆ F ₅	n/a	n/a	n/a	-3.4	-4.3	-3.6	-1.9	-2.9	-2.1
P (O) (C ₃ F ₇) ₂	2.8	1.5	2.5	n/a	n/a	n/a	1.8	0.6	1.5
OP (O) (C ₃ F ₇) ₂	-2.7	-3.6	-2.8	n/a	n/a	n/a	-3.4	-4.3	-3.6
NHP (O) (C ₃ F ₇) ₂	-3.3	-4.2	-3.4	n/a	n/a	n/a	-4.0	-4.9	-4.1
CH ₂ Mn (CO) ₅	-7.9	-8.5	-7.8	n/a	n/a	n/a	-8.3	-9.0	-8.3
C ₆ H ₂ -2,4,6- (NO ₂) ₃	n/a	n/a	n/a	-2.8	-3.7	-3.0	-1.3	-2.3	-1.5
C ₆ H ₄ -3-Br	n/a	n/a	n/a	-4.0	-4.8	-4.1	-2.4	-3.4	-2.6
C ₆ H ₄ -4-Br	n/a	n/a	n/a	-4.3	-5.1	-4.4	-2.7	-3.7	-2.9
C ₆ H ₄ -3-Cl	n/a	n/a	n/a	-4.7	-5.5	-4.8	-3.2	-4.1	-3.3
C ₆ H ₄ -4-Cl	n/a	n/a	n/a	-4.3	-5.1	-4.4	-2.7	-3.7	-2.9
C ₆ H ₄ -3-F	n/a	n/a	n/a	-4.7	-5.5	-4.8	-3.2	-4.1	-3.3
C ₆ H ₄ -4-F	n/a	n/a	n/a	-5.0	-5.8	-5.1	-3.4	-4.3	-3.6
OC ₆ H ₄ -4-F	n/a	n/a	n/a	-4.4	-5.3	-4.6	-2.9	-3.8	-3.0
C ₆ H ₄ -3-I	n/a	n/a	n/a	-5.2	-6.0	-5.3	-3.6	-4.5	-3.7
C ₆ H ₄ -4-I	n/a	n/a	n/a	-4.6	-5.4	-4.7	-3.0	-3.9	-3.1
C ₆ H ₄ -3-NO ₂	n/a	n/a	n/a	-3.9	-4.7	-4.0	-2.3	-3.3	-2.5
C ₆ H ₄ -4-NO ₂	n/a	n/a	n/a	-3.4	-4.3	-3.6	-1.9	-2.9	-2.1
SC ₆ H ₄ -4-NO ₂	-2.8	-3.8	-3.0	n/a	n/a	n/a	-3.6	-4.5	-3.7
SOC ₆ H ₄ -4-NO ₂	-0.3	-1.4	-0.5	n/a	n/a	n/a	-1.2	-2.2	-1.4
2-benzotriazolyl	n/a	n/a	n/a	-2.8	-3.7	-3.0	-1.3	-2.3	-1.5
C ₆ H ₅	n/a	n/a	n/a	-5.3	-6.1	-5.4	-3.7	-4.6	-3.8
N (O) =NSO ₂ C ₆ H ₅	1.5	0.3	1.2	n/a	n/a	n/a	0.5	-0.6	0.2
N=NC ₆ H ₅	0.3	-0.8	0.0	n/a	n/a	n/a	-0.6	-1.7	-0.8
OC ₆ H ₅	-7.0	-7.7	-7.0	n/a	n/a	n/a	-7.5	-8.2	-7.5
SOC ₆ H ₅	-2.1	-3.1	-2.3	n/a	n/a	n/a	-2.9	-3.8	-3.0
2- (5-acetylfuryl)	n/a	n/a	n/a	-6.8	-7.5	-6.8	-5.1	-5.9	-5.2
2- (6-methylpyronyl)	n/a	n/a	n/a	-2.4	-3.3	-2.6	-0.9	-1.9	-1.1
SO ₂ C ₆ H ₅	0.4	-0.7	0.2	n/a	n/a	n/a	-0.5	-1.5	-0.7
OSO ₂ C ₆ H ₅	-1.7	-2.7	-1.8	n/a	n/a	n/a	-2.4	-3.4	-2.6
SC ₆ H ₅	-4.5	-5.3	-4.5	n/a	n/a	n/a	-5.1	-5.9	-5.2
NHC ₆ H ₅	-12.6	-13.0	-12.4	n/a	n/a	n/a	-12.8	-13.3	-12.6
NHSO ₂ C ₆ H ₅	-4.5	-5.3	-4.5	n/a	n/a	n/a	-5.1	-5.9	-5.2

SO ₂ NHC ₆ H ₅	1.0	-0.1	0.7	n/a	n/a	n/a	0.1	-1.0	-0.2
2-(5-ethylfuryl)	n/a	n/a	n/a	-8.2	-8.9	-8.3	-6.5	-7.3	-6.5
1-(2,5-dimethylpyrryl)	n/a	n/a	n/a	-5.5	-6.2	-5.6	-3.9	-4.7	-4.0
1-cyclohexenyl	n/a	n/a	n/a	-3.6	-4.4	-3.7	-2.0	-3.0	-2.2
cyclohexyl	-3.7	-4.6	-3.8	n/a	n/a	n/a	-4.4	-5.3	-4.5
N(C ₃ H ₇) ₂	-15.7	-16.0	-15.4	n/a	n/a	n/a	-15.8	-16.0	-15.5
(CH ₂) ₄ NMe ₂	-3.3	-4.2	-3.4	n/a	n/a	n/a	-4.0	-4.9	-4.1
PO(isopropyl) ₂	-0.3	-1.4	-0.5	n/a	n/a	n/a	-1.2	-2.2	-1.4
P(isopropyl) ₂	-0.8	-1.8	-1.0	n/a	n/a	n/a	-1.6	-2.6	-1.8
P(O)(OPr) ₂	1.5	0.3	1.2	n/a	n/a	n/a	0.5	-0.6	0.2
Ge(Et) ₃	-1.5	-2.5	-1.7	n/a	n/a	n/a	-2.3	-3.3	-2.5
Si(OEt) ₃	-0.3	-1.4	-0.5	n/a	n/a	n/a	-1.2	-2.2	-1.4
Sn(Et) ₃	-1.5	-2.5	-1.7	n/a	n/a	n/a	-2.3	-3.3	-2.5
P(=NSO ₂ CF ₃)(C ₃ F ₇) ₂	2.8	1.5	2.5	n/a	n/a	n/a	1.8	0.6	1.5
Si(NMe ₂) ₃	-1.7	-2.7	-1.8	n/a	n/a	n/a	-2.4	-3.4	-2.6
2-benzoxazolyl	n/a	n/a	n/a	-2.8	-3.7	-3.0	-1.3	-2.3	-1.5
2-benzthiazolyl	n/a	n/a	n/a	-3.1	-4.0	-3.3	-1.6	-2.6	-1.8
C(O)C ₆ H ₅	n/a	n/a	n/a	-1.7	-2.6	-1.8	-0.2	-1.3	-0.4
OCOC ₆ H ₅	-3.0	-3.9	-3.1	n/a	n/a	n/a	-3.7	-4.6	-3.8
C(O)OC ₆ H ₅	n/a	n/a	n/a	-2.0	-2.9	-2.1	-0.5	-1.5	-0.7
N=CHC ₆ H ₅	-11.3	-11.8	-11.1	n/a	n/a	n/a	-11.6	-12.1	-11.4
CH=NC ₆ H ₅	n/a	n/a	n/a	-2.1	-3.0	-2.3	-0.6	-1.7	-0.8
NHCOC ₆ H ₅	-5.8	-6.6	-5.8	n/a	n/a	n/a	-6.4	-7.1	-6.4
C(O)NHC ₆ H ₅	n/a	n/a	n/a	0.1	-1.0	-0.1	1.5	0.3	1.2
C ₆ H ₄ -4-Me	n/a	n/a	n/a	-5.6	-6.4	-5.7	-4.0	-4.9	-4.1
CH ₂ C ₆ H ₅	-1.8	-2.8	-2.0	n/a	n/a	n/a	-2.6	-3.5	-2.7
N=NC ₆ H ₃ -5-Me-2-OH	-0.3	-1.4	-0.5	n/a	n/a	n/a	-1.2	-2.2	-1.4
C ₆ H ₄ -4-OMe	n/a	n/a	n/a	-6.5	-7.2	-6.6	-4.8	-5.7	-4.9
CH(OH)C ₆ H ₅	-2.2	-3.2	-2.4	n/a	n/a	n/a	-3.0	-3.9	-3.1
CH ₂ OC ₆ H ₅	-1.2	-2.2	-1.4	n/a	n/a	n/a	-2.0	-3.0	-2.2
CH ₂ SO ₂ C ₆ H ₅	-1.2	-2.2	-1.4	n/a	n/a	n/a	-2.0	-3.0	-2.2
C(Et) ₃	-4.3	-5.2	-4.4	n/a	n/a	n/a	-5.0	-5.8	-5.0
(CH ₂) ₆ CH ₃	-3.4	-4.3	-3.5	n/a	n/a	n/a	-4.1	-5.0	-4.2
SiMe(OSi(Me) ₃) ₂	-1.4	-2.4	-1.5	n/a	n/a	n/a	-2.2	-3.1	-2.3
CF ₂ CF ₂ C ₆ H ₄ -4-F	0.0	-1.1	-0.3	n/a	n/a	n/a	-0.9	-1.9	-1.1
C≡CC ₆ H ₅	n/a	n/a	n/a	-3.3	-4.2	-3.4	-1.7	-2.7	-1.9
CH=NCOC ₆ H ₅	n/a	n/a	n/a	-0.9	-1.9	-1.1	0.5	-0.6	0.2
CH=CHC ₆ H ₅	n/a	n/a	n/a	-5.9	-6.6	-6.0	-4.3	-5.1	-4.4
CH ₂ Fe(CO) ₂ (π-C ₅ H ₅)	-6.7	-7.4	-6.7	n/a	n/a	n/a	-7.2	-7.9	-7.2
CH=NNHCOC ₆ H ₅	n/a	n/a	n/a	-0.9	-1.9	-1.1	0.5	-0.6	0.2
N=CHC ₆ H ₄ -4-OCH ₃	-11.3	-11.8	-11.1	n/a	n/a	n/a	-11.6	-12.1	-11.4

NHCOC ₆ H ₄ -4-OCH ₃	-4.5	-5.3	-4.5	n/a	n/a	n/a	-5.1	-5.9	-5.2
SCH=NSO ₂ C ₆ H ₄ -4-Me	0.3	-0.8	0.0	n/a	n/a	n/a	-0.6	-1.7	-0.8
C ₆ H ₄ -4-Et	n/a	n/a	n/a	-5.6	-6.4	-5.7	-4.0	-4.9	-4.1
CH ₂ CH ₂ C ₆ H ₅	-2.7	-3.6	-2.8	n/a	n/a	n/a	-3.4	-4.3	-3.6
N=C (Me) NHC ₆ H ₅	-5.5	-6.3	-5.5	n/a	n/a	n/a	-6.1	-6.9	-6.1
Si (C ₆ H ₅) (Me) ₂	-0.9	-2.0	-1.1	n/a	n/a	n/a	-1.7	-2.7	-1.9
S (Me) =NSO ₂ C ₆ H ₄ -4-Me	0.3	-0.8	0.0	n/a	n/a	n/a	-0.6	-1.7	-0.8
2,4,6-trimethylpyridinium	n/a	n/a	n/a	-3.9	-4.7	-4.0	-2.3	-3.3	-2.5
PO (CMe ₃) ₂	0.9	-0.3	0.6	n/a	n/a	n/a	-0.1	-1.1	-0.3
PO (C ₄ H ₉) ₂	1.8	0.6	1.5	n/a	n/a	n/a	0.8	-0.3	0.5
PO (OC ₄ H ₉) ₂	2.2	1.0	1.9	n/a	n/a	n/a	1.2	0.1	0.9
P (CMe ₃) ₂	1.3	0.1	1.0	n/a	n/a	n/a	0.4	-0.7	0.1
C ₆ H ₅ Cr (CO) ₃	n/a	n/a	n/a	-6.6	-7.3	-6.7	-5.0	-5.8	-5.0
2-benzo-4-thiopyranyl	n/a	n/a	n/a	-3.3	-4.2	-3.4	-1.7	-2.7	-1.9
2- (benzothiopyranyl)	n/a	n/a	n/a	-3.9	-4.7	-4.0	-2.3	-3.3	-2.5
2- (benzo-1,4-pyranyl)	n/a	n/a	n/a	-3.6	-4.4	-3.7	-2.0	-3.0	-2.2
CH=CHCOC ₆ H ₄ -4-NO ₂	n/a	n/a	n/a	-5.8	-6.5	-5.8	-4.1	-5.0	-4.2
CH ₂ Mo (CO) ₃ (C ₅ H ₅)	-6.7	-7.4	-6.7	n/a	n/a	n/a	-7.2	-7.9	-7.2
CH=CHCOC ₆ H ₅	n/a	n/a	n/a	-6.3	-7.1	-6.4	-4.7	-5.5	-4.8
C ₆ H ₄ -4-CHMe ₂	n/a	n/a	n/a	-5.2	-6.0	-5.3	-3.6	-4.5	-3.7
Si (OSiMe ₃) ₃	0.0	-1.1	-0.3	n/a	n/a	n/a	-0.9	-1.9	-1.1
ferrocenyl	n/a	n/a	n/a	-4.7	-5.5	-4.8	-3.2	-4.1	-3.3
C ₆ H ₄ -4-CMe ₃	n/a	n/a	n/a	-5.0	-5.8	-5.1	-3.4	-4.3	-3.6
1-adamantyl	-1.9	-2.9	-2.1	n/a	n/a	n/a	-2.7	-3.7	-2.9
1-dibenzarsenyl	-2.5	-3.5	-2.7	n/a	n/a	n/a	-3.3	-4.2	-3.4
1-dibenzoarsoxyl	-3.0	-3.9	-3.1	n/a	n/a	n/a	-3.7	-4.6	-3.8
1-dibenzoarsazinyl	-2.4	-3.4	-2.5	n/a	n/a	n/a	-3.2	-4.1	-3.3
As (C ₆ H ₅) ₂	-0.3	-1.4	-0.5	n/a	n/a	n/a	-1.2	-2.2	-1.4
AsO (C ₆ H ₅) ₂	1.2	0.0	0.9	n/a	n/a	n/a	0.2	-0.9	0.0
P (C ₆ H ₅) ₂ (BCl ₃)	0.4	-0.7	0.2	n/a	n/a	n/a	-0.5	-1.5	-0.7
N (C ₆ H ₅) ₂	-6.1	-6.9	-6.1	n/a	n/a	n/a	-6.7	-7.4	-6.7
PO (C ₆ H ₅) ₂	2.0	0.8	1.7	n/a	n/a	n/a	1.1	-0.1	0.8
P (C ₆ H ₅) ₂	0.3	-0.8	0.0	n/a	n/a	n/a	-0.6	-1.7	-0.8
PS (C ₆ H ₅) ₂	2.5	1.3	2.2	n/a	n/a	n/a	1.5	0.3	1.2
P (N (C ₃ H ₇) ₂) C ₆ H ₄ -3-F	-0.5	-1.5	-0.7	n/a	n/a	n/a	-1.3	-2.3	-1.5
	n/a	n/a	n/a	-3.3	-4.2	-3.4	-1.7	-2.7	-1.9

n/a	n/a	n/a	-3.4	-4.3	-3.6	-1.9	-2.9	-2.1
n/a	n/a	n/a	-2.8	-3.7	-3.0	-1.3	-2.3	-1.5
CH (C ₆ H ₅) ₂	-1.9	-2.9	-2.1	n/a	n/a	n/a	-2.7	-3.7	-2.9
-2.4	-3.4	-2.5	n/a	n/a	n/a	-3.2	-4.1	-3.3
PO (C ₆ H ₅) C ₆ H ₄ -4-Me	2.0	0.8	1.7	n/a	n/a	n/a	1.1	-0.1	0.8
CH ₂ PO (C ₆ H ₅) ₂	-4.0	-4.9	-4.1	n/a	n/a	n/a	-4.7	-5.5	-4.8
PS (C ₆ H ₅) C ₆ H ₄ -4-Me	2.9	1.7	2.6	n/a	n/a	n/a	1.9	0.7	1.6
Si (Me) (C ₆ H ₅) ₂	-0.8	-1.8	-1.0	n/a	n/a	n/a	-1.6	-2.6	-1.8
C (O) OCH (C ₆ H ₅) ₂	n/a	n/a	n/a	0.7	-0.4	0.4	2.0	0.9	1.7
PO (C ₆ H ₄ -4-Me) ₂	1.3	0.1	1.0	n/a	n/a	n/a	0.4	-0.7	0.1
PS (C ₆ H ₄ -4-Me) ₂	-0.6	-1.7	-0.8	n/a	n/a	n/a	-1.5	-2.5	-1.7
Ge (C ₆ H ₅) ₃	-0.9	-2.0	-1.1	n/a	n/a	n/a	-1.7	-2.7	-1.9
2-methyl-4,6-diphenylpyridinium	n/a	n/a	n/a	-2.1	-3.0	-2.3	-0.6	-1.7	-0.8
N=P (C ₆ H ₅) ₃	-11.0	-11.5	-10.8	n/a	n/a	n/a	-11.3	-11.8	-11.2
Si (C ₆ H ₅) ₃	1.0	-0.1	0.7	n/a	n/a	n/a	0.1	-1.0	-0.2
Sn (C ₆ H ₅) ₃	-6.2	-7.0	-6.3	n/a	n/a	n/a	-6.8	-7.5	-6.8
C (C ₆ H ₅) ₃	-0.9	-2.0	-1.1	n/a	n/a	0.0	-1.7	-2.7	-1.9
2,4,6-triphenylpyridinium	n/a	n/a	n/a	-3.7	-4.6	-3.8	-2.2	-3.1	-2.3

Table S2. Estimated gas phase standard state (298.15 K, 1 atm) hydration equilibrium constants ($\log K_{\text{hydr}, (g)}$) for various aldehydes with electron withdrawing and electron releasing substituents using training set correlations developed between Swain-Lupton positively charged reaction center resonance effect (R^+) parameters and $\log K_{\text{hydr}, (g)}$ calculated at the CBS-Q//B3, G4MP2, and G4 levels of theory. Estimated $\log K_{\text{hydr}, (g)}$ presented in the table below are calculated from Swain-Lupton resonance effect (R^+) parameters given in ref. (1).

substituent	CBS-Q//B3	G4MP2	G4
Br	-4.0	-4.9	-4.1
SiBr ₃	-1.9	-2.9	-2.1
Cl	-4.0	-4.9	-4.2
P(O)Cl ₂	-4.1	-5.0	-4.2
PCl ₂	-0.8	-1.8	-1.0
P(S)Cl ₂	-4.0	-4.9	-4.1
GeCl ₃	-2.3	-3.3	-2.5
SiCl ₃	-0.7	-1.8	-0.9
F	-5.6	-6.4	-5.7
I	-3.8	-4.7	-3.9
NO ₂	-0.6	-1.7	-0.9
H	-1.7	-2.7	-1.9
OH	-11.1	-11.7	-11.0
SH	-4.2	-5.1	-4.3
B(OH) ₂	1.4	0.3	1.1
NH ₂	-12.1	-12.6	-12.0
PH ₂	-1.9	-2.9	-2.1
SiH ₃	-1.1	-2.1	-1.3
C(O)Cl	0.8	-0.3	0.5
CF ₃	0.0	-1.0	-0.2
N=NCF ₃	0.1	-1.0	-0.1
CN	-0.6	-1.6	-0.8
N=C=O	-5.5	-6.3	-5.6
N=N-C≡N	1.9	0.7	1.5
C(O)H	1.3	0.2	1.0
C(O)OH	-1.1	-2.1	-1.3
CH ₂ Br	-2.6	-3.6	-2.8
CH ₂ Cl	-2.7	-3.7	-2.9
CH ₃	-4.1	-5.0	-4.2
SiCl ₂ (CH ₃)	-3.3	-4.2	-3.4
SiF ₂ (CH ₃)	-2.4	-3.3	-2.6
OCH ₃	-9.8	-10.4	-9.7
CH ₂ OH	-2.2	-3.2	-2.4
OSO ₂ CH ₃	-3.5	-4.4	-3.7
SCH ₃	-8.0	-8.7	-8.0
NHCH ₃	-15.1	-15.5	-14.9
C(O)CF ₃	0.6	-0.5	0.4
C≡CH	-2.0	-3.0	-2.2
CH ₂ CN	-1.8	-2.8	-2.0
CH=CH ₂	-3.9	-4.8	-4.0
OC(O)CH ₃	-6.3	-7.1	-6.4
C(O)OCH ₃	-0.6	-1.6	-0.8
NHC(O)CH ₃	-8.6	-9.3	-8.5
CH ₂ CH ₃	-4.0	-4.9	-4.1
OCH ₂ CH ₃	-9.8	-10.4	-9.7
CH ₂ OCH ₃	-3.0	-4.0	-3.2
SiCl(CH ₃) ₂	-2.7	-3.7	-2.9
SiF(CH ₃) ₂	-1.7	-2.7	-1.9

N(CH ₃) ₂	-15.7	-16.0	-15.4
SO ₂ N(CH ₃) ₂	1.5	0.3	1.2
N=NN(CH ₃) ₂	-4.9	-5.8	-5.0
SiH(CH ₃) ₂	-2.2	-3.2	-2.4
cyclopropyl	-4.9	-5.8	-5.0
CH ₂ CH=CH ₂	-2.9	-3.9	-3.1
C(O)OEt	-0.6	-1.7	-0.9
CH(CH ₃) ₂	-4.1	-5.0	-4.2
CH ₂ CH ₂ CH ₃	-4.0	-4.9	-4.1
OCH(CH ₃) ₂	-10.7	-11.3	-10.6
OCH ₂ CH ₂ CH ₃	-9.9	-10.5	-9.9
Si(CH ₃) ₂ OCH ₃	-2.5	-3.5	-2.7
SiCH ₃ (OCH ₃) ₂	-2.0	-3.0	-2.2
Si(OCH ₃) ₃	-1.5	-2.5	-1.7
Si(CH ₃) ₃	-1.6	-2.6	-1.8
Sn(CH ₃) ₃	-5.2	-6.0	-5.3
CH=C(CN) ₂	0.2	-0.9	-0.1
2-furyl	-5.4	-6.2	-5.5
2-thienyl	-5.9	-6.7	-6.0
3-thienyl	-5.2	-6.0	-5.3
CH=CHC(O)CH ₃	-1.1	-2.1	-1.3
cyclobutyl	-4.0	-4.9	-4.2
C(CH ₃) ₃	-3.0	-3.9	-3.1
(CH ₂) ₃ CH ₃	-3.8	-4.7	-3.9
N(Et) ₂	-17.4	-17.7	-17.1
CH ₂ Si(CH ₃) ₃	-6.4	-7.2	-6.4
cyclopentyl	-4.1	-5.0	-4.2
CH ₂ C(CH ₃) ₃	-3.4	-4.3	-3.5
C ₆ F ₅	-2.4	-3.3	-2.6
C ₆ H ₄ -4-Br	-4.6	-5.4	-4.7
C ₆ H ₄ -3-Cl	-4.3	-5.1	-4.4
C ₆ H ₄ -4-Cl	-4.5	-5.4	-4.6
C ₆ H ₄ -4-NO ₂	-3.4	-4.3	-3.5
SC ₆ H ₄ -4-NO ₂	-5.7	-6.5	-5.8
C ₆ H ₅	-4.0	-4.9	-4.1
N=NC ₆ H ₅	-5.4	-6.2	-5.5
OC ₆ H ₅	-8.3	-9.0	-8.3
SC ₆ H ₅	-8.1	-8.8	-8.1
NHC ₆ H ₅	-12.5	-13.0	-12.3
NHSO ₂ C ₆ H ₅	-10.9	-11.5	-10.8
cyclohexyl	-4.1	-5.0	-4.2
Si(OEt) ₃	-0.6	-1.7	-0.9
C(O)C ₆ H ₅	-0.2	-1.3	-0.4
OC(O)C ₆ H ₅	-4.2	-5.1	-4.3
NHC(O)C ₆ H ₅	-7.2	-8.0	-7.2
CH ₂ C ₆ H ₅	-5.1	-5.9	-5.2
C≡CC ₆ H ₅	-3.0	-4.0	-3.2
CH=CHC ₆ H ₅	-10.0	-10.6	-9.9
CH ₂ CH ₂ C ₆ H ₅	-3.7	-4.6	-3.9
Si(CH ₃) ₂ C ₆ H ₅	-1.5	-2.6	-1.8
ferrocenyl	-8.6	-9.3	-8.5
1-adamantyl	-4.0	-4.9	-4.2
PO(C ₆ H ₅) ₂	-0.2	-1.3	-0.4
P(C ₆ H ₅) ₂	2.8	1.6	2.5
CH(C ₆ H ₅) ₂	-3.0	-4.0	-3.2
Si(CH ₃)(C ₆ H ₅) ₂	-2.8	-3.8	-3.0
Ge(C ₆ H ₅) ₃	-4.3	-5.2	-4.5

$\text{N}=\text{P}(\text{C}_6\text{H}_5)_3$	-13.4	-13.9	-13.2
$\text{Si}(\text{C}_6\text{H}_5)_3$	-0.5	-1.5	-0.7
$\text{C}(\text{C}_6\text{H}_5)_3$	-3.4	-4.3	-3.5

Table S3. Estimated aqueous phase standard state (298.15 K, 1 M) hydration equilibrium constants ($\log K_{\text{hydr, (aq)}}$) for various aldehydes with electron withdrawing and electron releasing substituents using training set correlations developed between Swain-Lupton positively charged reaction center resonance effect (R^+) parameters and experimental $\log K_{\text{hydr, (aq)}}$ from the compilation in ref. (2). Estimated $\log K_{\text{hydr, (g)}}$ presented in the table below are calculated from Swain-Lupton resonance effect (R^+) parameters given in ref. (1).

substituent	$\log K_{\text{hydr, (aq)}}$
Br	-0.1
SiBr ₃	2.1
Cl	-0.2
P(O)Cl ₂	-0.3
PCl ₂	3.3
P(S)Cl ₂	-0.1
GeCl ₃	1.7
SiCl ₃	3.4
F	-1.9
I	0.1
NO ₂	3.4
O ⁻	-14.2
S ⁻	-18.4
H	2.3
OH	-7.8
SH	-0.4
B(OH) ₂	5.6
NH ₂	-8.8
PH ₂	2.1
SiH ₃	3.0
C(O)Cl	5.0
CF ₃	4.2
N=NCF ₃	4.3
CN	3.5
N=C=O	-1.7
N=N-C≡N	6.1
CO ₂ ⁻	3.0
C(O)OR	3.4
C(O)H	5.5
C(O)OH	3.0
CH ₂ Br	1.3
CH ₂ Cl	1.2
CH ₃	-0.3
SiCl ₂ (CH ₃)	0.6
SiF ₂ (CH ₃)	1.6
OCH ₃	-6.3
CH ₂ OH	1.7
OSO ₂ CH ₃	0.4
SCH ₃	-4.4
NHCH ₃	-12.1
C(O)CF ₃	4.8
C≡CH	2.0
CH ₂ CN	2.2
CH=CH ₂	0.0
OC(O)CH ₃	-2.6
C(O)OCH ₃	3.5
NHC(O)CH ₃	-5.0
CH ₂ CH ₃	-0.1

OCH ₂ CH ₃	-6.3
CH ₂ OCH ₃	0.9
SiCl(CH ₃) ₂	1.2
SiF(CH ₃) ₂	2.3
N(CH ₃) ₂	-12.6
SO ₂ N(CH ₃) ₂	5.7
N=NN(CH ₃) ₂	-1.2
SiH(CH ₃) ₂	1.7
cyclopropyl	-1.2
CH ₂ CH=CH ₂	1.0
C(O)OEt	3.4
CH(CH ₃) ₂	-0.3
CH ₂ CH ₂ CH ₃	-0.1
OCH(CH ₃) ₂	-7.3
OCH ₂ CH ₂ CH ₃	-6.5
N ⁺ (CH ₃) ₃	-1.3
Si(CH ₃) ₂ OCH ₃	1.4
SiCH ₃ (OCH ₃) ₂	2.0
Si(OCH ₃) ₃	2.6
Si(CH ₃) ₃	2.4
Sn(CH ₃) ₃	-1.4
CH=C(CN) ₂	4.3
2-furyl	-1.6
2-thienyl	-2.2
3-thienyl	-1.4
CH=CHC(O)CH ₃	3.0
cyclobutyl	-0.2
C(CH ₃) ₃	0.9
(CH ₂) ₃ CH ₃	0.1
N(Et) ₂	-14.5
CH ₂ Si(CH ₃) ₃	-2.7
cyclopentyl	-0.3
CH ₂ C(CH ₃) ₃	0.5
C ₆ F ₅	1.6
C ₆ H ₄ -4-Br	-0.8
C ₆ H ₄ -3-Cl	-0.4
C ₆ H ₄ -4-Cl	-0.7
C ₆ H ₄ -4-NO ₂	0.5
SC ₆ H ₄ -4-NO ₂	-2.0
C ₆ H ₅	-0.1
N=NC ₆ H ₅	-1.6
OC ₆ H ₅	-4.7
SC ₆ H ₅	-4.6
NHC ₆ H ₅	-9.2
NHSO ₂ C ₆ H ₅	-7.5
cyclohexyl	-0.3
Si(OEt) ₃	3.4
C(O)C ₆ H ₅	3.9
OC(O)C ₆ H ₅	-0.4
NHC(O)C ₆ H ₅	-3.6
CH ₂ C ₆ H ₅	-1.3
C≡CC ₆ H ₅	0.9
CH=CHC ₆ H ₅	-6.6
CH ₂ CH ₂ C ₆ H ₅	0.1
Si(CH ₃) ₂ C ₆ H ₅	2.5
ferrocenyl	-5.0
1-adamantyl	-0.2

$\text{PO}(\text{C}_6\text{H}_5)_2$	3.9
$\text{P}(\text{C}_6\text{H}_5)_2$	7.2
$\text{CH}(\text{C}_6\text{H}_5)_2$	0.9
$\text{Si}(\text{CH}_3)(\text{C}_6\text{H}_5)_2$	1.1
$\text{Ge}(\text{C}_6\text{H}_5)_3$	-0.5
$\text{N}=\text{P}(\text{C}_6\text{H}_5)_3$	-10.2
$\text{Si}(\text{C}_6\text{H}_5)_3$	3.6
$\text{C}(\text{C}_6\text{H}_5)_3$	0.5

GAUSSIAN 09 ARCHIVE ENTRIES

Gas phase standard state (298.15 K, 1 atm) lowest energy conformations of the aldehydes, aldehyde hydrates, aldehyde radicals, and deprotonated aldehyde anions under consideration optimized at the G4 level of theory.

ALDEHYDES

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H(O)CC≡N

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 2=-191.3252631\\MP4/GTBas2=-191.377374\\MP2/GTBas3=-191.4495687\\MP4/GTBa
 s3=-191.5098503\\HF/GTLargeXP=-190.8316926\\MP2/GTLargeXP=-191.716229\\HF/
 GFHFB1=-190.847024\\HF/GFHFB2=-190.850072\\G4=-191.8108357

H (O) CC≡CH

\\0,1\\O,0,-1.6099724018,-0.4157378415,-0.0001327565\\C,0,-0.72
 7387355,0.4087060699,0.0000492947\\C,0,0.6819454971,0.0893568659,0.0002
 276007\\C,0,1.8649163397,-0.1348965267,0.0002956119\\H,0,-0.9444660968,1
 .4954803994,0.0000753588\\H,0,2.9063840169,-0.3493089669,0.0003948904\\
 Version=EM64L-G09RevA.02\\State=1-A\\MP2/GTBas1=-190.0853476\\MP4/GTBas1=
 -190.1293394\\CCSD(T)/G3Bas1=-190.1258194\\MP2/GTBas2=-190.0986279\\MP4/G
 TBas2=-190.1430952\\MP2/GTBas3=-190.2098691\\MP4/GTBas3=-190.2611338\\HF/
 GTLargeXP=-189.6084228\\MP2/GTLargeXP=-190.4718413\\HF/GFHFB1=-189.62337
 51\\HF/GFHFB2=-189.6261963\\G4=-190.5713279

H (O) CF

\\0,1\\O,0,-0.0369977849,-0.7129678844,0.\\C,0,-0.0604358188,
 0.4674325955,0.\\H,0,-0.9443110341,1.1196131325,0.\\F,0,1.0417246378,1.2
 207021564,0.\\Version=EM64L-G09RevA.02\\State=1-A'\\MP2/GTBas1=-213.2188
 557\\MP4/GTBas1=-213.2443613\\CCSD(T)/G3Bas1=-213.2399117\\MP2/GTBas2=-21
 3.2365451\\MP4/GTBas2=-213.2631332\\MP2/GTBas3=-213.3524829\\MP4/GTBas3=-
 213.386874\\HF/GTLargeXP=-212.8297521\\MP2/GTLargeXP=-213.6099953\\HF/GFH
 FB1=-212.8494931\\HF/GFHFB2=-212.8534646\\G4=-213.707511

H (O) CH

\\0,1\\O,0,0.67455,0.,0.\\C,0,-0.52541,0.,0.\\H,0,-1.12193,0.937
 17,0.\\H,0,-1.12199,-0.93714,0.\\Version=EM64L-G09RevA.02\\State=1-A'\\MP
 2/GTBas1=-114.167049\\MP4/GTBas1=-114.1912206\\CCSD(T)/G3Bas1=-114.18996
 81\\MP2/GTBas2=-114.1761164\\MP4/GTBas2=-114.2005906\\MP2/GTBas3=-114.247
 9948\\MP4/GTBas3=-114.277772\\HF/GTLargeXP=-113.9116364\\MP2/GTLargeXP=-1
 14.3970394\\HF/GFHFB1=-113.9210862\\HF/GFHFB2=-113.9230227\\G4=-114.45319
 06

H (O) COH

\\0,1\\C,0,-0.13472,0.39751,-0.00001\\O,0,-1.13529,-0.26176,0.\\
 H,0,-0.09245,1.4971,0.00001\\O,0,1.11773,-0.09115,0.\\H,0,1.04119,-1.058
 9,0.\\Version=EM64L-G09RevA.02\\State=1-A\\MP2/GTBas1=-189.2412506\\MP4/G

TBas1=-189.269522\CCSD(T)/G3Bas1=-189.2663043\MP2/GTBas2=-189.2559895\
MP4/GTBas2=-189.2851756\MP2/GTBas3=-189.3734005\MP4/GTBas3=-189.410315
9\HF/GTLargeXP=-188.8401299\MP2/GTLargeXP=-189.6091779\HF/GFHFB1=-188.
8560595\HF/GFHFB2=-188.8593944\G4=-189.692992

H(O)CCH₃

\0,1\O,0,1.22542,-0.28574,0.00002\C,0,0.24234,0.40851,-0.000
09\C,0,-1.17236,-0.135,-0.00005\H,0,0.33121,1.51903,0.00013\H,0,-1.319
08,-0.76579,0.88285\H,0,-1.91813,0.66298,-0.00314\H,0,-1.31721,-0.7713
7,-0.87918\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-153.3447044
\MP4/GTBas1=-153.3848162\CCSD(T)/G3Bas1=-153.3833453\MP2/GTBas2=-153.3
557016\MP4/GTBas2=-153.3964186\MP2/GTBas3=-153.4622611\MP4/GTBas3=-153
.5103435\HF/GTLargeXP=-152.9715057\MP2/GTLargeXP=-153.6710617\HF/GFHFB
1=-152.9840494\HF/GFHFB2=-152.9866332\G4=-153.7423328

H(O)CNO₂

\0,1\O,0,1.8310647971,0.1274221021,0.0002984937\C,0,0.8767
104291,-0.5587156959,-0.0004933916\N,0,-0.5547915666,0.0464530838,-0.0
005900267\O,0,-0.660353409,1.2525145671,0.0002314686\O,0,-1.441200099,
-0.7944661093,0.0003471253\H,0,0.7837198483,-1.6550179478,0.0006463306
\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-318.1765655\MP4/GTBas
1=-318.2211716\CCSD(T)/G3Bas1=-318.2072307\MP2/GTBas2=-318.199617\MP4/
GTBas2=-318.2459563\MP2/GTBas3=-318.3771763\MP4/GTBas3=-318.4352705\HF
/GTLargeXP=-317.4533794\MP2/GTLargeXP=-318.7631093\HF/GFHFB1=-317.4801
082\HF/GFHFB2=-317.4854427\G4=-318.9094465

H(O)CC₆H₅

\0,1\O,0,2.84093,-0.39419,-0.00001\C,0,1.99011,0.46508,0.\C,
0,0.53288,0.21232,0.00001\C,0,-0.35869,1.28832,0.\C,0,-1.73084,1.0596,
-0.00001\C,0,-2.21242,-0.24816,-0.00001\C,0,-1.32546,-1.32749,0.00002\
C,0,0.04325,-1.0997,-0.00002\H,0,2.26655,1.54417,0.00008\H,0,0.02991,2
.30308,0.\H,0,-2.4229,1.89476,-0.00002\H,0,-3.28241,-0.42891,-0.00001\
H,0,-1.70769,-2.34274,0.00003\H,0,0.75618,-1.91669,0.\\Version=EM64L-G
09RevA.02\State=1-A\MP2/GTBas1=-344.4857609\MP4/GTBas1=-344.5767913\CC
SD(T)/G3Bas1=-344.5717365\MP2/GTBas2=-344.5070678\MP4/GTBas2=-344.5985
712\MP2/GTBas3=-344.7266056\MP4/GTBas3=-344.8298653\HF/GTLargeXP=-343.
5427929\MP2/GTLargeXP=-345.2220455\HF/GFHFB1=-343.5698515\HF/GFHFB2=-3
43.5748893\G4=-345.3849641

H(O)CCF₃

\0,1\O,0,2.0418013557,0.1169473372,-0.0007011282\C,0,1.065
2513351,-0.5717400145,-0.0000672966\C,0,-0.3650064411,0.0069227823,-0.
000041308\F,0,-0.3670091377,1.3292883894,-0.0011921948\F,0,-1.01774500
58,-0.4360638742,-1.0829101046\F,0,-1.016880837,-0.4341720763,1.084134
0245\H,0,1.0821187308,-1.6800025439,0.0005980076\\Version=EM64L-G09Rev
A.02\State=1-A\MP2/GTBas1=-450.4162254\MP4/GTBas1=-450.464221\CCSD(T)/
G3Bas1=-450.4560568\MP2/GTBas2=-450.4508125\MP4/GTBas2=-450.5015984\MP
2/GTBas3=-450.6913399\MP4/GTBas3=-450.7574524\HF/GTLargeXP=-449.651765
4\MP2/GTLargeXP=-451.2239411\HF/GFHFB1=-449.6932712\HF/GFHFB2=-449.701
9678\G4=-451.4292713

H(O)CSi(CH₃)₃

\0,1\O,0,2.39891,0.15152,-0.00075\C,0,1.3897,0.82673,-0.
00445\Si,0,-0.35391,-0.01274,-0.00007\C,0,-0.44616,-1.06467,1.5568\C,0
, -1.67929,1.32524,-0.01064\C,0,-0.44328,-1.08712,-1.54163\H,0,1.49154,
1.94526,-0.0103\H,0,-0.41806,-0.44933,2.46179\H,0,-1.37018,-1.65223,1.
58217\H,0,0.39775,-1.76005,1.59879\H,0,-1.59835,1.96145,-0.89858\H,0,-

2.68437,0.89011,-0.0092\H,0,-1.60075,1.97274,0.86932\H,0,0.40177,-1.78169,-1.57284\H,0,-1.36635,-1.67643,-1.55941\H,0,-0.41527,-0.4848,-2.45533\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-521.8579273\MP4/GTBas1=-521.946977\CCSD(T)/G3Bas1=-521.9472332\MP2/GTBas2=-521.8763906\MP4/GTBas2=-521.9665986\MP2/GTBas3=-522.0989823\MP4/GTBas3=-522.204844\HF/GTLargeXP=-521.1999787\MP2/GTLargeXP=-522.7526968\HF/GFHFB1=-521.2229165\HF/GFHFB2=-521.2290204\G4=-522.8890342

H(O) CBr

\\0,1\O,0,-0.2656486928,-0.9578789517,0.\C,0,-0.3338060295,0.216892248,0.\H,0,-1.2406723716,0.835382188,0.\Br,0,1.2401070939,1.4003845157,0.\\Version=EM64L-G09RevA.02\State=1-A'\MP2/GTBas1=-2685.9700584\MP4/GTBas1=-2685.9954121\CCSD(T)/G3Bas1=-2685.990229\MP2/GTBas2=-2685.9797279\MP4/GTBas2=-2686.0056445\MP2/GTBas3=-2686.0816099\MP4/GTBas3=-2686.1191885\HF/GTLargeXP=-2685.7430054\MP2/GTLargeXP=-2687.3506579\HF/GFHFB1=-2685.8165482\HF/GFHFB2=-2685.8186501\G4=-2687.5040536

H(O) CCl

\\0,1\O,0,-0.2269587606,-0.9329054816,0.\C,0,-0.2985725044,0.2436769148,0.\H,0,-1.207952019,0.8573826973,0.\Cl,0,1.133453284,1.3266258694,0.\\Version=EM64L-G09RevA.02\State=1-A'\MP2/GTBas1=-573.2152426\MP4/GTBas1=-573.2513586\CCSD(T)/G3Bas1=-573.2479646\MP2/GTBas2=-573.2254556\MP4/GTBas2=-573.2622287\MP2/GTBas3=-573.3414633\MP4/GTBas3=-573.390788\HF/GTLargeXP=-572.8584714\MP2/GTLargeXP=-573.8453658\HF/GFHFB1=-572.8773358\HF/GFHFB2=-572.8801951\G4=-573.9580612

H(O) CSiCl₃

\\0,1\O,0,1.5748076873,-0.2487789776,-0.2413130607\C,0,0.6482192302,0.5154934741,-0.1597511343\Si,0,-1.1793514043,-0.0931674092,-0.157738073\H,0,0.8113588837,1.616347265,-0.0813667315\Cl,0,-1.2476227259,-2.12560977,-0.3095390531\Cl,0,-2.1472167356,0.7790760329,-1.7462654684\Cl,0,-2.0595649353,0.5267293848,1.592093521\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-1781.5693615\MP4/GTBas1=-1781.6429187\CCSD(T)/G3Bas1=-1781.6407318\MP2/GTBas2=-1781.587029\MP4/GTBas2=-1781.6618989\MP2/GTBas3=-1781.8396031\MP4/GTBas3=-1781.9453245\HF/GTLargeXP=-1780.9863251\MP2/GTLargeXP=-1783.3781735\HF/GFHFB1=-1781.0285693\HF/GFHFB2=-1781.0357427\G4=-1783.6357668

H(O) CSiF₃

\\0,1\O,0,1.5911693361,-0.2401109682,-0.2484312756\C,0,0.6338706117,0.4908406946,-0.1419013911\Si,0,-1.129998866,-0.224672344,-0.0933483331\H,0,0.7731800743,1.5956666389,-0.0719297942\F,0,-1.0852189942,-1.7942759964,-0.12959928\F,0,-1.9632458014,0.2924998304,-1.328504414\F,0,-1.8699963605,0.2374421446,1.2205944879\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-701.6218003\MP4/GTBas1=-701.6635038\CCSD(T)/G3Bas1=-701.6566583\MP2/GTBas2=-701.6566322\MP4/GTBas2=-701.7014798\MP2/GTBas3=-701.9034117\MP4/GTBas3=-701.9650052\HF/GTLargeXP=-700.928978\MP2/GTLargeXP=-702.7075527\HF/GFHFB1=-700.9723571\HF/GFHFB2=-700.9848527\G4=-702.9220139

H(O) CSiH₃

\\0,1\O,0,1.6074225416,-0.2265670939,-0.2317407441\C,0,0.6242128207,0.4718989665,-0.1434839702\Si,0,-1.1658972481,-0.2486648978,-0.0912968037\H,0,0.7395072032,1.5846233773,-0.0907773897\H,0,-1.1063495281,-1.7256691247,-0.1365479321\H,0,-1.9211688531,0.2852149933,-1.2533740357\H,0,-1.8279569362,0.2165337793,1.1541108755\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-404.3158967\MP4/GTBas1=-404.3586374\CCS

D(T)/G3Bas1=-404.3588061\MP2/GTBas2=-404.3276721\MP4/GTBas2=-404.3710646\MP2/GTBas3=-404.4396475\MP4/GTBas3=-404.4935855\HF/GTLargeXP=-404.0141073\MP2/GTLargeXP=-404.9074009\HF/GFHFB1=-404.0284121\HF/GFHFB2=-404.0321803\G4=-405.0022629

H(O) CCB₃

\0,1\O,0,1.5990141455,0.1546011809,-0.303444944\C,0,0.5351871933,0.6628185805,-0.1232838505\C,0,-0.8089970963,-0.0897955306,-0.2064716587\H,0,0.3897490469,1.7312223131,0.123972987\Br,0,-0.5820527422,-1.9561546087,-0.6357103015\Br,0,-1.8511368385,0.8387863577,-1.587198885\Br,0,-1.6553937087,0.1415917071,1.5495066528\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-7868.6802671\MP4/GTBas1=-7868.7234038\CCSD(T)/G3Bas1=-7868.7113333\MP2/GTBas2=-7868.6966543\MP4/GTBas2=-7868.7408967\MP2/GTBas3=-7868.8947298\MP4/GTBas3=-7868.9656149\HF/GTLargeXP=-7868.3922247\MP2/GTLargeXP=-7872.4676064\HF/GFHFB1=-7868.5960833\HF/GFHFB2=-7868.5991742\G4=-7872.8345558

H(O) CCCl₃

\0,1\O,0,1.5828141277,0.1418248422,-0.3113862956\C,0,0.5246382964,0.6564725686,-0.1253093049\C,0,-0.8295810775,-0.0944226918,-0.2056916493\H,0,0.3799664072,1.7240646741,0.1255110177\Cl,0,-0.6252309307,-1.7992634986,-0.6045026588\Cl,0,-1.7970943208,0.7502984216,-1.4604333865\Cl,0,-1.6091325023,0.1041056839,1.3991622774\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-1530.4102128\MP4/GTBas1=-1530.4867581\CCSD(T)/G3Bas1=-1530.4810391\MP2/GTBas2=-1530.4276066\MP4/GTBas2=-1530.5055681\MP2/GTBas3=-1530.6644781\MP4/GTBas3=-1530.771584\HF/GTLargeXP=-1529.7341388\MP2/GTLargeXP=-1531.9412376\HF/GFHFB1=-1529.7741545\HF/GFHFB2=-1529.7797761\G4=-1532.1885416

H(O) CC=CF₃

\0,1\O,0,-1.8137383149,-0.3768802041,-0.0042089854\C,0,-0.9445032518,0.4587741238,-0.0016204555\C,0,0.4711878272,0.1421817399,0.0012172457\C,0,1.6513997196,-0.091453213,0.0035084797\H,0,-1.165549979,1.5433601893,-0.0018554472\C,0,3.0881235443,-0.3922565055,0.0069149193\F,0,3.8147540324,0.7294745767,-0.0090049251\F,0,3.421937448,-1.1151137859,-1.0654406121\F,0,3.4226789742,-1.0848469211,1.0988597807\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-526.3294276\MP4/GTBas1=-526.3965792\CCSD(T)/G3Bas1=-526.3857805\MP2/GTBas2=-526.366768\MP4/GTBas2=-526.4368162\MP2/GTBas3=-526.6475524\MP4/GTBas3=-526.7343187\HF/GTLargeXP=-525.3396679\MP2/GTLargeXP=-527.2923827\HF/GFHFB1=-525.3868119\HF/GFHFB2=-525.3963367\G4=-527.5406005

H(O) CC=CH₃

\0,1\O,0,-1.792302099,-0.3779722773,-0.002880243\C,0,-0.903917753,0.4436646488,-0.0017577942\C,0,0.5008105085,0.1305266514,0.0013539443\C,0,1.6870546394,-0.0956100491,0.0038669548\H,0,-1.1256296803,1.5307636368,-0.0031229966\C,0,3.1086763433,-0.389675279,0.0069272274\H,0,3.7091203506,0.5254950336,-0.0055133707\H,0,3.3809130562,-0.9889186303,-0.8687161961\H,0,3.3816586565,-0.9650637349,0.8982224741\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-229.2628387\MP4/GTBas1=-229.3222449\CCSD(T)/G3Bas1=-229.318309\MP2/GTBas2=-229.2770999\MP4/GTBas2=-229.3372617\MP2/GTBas3=-229.4247032\MP4/GTBas3=-229.4934949\HF/GTLargeXP=-228.6681788\MP2/GTLargeXP=-229.7464233\HF/GFHFB1=-228.6862535\HF/GFHFB2=-228.6897187\G4=-229.8601852

H (O) CC (C≡N)₃

\\0,1\\O,0,2.1774147524,0.1913944173,-0.0154976063\\C,0,1.214
9468141,-0.4987024492,0.002254462\\C,0,-0.2736406591,0.1042182048,0.027
0881623\\C,0,-0.2307809479,1.5716412653,0.0248475925\\C,0,-0.9532085337,
-0.416082144,-1.1706118037\\C,0,-0.9116352796,-0.4134166948,1.248669712
8\\H,0,1.2091569459,-1.6028149876,0.0040651228\\N,0,-1.350224401,-0.8596
981146,2.2185152894\\N,0,-1.4256473728,-0.8640417346,-2.1236423641\\N,0,
-0.1822913183,2.7235822375,0.0235214322\\Version=EM64L-G09RevA.02\\Stat
e=1-A\\MP2/GTbas1=-429.3217339\\MP4/GTbas1=-429.4089354\\CCSD(T)/G3bas1=-
429.3916762\\MP2/GTbas2=-429.3455693\\MP4/GTbas2=-429.4339665\\MP2/GTbas3
=-429.5650689\\MP4/GTbas3=-429.6661797\\HF/GTLargeXP=-428.1870955\\MP2/GT
LargeXP=-430.1433967\\HF/GFHFB1=-428.2181175\\HF/GFHFB2=-428.2237735\\G4=
-430.3619253

H (O) CC₆H₄-4-Br

\\0,1\\O,0,2.8907714491,-0.3122661605,-0.0000110152\\C,0,2.0
341790571,0.5404777762,0.0000097924\\C,0,0.5792717447,0.2707503704,0.00
00094\\C,0,-0.3288337391,1.331998863,0.0000151299\\C,0,-1.6987230388,1.0
931805408,0.0000147299\\C,0,-2.1462004119,-0.2250326598,0.0000085534\\C,
0,-1.2578158161,-1.3015445735,0.000002744\\C,0,0.1050706081,-1.04662469
86,0.0000032476\\H,0,2.2990819561,1.6217349643,-0.0000032485\\H,0,0.0397
030373,2.3539811997,0.0000198416\\H,0,-2.4079212873,1.9114072437,0.0000
188838\\Br,0,-4.0179529038,-0.5698966212,0.000005885\\H,0,-1.6342806797,
-2.3169147491,-0.0000024583\\H,0,0.8252200242,-1.8573314955,-0.00000148
56\\Version=EM64L-G09RevA.02\\State=1-A\\MP2/GTbas1=-2916.2735593\\MP4/GT
bas1=-2916.3645153\\CCSD(T)/G3bas1=-2916.3560394\\MP2/GTbas2=-2916.29614
78\\MP4/GTbas2=-2916.3878027\\MP2/GTbas3=-2916.5462298\\MP4/GTbas3=-2916.
6559576\\HF/GTLargeXP=-2915.3575377\\MP2/GTLargeXP=-2918.1619482\\HF/GFHFB
1=-2915.4483408\\HF/GFHFB2=-2915.4535157\\G4=-2918.4229183

H (O) CC₆H₄-4-Cl

\\0,1\\O,0,2.8806587224,-0.3136654317,0.0000603259\\C,0,2.02
32400576,0.5385064673,-0.0000483184\\C,0,0.5689186876,0.2686062099,-0.0
000220086\\C,0,-0.3392875098,1.3300594191,-0.0000061129\\C,0,-1.70846509
33,1.0912764448,0.0000126507\\C,0,-2.1567584312,-0.2270579145,0.0000172
786\\C,0,-1.2679053452,-1.3037523595,0.0000027353\\C,0,0.0944132456,-1.0
489768939,-0.0000163269\\H,0,2.287769054,1.6199243709,0.0000671608\\H,0,
0.0295149517,2.3518534214,-0.0000103061\\H,0,-2.4216922757,1.9060211146
,0.0000239276\\Cl,0,-3.8743993828,-0.5422176988,0.0000418895\\H,0,-1.649
3675233,-2.3174056472,0.0000064489\\H,0,0.8149408425,-1.8592515022,-0.0
000293445\\Version=EM64L-G09RevA.02\\State=1-A\\MP2/GTbas1=-803.5178862\\
MP4/GTbas1=-803.6202459\\CCSD(T)/G3bas1=-803.6137649\\MP2/GTbas2=-803.54
04527\\MP4/GTbas2=-803.6436063\\MP2/GTbas3=-803.8030817\\MP4/GTbas3=-803.
9251082\\HF/GTLargeXP=-802.4718437\\MP2/GTLargeXP=-804.6538867\\HF/GFHFB1
=-802.5080065\\HF/GFHFB2=-802.5140541\\G4=-804.8751126

H (O) CC₆H₄-4-F

\\0,1\\O,0,2.8526769151,-0.3182044945,-0.0000023935\\C,0,1.99
27031001,0.5322032808,0.0000078478\\C,0,0.5405977438,0.2630807697,0.000
0088816\\C,0,-0.3677031197,1.3257388127,0.0000142103\\C,0,-1.7363611083,
1.0873874712,0.0000139396\\C,0,-2.1767775888,-0.230435655,0.0000081503\\
C,0,-1.2960944973,-1.3097174358,0.0000027409\\C,0,0.0656589509,-1.05556
76913,0.0000032114\\H,0,2.2565591566,1.6142483467,0.0000025901\\H,0,0.00
34740024,2.3465639802,0.000018127\\H,0,-2.461185239,1.8924591046,0.0000
177784\\F,0,-3.4874624503,-0.4714907887,0.000007408\\H,0,-1.6923881839,-
2.3181823568,-0.0000015428\\H,0,0.7878823183,-1.864153344,-0.000000949\\
\\Version=EM64L-G09RevA.02\\State=1-A\\MP2/GTbas1=-443.5043284\\MP4/GTbas1

=-443.5984733\CCSD(T)/G3Bas1=-443.5908352\MP2/GTBas2=-443.5347097\MP4/
GTBas2=-443.6301682\MP2/GTBas3=-443.7979962\MP4/GTBas3=-443.9078565\HF/
GTLargeXP=-442.4317648\MP2/GTLargeXP=-444.4023976\HF/GFHFB1=-442.4683
539\HF/GFHFB2=-442.4753332\G4=-444.6109241

H(O)CC₆H₄-4-CH₃

\0,1\O,0,2.911927006,-0.3053946958,0.0023526193\C,0,2.048952
9428,0.5425514134,0.0015045067\C,0,0.5971626702,0.2727258365,0.0002355
875\C,0,-0.3114617116,1.3322315362,-0.0005809708\C,0,-1.6800556706,1.0
847035316,-0.001653841\C,0,-2.1686557755,-0.2243359387,-0.0020454026\C
,0,-1.247126983,-1.2839793865,-0.0010299832\C,0,0.115873747,-1.0437050
685,0.0000239099\H,0,2.3110527515,1.6254262309,0.0016068861\H,0,0.0585
004814,2.3540259151,-0.0001998395\H,0,-2.3794504344,1.9149962881,-0.00
21418649\C,0,-3.6497780666,-0.5043606393,-0.0045343963\H,0,-1.61438524
42,-2.3062304072,-0.0009924915\H,0,0.8340649234,-1.856263221,0.0008694
924\H,0,-4.2334193903,0.4193263857,0.0084816926\H,0,-3.9407687659,-1.1
005158912,0.867565584\H,0,-3.9421124802,-1.0758218893,-0.8927214887\\
Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-383.6570575\MP4/GTBas1=-
383.7633724\CCSD(T)/G3Bas1=-383.7581772\MP2/GTBas2=-383.6796732\MP4/GT
Bas2=-383.7867636\MP2/GTBas3=-383.9353306\MP4/GTBas3=-384.0561292\HF/G
TLargeXP=-382.592673\MP2/GTLargeXP=-384.4907191\HF/GFHFB1=-382.6227605
\HF/GFHFB2=-382.6284014\G4=-384.6691954

H(O)CPF₄

\0,1\C,0,-1.7822718338,1.1109544975,-0.0345187683\O,0,-2.29
22269271,2.1198889307,0.3591252564\P,0,0.0090931816,0.6200956764,0.309
5178448\F,0,-0.507235653,-0.6952081282,1.0138815648\F,0,0.2771964438,0
.5840747509,-1.2460192619\F,0,0.2740953135,1.9201289896,1.1374408667\F
,0,1.4973001363,0.1575893396,0.5643665786\H,0,-2.3376606614,0.36619594
35,-0.6485040812\\Version=AM64L-G09RevA.02\State=1-A\MP2/GTBas1=-852.9
629704\MP4/GTBas1=-853.0121359\CCSD(T)/G3Bas1=-853.0021268\MP2/GTBas2=
-853.0024419\MP4/GTBas2=-853.0558359\MP2/GTBas3=-853.323828\MP4/GTBas3
=-853.3978232\HF/GTLargeXP=-852.1037716\MP2/GTLargeXP=-854.251081\HF/G
FHFB1=-852.1599278\HF/GFHFB2=-852.1769558\G4=-854.5179502

H(O)CGeH₃

\0,1\C,0,-1.6481407402,0.859837617,-0.1315794114\O,0,-2.3008
985525,1.6054861903,0.5512604592\Ge,0,0.2272509751,0.3264504796,0.3486
915211\H,0,-2.0794006505,0.4361254342,-1.0713495263\H,0,0.6121123734,1
.0160530617,1.6601319616\H,0,1.1743181013,0.7440320559,-0.7877923432\H
,0,0.2923287352,-1.2024043052,0.4945469876\\Version=AM64L-G09RevA.02\S
tate=1-A\MP2/GTBas1=-2190.6465938\MP4/GTBas1=-2190.6797099\CCSD(T)/G3B
as1=-2190.67603\MP2/GTBas2=-2190.6569092\MP4/GTBas2=-2190.6905751\MP2/
GTBas3=-2190.7671059\MP4/GTBas3=-2190.811049\HF/GTLargeXP=-2190.411903
6\MP2/GTLargeXP=-2192.0188326\HF/GFHFB1=-2190.4829699\HF/GFHFB2=-2190.
4852479\G4=-2192.1561993

ALDEHYDE HYDRATES

H(HO)₂CC(O)CH₃

\0,1\O,0,-1.63714,0.77491,0.2528\C,0,-0.70135,-0.2344,0.3873
\O,0,-0.9062,-1.31566,-0.50495\C,0,0.70883,0.29048,0.03163\C,0,1.86345
, -0.6578,0.19664\O,0,0.81071,1.41952,-0.39157\H,0,-0.73256,-0.59164,1.
42973\H,0,-1.20484,1.46312,-0.28139\H,0,-1.83146,-1.5721,-0.42194\H,0,
1.67889,-1.55126,-0.40777\H,0,2.79622,-0.17854,-0.10158\H,0,1.92925,-0
.98936,1.23924\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-342.588
3373\MP4/GTBas1=-342.6552211\CCSD(T)/G3Bas1=-342.6517947\MP2/GTBas2=-3

42.6160406\MP4/GTBas2=-342.6849167\MP2/GTBas3=-342.8464038\MP4/GTBas3=-342.9297091\HF/GTLargeXP=-341.810318\MP2/GTLargeXP=-343.2909376\HF/GFHFBI=-341.8381304\HF/GFHFB2=-341.8441424\G4=-343.4406977

H (HO)₂CNH₂

\0,1\O,0,-0.5536283267,1.1904605009,-0.0346177102\C,0,-0.0695081799,-0.0426351252,0.4110348163\O,0,-0.7737807936,-1.1334908674,-0.1267557175\N,0,1.2924629458,-0.2249863424,-0.0295096263\H,0,-0.2037363474,-0.00399203,1.5063647892\H,0,-0.2843685294,1.2501983774,-0.9618928617\H,0,-1.7005241965,-1.0028706979,0.0992143078\H,0,1.5769198087,-1.1871608724,0.1204988339\H,0,1.9105536189,0.3781070571,0.5021131685\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-245.5889312\MP4/GTBas1=-245.6323536\CCSD(T)/G3Bas1=-245.6321082\MP2/GTBas2=-245.614779\MP4/GTBas2=-245.6596749\MP2/GTBas3=-245.7856448\MP4/GTBas3=-245.8412576\HF/GTLargeXP=-245.050178\MP2/GTLargeXP=-246.1031731\HF/GFHFB1=-245.0706143\HF/GFHFB2=-245.0751974\G4=-246.2032821

H (HO)₂CC (CH₃)₃

\0,1\O,0,-1.5805372498,-1.1504263599,-0.1026466034\C,0,-0.8556477033,0.0021703036,-0.4711384562\O,0,-1.4768904661,1.1635180185,0.0326820247\C,0,0.61592173,-0.0010996144,0.0043293713\C,0,1.3125409867,-1.2372176701,-0.5893014003\C,0,1.302348095,1.2783175586,-0.5058398294\C,0,0.6777981142,-0.0479324763,1.5421480957\H,0,-0.8783743798,-0.009322498,-1.5712849925\H,0,-1.6173062743,-1.1642486059,0.8614504898\H,0,-2.3912434301,1.1459948204,-0.2700218375\H,0,1.3163622026,-1.2013842048,-1.6846623144\H,0,2.3538384885,-1.2871290689,-0.2548037621\H,0,0.8062337551,-2.1576222187,-0.2876578086\H,0,0.8438693234,2.1717420597,-0.0766536309\H,0,2.3655046361,1.271924881,-0.2431259506\H,0,1.2313169031,1.3538951757,-1.5971088638\H,0,0.2695611215,-0.986030521,1.9369370854\H,0,1.7166100393,0.0121101457,1.8817378898\H,0,0.1236041078,0.7841502749,1.9835304929\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-347.0668178\MP4/GTBas1=-347.1622196\CCSD(T)/G3Bas1=-347.1629164\MP2/GTBas2=-347.0922064\MP4/GTBas2=-347.1898094\MP2/GTBas3=-347.3712417\MP4/GTBas3=-347.4853195\HF/GTLargeXP=-346.1795641\MP2/GTLargeXP=-347.8527742\HF/GFHFB1=-346.207579\HF/GFHFB2=-346.213698\G4=-347.9918691

H (HO)₂CC≡N

\0,1\O,0,-0.99504,1.18814,-0.0738\C,0,-0.41615,-0.0032,0.37279\O,0,-0.96362,-1.1458,-0.22217\C,0,1.04029,-0.04178,0.08844\N,0,2.17441,-0.01988,-0.12488\H,0,-0.55797,0.00547,1.46146\H,0,-0.84724,1.25093,-1.02652\H,0,-1.89128,-1.18607,0.03961\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-282.3884741\MP4/GTBas1=-282.4371257\CCSD(T)/G3Bas1=-282.4331695\MP2/GTBas2=-282.4106618\MP4/GTBas2=-282.4607187\MP2/GTBas3=-282.5831212\MP4/GTBas3=-282.6437367\HF/GTLargeXP=-281.7377437\MP2/GTLargeXP=-282.948991\HF/GFHFB1=-281.7603557\HF/GFHFB2=-281.7650628\G4=-283.0781246

H (HO)₂CN (CH₃)₂

\0,1\O,0,-1.02693,-0.98627,0.89831\C,0,-0.6647,-0.36444,-0.33037\O,0,-1.5706,0.6634,-0.63344\N,0,0.65326,0.19513,-0.38588\C,0,0.88931,1.3096,0.52181\C,0,1.69918,-0.81289,-0.32321\H,0,-0.71609,-1.18631,-1.05715\H,0,-1.00836,-0.3018,1.57879\H,0,-2.44717,0.3109,-0.44641\H,0,0.97761,1.00451,1.58182\H,0,1.82783,1.80103,0.24833\H,0,0.07907,2.03354,0.42803\H,0,1.50893,-1.59321,-1.0667\H,0,2.66193,-0.34862,-0.55876\H,0,1.78085,-1.29658,0.66492\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-323.904725\MP4/GTBas1=-323.9803712\CCSD(T)/G3Bas1=-323.9804354\MP2/GTBas2=-323.9313135\MP4/GTBas2=-324.0091532\MP2/GTBas3=-324.173

7535\MP4/GTBas3=-324.266317\HF/GTLargeXP=-323.1210068\MP2/GTLargeXP=-324.6077384\HF/GFHFB1=-323.1469176\HF/GFHFB2=-323.1527057\G4=-324.7395894

H (HO)₂CCH=CH₂

\0,1\O,0,-1.0314218706,1.2601107376,0.5403019286\C,0,-0.4771562058,-0.0262570607,0.3373810443\O,0,-1.3982551093,-0.9000131176,-0.2633794842\C,0,0.7635960299,0.0456957239,-0.51089061\H,0,-0.222792558,-0.3617922384,1.3547517944\H,0,-1.1661110069,1.6441180445,-0.3353735229\H,0,-2.1870371726,-0.8946909129,0.289041713\C,0,0.9532143797,-0.6163022767,-1.6459690095\H,0,1.8637846031,-0.4989883374,-2.2239642607\H,0,0.2050807242,-1.3012344874,-2.027393573\H,0,1.5157081863,0.7287839251,-0.1238960201\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-267.5205107\MP4/GTBas1=-267.5812095\CCSD(T)/G3Bas1=-267.5818016\MP2/GTBas2=-267.5448345\MP4/GTBas2=-267.6067583\MP2/GTBas3=-267.7322169\MP4/GTBas3=-267.8056701\HF/GTLargeXP=-266.8940723\MP2/GTLargeXP=-268.0931861\HF/GFHFB1=-266.916241\HF/GFHFB2=-266.9209863\G4=-268.2120315

H (HO)₂CC≡CH

\0,1\O,0,-1.03629,1.18417,-0.08401\C,0,-0.44168,-0.00685,0.37444\O,0,-1.00486,-1.1479,-0.22797\C,0,1.00286,-0.04082,0.11523\C,0,2.18438,-0.02342,-0.09687\H,0,-0.62549,0.00128,1.458\H,0,-0.80211,1.27854,-1.01588\H,0,-1.94717,-1.12875,-0.02236\H,0,3.23065,-0.01477,-0.28074\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-266.2985684\MP4/GTBas1=-266.3513857\CCSD(T)/G3Bas1=-266.3497105\MP2/GTBas2=-266.3220529\MP4/GTBas2=-266.3761287\MP2/GTBas3=-266.4959001\MP4/GTBas3=-266.5601877\HF/GTLargeXP=-265.6774224\MP2/GTLargeXP=-266.8526387\HF/GFHFB1=-265.6992852\HF/GFHFB2=-265.7038277\G4=-266.9762816

H (HO)₂CF

\0,1\H,0,-0.8077208055,0.9480243897,-0.9074639808\O,0,-0.993966352,0.0262632885,-0.682950602\H,0,1.6716745856,0.1177648548,0.8014838101\O,0,1.1299324989,0.176590851,0.0063439474\C,0,-0.1243634747,-0.3303250722,0.3010640161\H,0,-0.1485480454,-1.4234768687,0.3928991814\F,0,-0.5143384068,0.1777285568,1.5259436278\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-289.4285494\MP4/GTBas1=-289.46358\CCSD(T)/G3Bas1=-289.4614169\MP2/GTBas2=-289.4565458\MP4/GTBas2=-289.4934858\MP2/GTBas3=-289.6333926\MP4/GTBas3=-289.6816914\HF/GTLargeXP=-288.8981628\MP2/GTLargeXP=-289.9859044\HF/GFHFB1=-288.9244932\HF/GFHFB2=-288.9301965\G4=-290.109065

H (HO)₂CH

\0,1\O,0,1.0078007319,-0.4955545364,-0.0646313461\C,0,0.0273740415,0.4753355049,0.1919887696\O,0,-1.2470356889,-0.0741840055,0.4009556925\H,0,0.2408486635,1.053419586,1.1010626449\H,0,0.0551556043,1.145018433,-0.6780228501\H,0,1.0440363086,-1.0745123077,0.705404246\H,0,-1.4873496609,-0.5503126743,-0.4021671568\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-190.3874521\MP4/GTBas1=-190.4202761\CCSD(T)/G3Bas1=-190.4203064\MP2/GTBas2=-190.4068996\MP4/GTBas2=-190.4408556\MP2/GTBas3=-190.540777\MP4/GTBas3=-190.5835897\HF/GTLargeXP=-189.9872584\MP2/GTLargeXP=-190.7848681\HF/GFHFB1=-190.0037478\HF/GFHFB2=-190.0074233\G4=-190.8629821

H (HO)₂COH

\0,1\O,0,-1.2597990819,0.2934383737,-0.7943850379\O,0,0.9952324556,0.3342879691,-1.0011818975\H,0,-1.1664103259,1.2220908276,-1.0467200781\H,0,1.7455138954,0.4971579002,-0.4186459632\C,0,-0.0659214689

, -0.0675433263, -0.1962752426\H, 0, -0.1136406354, -1.1628632656, -0.0886660998\O, 0, 0.134774547, 0.5485366878, 1.0542921305\H, 0, -0.5840093858, 0.2739148334, 1.6340421886\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-265.4354107\MP4/GTBas1=-265.473293\CCSD(T)/G3Bas1=-265.4724109\MP2/GTBas2=-265.4613728\MP4/GTBas2=-265.5009758\MP2/GTBas3=-265.6402941\MP4/GTBas3=-265.6911685\HF/GTLargeXP=-264.8925137\MP2/GTLargeXP=-265.9714631\HF/GFHFB1=-264.9152281\HF/GFHFB2=-264.9203131\G4=-266.0822264

H (HO)₂CCH₃

\\0,1\O,0,-0.73485,1.1648,-0.03209\C,0,-0.04767,-0.00203,0.36114\O,0,-0.65086,-1.15918,-0.17203\C,0,1.40619,-0.01146,-0.08356\H,0,-0.11685,0.00742,1.45867\H,0,-0.66738,1.22062,-0.9934\H,0,-1.57494,-1.14478,0.10132\H,0,1.91782,0.87835,0.28983\H,0,1.91677,-0.90312,0.28902\H,0,1.45913,-0.02253,-1.17798\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-229.562765\MP4/GTBas1=-229.611507\CCSD(T)/G3Bas1=-229.6116448\MP2/GTBas2=-229.583497\MP4/GTBas2=-229.6336602\MP2/GTBas3=-229.7529907\MP4/GTBas3=-229.8139849\HF/GTLargeXP=-229.0421302\MP2/GTLargeXP=-230.0561797\HF/GFHFB1=-229.0615154\HF/GFHFB2=-229.0658121\G4=-230.1501925

H (HO)₂CNO₂

\\0,1\H,0,0.45005789,-1.4282008119,-0.187156093\O,0,1.2418109377,0.350500771,-0.6597259294\O,0,-1.5506077507,-0.1953458926,-1.1856716897\C,0,0.4259772471,-0.3909305328,0.155394774\N,0,-1.0753590245,0.0629983234,-0.1049825268\H,0,1.451430725,1.1707979161,-0.1931018111\H,0,-0.1072381982,0.2527145755,1.8431507018\O,0,-1.6238918379,0.6731297792,0.8095464562\O,0,0.6606400116,-0.2362841279,1.4877261181\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-394.3998079\MP4/GTBas1=-394.4535471\CCSD(T)/G3Bas1=-394.4425847\MP2/GTBas2=-394.430962\MP4/GTBas2=-394.4872991\MP2/GTBas3=-394.6736354\MP4/GTBas3=-394.7452299\HF/GTLargeXP=-393.5346289\MP2/GTLargeXP=-395.1523325\HF/GFHFB1=-393.5678188\HF/GFHFB2=-393.5749032\G4=-395.3239854

H (HO)₂CC₆H₅

\\0,1\H,0,-3.267317179,0.6262299649,0.9752465529\O,0,-2.3141718804,0.5196890651,1.0652298889\H,0,3.5715774965,-0.1160489098,0.0167377237\H,0,2.3230966701,-1.2086862314,-1.8303486663\O,0,-2.4063482795,-0.9407633374,-0.7500734337\C,0,2.4893152412,-0.0489550936,-0.023854583\C,0,1.788715026,-0.6619099014,-1.0602338888\H,0,2.333664288,1.1272510245,1.7716007803\C,0,1.793973275,0.6497707623,0.9601147205\C,0,0.4002948477,-0.576254277,-1.110374672\H,0,-0.151442852,-1.0553746299,-1.9115662076\H,0,-2.1072437963,-1.6819903243,-0.2079498112\C,0,0.4050126391,0.7378622812,0.9103769563\C,0,-0.3017473549,0.1220403073,-0.1243706939\H,0,-0.1404192504,1.2764106296,1.6749701358\C,0,-1.8138652245,0.2228484546,-0.2167721347\H,0,-2.0990236668,1.0085702154,-0.9327826673\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-420.6953651\MP4/GTBas1=-420.7951959\CCSD(T)/G3Bas1=-420.7920983\MP2/GTBas2=-420.7275621\MP4/GTBas2=-420.8286958\MP2/GTBas3=-421.0088744\MP4/GTBas3=-421.1250646\HF/GTLargeXP=-419.6036159\MP2/GTLargeXP=-421.5990253\HF/GFHFB1=-419.637358\HF/GFHFB2=-419.6440864\G4=-421.7862721

H (HO)₂CCF₃

\\0,1\O,0,-1.47426,-1.1705,-0.04919\C,0,-0.84773,0.00631,-0.45916\O,0,-1.41623,1.15763,0.09151\C,0,0.62536,0.0133,-0.01889\F,0,1.28836,-0.98003,-0.61743\F,0,1.23124,1.16048,-0.31845\F,0,0.70823,-0.17672,1.30868\H,0,-0.87893,-0.00123,-1.55629\H,0,-1.37291,-1.22724,0.91056\H,0,-2.34048,1.18029,-0.17974\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-526.6434998\MP4/GTBas1=-526.7002181\CCSD(T)/G3Bas1=-526.693

8565\MP2/GTbas2=-526.686996\MP4/GTbas2=-526.7474307\MP2/GTbas3=-526.99
13399\MP4/GTbas3=-527.0704029\HF/GTLargeXP=-525.7324261\MP2/GTLargeXP=
-527.6170329\HF/GFHFB1=-525.780351\HF/GFHFB2=-525.7907059\G4=-527.8458
771

H(HO)₂CSi(CH₃)₃

\\0,1\O,0,-1.9037,-1.15419,-0.1234\C,0,-1.20056,0.01384,-
0.53863\O,0,-1.78983,1.18419,-0.00206\Si,0,0.64287,0.00168,0.00193\C,0
,1.49453,-1.44982,-0.84211\C,0,1.45203,1.62921,-0.48426\C,0,0.66778,-0
.21586,1.87593\H,0,-1.30251,-0.00495,-1.63464\H,0,-1.83876,-1.19459,0.
83814\H,0,-2.71343,1.20368,-0.28327\H,0,1.49642,-1.3337,-1.93122\H,0,2
.53737,-1.54017,-0.51942\H,0,0.98942,-2.39291,-0.6113\H,0,0.93676,2.47
384,-0.01771\H,0,2.503,1.66009,-0.17682\H,0,1.42232,1.78024,-1.56874\H
,0,0.25107,-1.18107,2.18543\H,0,1.69142,-0.17273,2.26289\H,0,0.09217,0
.57458,2.3678\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTbas1=-598.0760
3\MP4/GTbas1=-598.1735104\CCSD(T)/G3bas1=-598.1752739\MP2/GTbas2=-598.
1043607\MP4/GTbas2=-598.2038595\MP2/GTbas3=-598.3904251\MP4/GTbas3=-59
8.5088642\HF/GTLargeXP=-597.2686935\MP2/GTLargeXP=-599.1388421\HF/GFHFB
B1=-597.2984029\HF/GFHFB2=-597.3062171\G4=-599.2982877

H(HO)₂CBR

\\0,1\H,0,-0.043729552,-0.3885228873,-1.5844540384\O,0,0.2
789092526,-0.5691470979,-0.6935536747\H,0,-1.4169331716,-1.6118762217,
-0.0624797056\C,0,-0.7859310727,-0.7471487687,0.1429685108\Br,0,-2.143
6337503,0.8139555481,-0.2114180619\O,0,-0.390561038,-0.7681605592,1.42
64777778\H,0,0.2603693321,-0.0633800132,1.553539192\\Version=EM64L-G09
RevA.02\State=1-A\MP2/GTbas1=-2762.1797537\MP4/GTbas1=-2762.2134658\CC
SD(T)/G3bas1=-2762.2106806\MP2/GTbas2=-2762.1974418\MP4/GTbas2=-2762.2
325533\MP2/GTbas3=-2762.363656\MP4/GTbas3=-2762.4141151\HF/GTLargeXP=-
2761.8099916\MP2/GTLargeXP=-2763.7256412\HF/GFHFB1=-2761.8902695\HF/GF
HFB2=-2761.8941137\G4=-2763.9035248

H(HO)₂CCl

\\0,1\H,0,-0.3594711681,-0.6245239532,-1.7555290376\O,0,0.
241354491,-0.2857076294,-1.0818285259\H,0,-0.5343309703,-1.379879292,0
.5160086408\C,0,-0.3681520167,-0.3674002629,0.1443833373\Cl,0,-2.14368
91997,0.2938655797,-0.0325563664\O,0,0.3300179951,0.3301190694,1.06356
10106\H,0,0.5719108686,1.1802364884,0.6702309412\\Version=EM64L-G09Rev
A.02\State=1-A\MP2/GTbas1=-649.423463\MP4/GTbas1=-649.4682848\CCSD(T)/
G3bas1=-649.4672604\MP2/GTbas2=-649.4424584\MP4/GTbas2=-649.4887521\MP
2/GTbas3=-649.6229305\MP4/GTbas3=-649.6852388\HF/GTLargeXP=-648.924797
3\MP2/GTLargeXP=-650.2198467\HF/GFHFB1=-648.9506593\HF/GFHFB2=-648.955
1466\G4=-650.3573322

H(HO)₂CSiCl₃

\\0,1\O,0,-0.9766543056,1.1398916225,0.0059858971\C,0,-
0.3573293349,0.0380918263,0.6274106023\O,0,-0.9507215713,-1.1875021822
,0.2880222849\Si,0,1.4805589249,-0.0862089796,0.1268506251\H,0,-0.4285
136184,0.2495353302,1.7036166806\H,0,-0.9156401578,1.0127559953,-0.950
3786656\H,0,-1.8682029965,-1.1716901424,0.5886755743\Cl,0,1.5748590939
, -0.0070229283,-1.9310883918\Cl,0,2.3642688749,-1.8141091817,0.7856398
085\Cl,0,2.5041650907,1.51688864,0.8987555846\\Version=EM64L-G09RevA.0
2\State=1-A\MP2/GTbas1=-1857.7922317\MP4/GTbas1=-1857.8739646\CCSD(T)/
G3bas1=-1857.8734151\MP2/GTbas2=-1857.8198161\MP4/GTbas2=-1857.9036693
\MP2/GTbas3=-1858.1358925\MP4/GTbas3=-1858.2539769\HF/GTLargeXP=-1857.
0599586\MP2/GTLargeXP=-1859.7677825\HF/GFHFB1=-1857.1090337\HF/GFHFB2=
-1857.1178597\G4=-1860.0486461

H(HO)₂CSiF₃

\\0,1\O,0,-0.9816552425,1.1459732473,-0.0018401329\C,0,-
0.3401348526,0.0321583708,0.5972802696\O,0,-0.9635420661,-1.1904556288
,0.2845028785\Si,0,1.434293955,-0.0857831689,-0.0157148764\H,0,-0.3821
699698,0.2468020454,1.6742840416\H,0,-0.9452484811,1.0262759178,-0.959
6010535\H,0,-1.8686232509,-1.1609169167,0.6196725187\F,0,1.4160710109,
0.0748988246,-1.5892694529\F,0,2.1500036342,-1.4432360947,0.3407048762
\F,0,2.3064852629,1.0867734031,0.578740931\\Version=EM64L-G09RevA.02\St
ate=1-A\MP2/GTBas1=-777.845442\MP4/GTBas1=-777.895718\CCSD(T)/G3Bas1=
-777.890281\MP2/GTBas2=-777.8891196\MP4/GTBas2=-777.9434181\MP2/GTBas3
=-778.1998887\MP4/GTBas3=-778.2743646\HF/GTLargeXP=-777.0046486\MP2/GT
LargeXP=-779.0977706\HF/GFHFB1=-777.0544895\HF/GFHFB2=-777.0686146\G4=
-779.3353461

H(HO)₂CSiH₃

\\0,1\O,0,-0.9842784969,1.1670601244,0.068818358\C,0,-0.32
23316683,0.0241285817,0.5897148689\O,0,-0.9680603171,-1.174509224,0.21
92845781\Si,0,1.4824750319,-0.092769355,-0.0372063423\H,0,-0.357441191
1,0.1757538482,1.6782117423\H,0,-0.9872510224,1.0833884777,-0.89278416
18\H,0,-1.8722570378,-1.1401507798,0.5571493261\H,0,1.4406094037,-0.04
55607911,-1.522105597\H,0,2.1486421974,-1.3417824025,0.4054521126\H,0,
2.2453831005,1.0769315203,0.462235115\\Version=EM64L-G09RevA.02\State=
1-A\MP2/GTBas1=-480.5342514\MP4/GTBas1=-480.5852797\CCSD(T)/G3Bas1=-48
0.5867287\MP2/GTBas2=-480.5549829\MP4/GTBas2=-480.6074906\MP2/GTBas3=-
480.7314986\MP4/GTBas3=-480.7979569\HF/GTLargeXP=-480.084301\MP2/GTLar
geXP=-481.2933119\HF/GFHFB1=-480.1053996\HF/GFHFB2=-480.1109226\G4=-48
1.4107406

H(HO)₂CCBr₃

\\0,1\O,0,-0.7420785674,1.2575272107,-0.0029971201\C,0,-0.
150079426,0.1451969979,0.5810604339\O,0,-0.7688159484,-1.0486085168,0.
2099595551\C,0,1.356702499,0.0081551317,0.2030627882\H,0,-0.1850354904
,0.3194110803,1.6642885245\H,0,-0.7029329321,1.138831614,-0.9632334779
\H,0,-1.6996268892,-0.9742031841,0.4488331991\Br,0,1.5244222739,-0.199
2314666,-1.7457782849\Br,0,2.1338012724,-1.5383206308,1.1064226683\Br,
0,2.2918732082,1.6275117637,0.7680417139\\Version=EM64L-G09RevA.02\Sta
te=1-A\MP2/GTBas1=-7944.9001461\MP4/GTBas1=-7944.9512791\CCSD(T)/G3Bas
1=-7944.9414097\MP2/GTBas2=-7944.925943\MP4/GTBas2=-7944.9791768\MP2/G
TBas3=-7945.1882701\MP4/GTBas3=-7945.2713884\HF/GTLargeXP=-7944.462740
4\MP2/GTLargeXP=-7948.8543195\HF/GFHFB1=-7944.6730741\HF/GFHFB2=-7944.
6778714\G4=-7949.2452097

H(HO)₂CCCl₃

\\0,1\O,0,-0.7220735814,1.2594150866,-0.011866658\C,0,-0.1
380129931,0.1467400962,0.5780963987\O,0,-0.7537562805,-1.0482538475,0.
2083763248\C,0,1.3700703007,0.0062057792,0.197971497\H,0,-0.1704608876
,0.3249537006,1.6604637083\H,0,-0.6843190646,1.1340563554,-0.970630461
8\H,0,-1.6814595497,-0.9802144749,0.4600556269\Cl,0,1.523397999,-0.182
6405006,-1.583139113\Cl,0,2.082815266,-1.4090166887,1.0187420881\Cl,0,
2.2320387913,1.4850444936,0.711610589\\Version=EM64L-G09RevA.02\State=
1-A\MP2/GTBas1=-1606.6317777\MP4/GTBas1=-1606.7164635\CCSD(T)/G3Bas1=-
1606.7129894\MP2/GTBas2=-1606.6592284\MP4/GTBas2=-1606.7462588\MP2/GTB
as3=-1606.9588574\MP4/GTBas3=-1607.0782725\HF/GTLargeXP=-1605.807104\MP
2/GTLargeXP=-1608.3293765\HF/GFHFB1=-1605.8537889\HF/GFHFB2=-1605.861
0762\G4=-1608.6006411

H (HO)₂CC≡CF₃

\\0,1\H,0,2.1309339305,0.5322231512,-0.2525122599\O,0,1.821
6219716,1.2260953083,-0.8490180279\F,0,-1.5991211461,-2.4367267206,0.3
520062546\F,0,-2.8938559512,-1.4158003725,-1.0467423844\C,0,-0.3928335
515,0.6853323244,-0.1504188128\C,0,-1.201775159,-0.1950165384,-0.04938
63191\C,0,0.6253925781,1.7355768466,-0.3193559841\C,0,-2.1894320828,-1
.2650204323,0.0819087018\H,0,0.2791495492,2.4574355756,-1.0720485418\O
,0,0.8016868034,2.3413311723,0.9352145677\H,0,1.4174467249,3.073118955
2,0.8082918547\F,0,-3.0548136672,-1.0086892698,1.0701209513\\Version=E
M64L-G09RevA.02\State=1-A\MP2/GTBas1=-602.5454431\MP4/GTBas1=-602.6214
319\CCSD(T)/G3Bas1=-602.6126048\MP2/GTBas2=-602.5934817\MP4/GTBas2=-60
2.673185\MP2/GTBas3=-602.9360723\MP4/GTBas3=-603.0358593\HF/GTLargeXP=
-601.4119584\MP2/GTLargeXP=-603.6759285\HF/GFHFB1=-601.4659453\HF/GFHF
B2=-601.477165\G4=-603.9483868

H (HO)₂CC≡CH₃

\\0,1\O,0,-1.1702728566,1.1930520988,0.020865892\C,0,-0.57936
81585,-0.0326181263,0.3926761376\O,0,-1.1540578877,-1.1210215391,-0.29
61593687\C,0,0.8636662623,-0.0574854091,0.1391654465\C,0,2.0489807926,
-0.0346659745,-0.0658757292\H,0,-0.7758998044,-0.1047999799,1.47195226
08\H,0,-0.9143659569,1.361355278,-0.8945435686\H,0,-2.0988833574,-1.09
46374054,-0.1032075126\C,0,3.4827143284,-0.0174192985,-0.3128161897\H,
0,3.8195825145,0.9778469433,-0.6223627362\H,0,3.7556884525,-0.72404362
5,-1.1038657367\H,0,4.0416356711,-0.2928229623,0.5880111047\\Version=E
M64L-G09RevA.02\State=1-A\MP2/GTBas1=-305.4742315\MP4/GTBas1=-305.5425
377\CCSD(T)/G3Bas1=-305.5405926\MP2/GTBas2=-305.4988299\MP4/GTBas2=-30
5.5686667\MP2/GTBas3=-305.7088069\MP4/GTBas3=-305.7906865\HF/GTLargeXP
=-304.7349198\MP2/GTLargeXP=-306.1252685\HF/GFHFB1=-304.7598851\HF/GFH
FB2=-304.7650709\G4=-306.2633481

H (HO)₂CC (C≡N)₃

\\0,1\N,0,0.1840465438,2.5207625251,-1.1805449806\N,0,-1.41
71582364,-1.3646175813,-2.1545374995\C,0,0.2669698182,1.3873373152,-0.
9813040773\C,0,-0.6616541719,-0.7773407242,-1.5107920466\C,0,0.3065708
934,-0.0533269493,-0.6669739863\C,0,1.6583336686,-0.5993531005,-0.8781
980587\N,0,2.7069318355,-1.0559761717,-1.0279041537\H,0,-0.1571080646,
-1.3119824714,1.0585726847\C,0,-0.114238737,-0.2342240541,0.8639382782
\O,0,0.8833276004,0.4203183244,1.5740181946\O,0,-1.3848583526,0.256593
6688,1.092801723\H,0,-1.3581234811,1.2221823689,1.0247918518\H,0,0.769
5006836,0.2334368502,2.5130520702\\Version=EM64L-G09RevA.02\State=1-A\
MP2/GTBas1=-505.5500316\MP4/GTBas1=-505.6452251\CCSD(T)/G3Bas1=-505.63
0472\MP2/GTBas2=-505.583224\MP4/GTBas2=-505.6805481\MP2/GTBas3=-505.86
63263\MP4/GTBas3=-505.9796803\HF/GTLargeXP=-504.2690606\MP2/GTLargeXP=
-506.5376721\HF/GFHFB1=-504.3067282\HF/GFHFB2=-504.3140933\G4=-506.780
0376

H (HO)₂CC₆H₄-4-Br

\\0,1\H,0,-2.0217325355,-1.5648027314,0.6382754991\O,0,-2.
2836228107,-0.7038932349,0.9893582194\O,0,-2.2319624755,0.2304087731,-
1.1472152094\Br,0,4.4769706438,-0.2195274125,-0.1416286997\H,0,2.47822
95047,-0.7122284462,1.992370024\H,0,-3.1813117777,0.3760450774,-1.0728
122309\C,0,1.9179181734,-0.3854639057,1.1249977252\C,0,2.5757296384,-0
.0701552271,-0.059074301\H,0,0.0037509432,-0.5247298362,2.0890909374\C
,0,0.5315378026,-0.2762502191,1.175175236\C,0,1.8744589981,0.349788773
8,-1.1837337237\H,0,2.4019085637,0.5886621324,-2.099110474\C,0,-0.1954
049441,0.1418128658,0.058279955\C,0,0.4877058302,0.4560035807,-1.11742
28659\H,0,-0.0715545425,0.7775226092,-1.9868087065\C,0,-1.7049484754,0

.2748947937,0.1562515574\H,0,-1.9693125368,1.222742407,0.6487770578\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-2992.4841246\MP4/GTBas1=-2992.5838983\CCSD(T)/G3Bas1=-2992.5774971\MP2/GTBas2=-2992.5174906\MP4/GTBas2=-2992.6188162\MP2/GTBas3=-2992.8293166\MP4/GTBas3=-2992.9520041\HF/GTLargeXP=-2991.4195301\MP2/GTLargeXP=-2994.5394249\HF/GFHFB1=-2991.517018\HF/GFHFB2=-2991.5238804\G4=-2994.8248221

H(HO)₂CC₆H₄-4-C1

\\0,1\C,0,-2.54063,-0.03712,0.31715\C,0,-1.02791,-0.00582,0.18947\C,0,-0.33059,1.19955,0.09436\C,0,1.05805,1.21141,0.00105\C,0,1.74822,0.00411,0.00828\C,0,1.07557,-1.20956,0.10544\C,0,-0.31256,-1.2055,0.19612\H,0,-0.88111,2.13159,0.08568\H,0,1.60106,2.14532,-0.07839\C1,0,3.4968,0.01099,-0.10837\H,0,1.63111,-2.13939,0.10837\H,0,-0.85159,-2.14355,0.26631\O,0,-3.04562,1.17622,-0.18487\O,0,-3.11742,-1.15081,-0.32626\H,0,-2.82877,-0.16964,1.37093\H,0,-2.83433,-1.1218,-1.24932\H,0,-3.99846,1.16495,-0.04343\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-879.7282334\MP4/GTBas1=-879.8394113\CCSD(T)/G3Bas1=-879.8349961\MP2/GTBas2=-879.761601\MP4/GTBas2=-879.8744256\MP2/GTBas3=-880.0860208\MP4/GTBas3=-880.2209814\HF/GTLargeXP=-878.5335426\MP2/GTLargeXP=-881.0312445\HF/GFHFB1=-878.5764067\HF/GFHFB2=-878.5841307\G4=-881.2768834

H(HO)₂CC₆H₄-4-F

\\0,1\C,0,-1.7182676997,-0.0775474154,0.2053907218\C,0,-0.2045619358,-0.0226520929,0.1092938367\C,0,0.4823728036,1.1929893546,0.1294554907\C,0,1.8721642397,1.2240423738,0.0635447906\C,0,2.5673108661,0.0259953346,-0.0178857391\C,0,1.9122522281,-1.1973808539,-0.0363317284\C,0,0.5227330282,-1.2130972563,0.0284403325\H,0,-0.0786927637,2.1166719436,0.1894143214\H,0,2.4198263564,2.159149341,0.0722956837\F,0,3.9033336042,0.0502226119,-0.0814806732\H,0,2.4893178144,-2.1122171199,-0.1018687625\H,0,-0.0093137433,-2.1574584666,0.009581145\O,0,-2.2272157457,1.1710289528,-0.1984836577\O,0,-2.2726073873,-1.1350634355,-0.5450649583\H,0,-2.0280415903,-0.304227548,1.2367859721\H,0,-1.9619241397,-1.0282933927,-1.4533735736\H,0,-3.1825059352,1.1366776689,-0.0793032019\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-519.7142149\MP4/GTBas1=-519.8170652\CCSD(T)/G3Bas1=-519.8114508\MP2/GTBas2=-519.7556046\MP4/GTBas2=-519.8606424\MP2/GTBas3=-520.0802333\MP4/GTBas3=-520.202917\HF/GTLargeXP=-518.4923751\MP2/GTLargeXP=-520.7793565\HF/GFHFB1=-518.5356397\HF/GFHFB2=-518.5443028\G4=-521.0122102

H(HO)₂CC₆H₄-4-CH₃

\\0,1\H,0,2.7896500259,-1.2623773316,0.3817871643\H,0,-3.6366511583,1.2581913186,-0.0763097777\C,0,2.5025638018,-0.2254322558,0.149809618\H,0,0.8896282661,-0.1959860485,-2.0668552957\C,0,0.319588613,-0.1164251493,-1.1496784579\C,0,0.9925572051,-0.1006593976,0.0725737581\H,0,-1.575538791,-0.0384714026,-2.1504550535\C,0,-1.0684567672,-0.0263871362,-1.1897211059\C,0,0.2461273923,-0.0011866858,1.2490969187\H,0,0.7616066872,0.0083252363,2.2032785284\H,0,3.9931136386,0.037130105,-1.0356861594\C,0,-1.8231784945,0.0794373827,-0.0186162558\C,0,-1.1407981164,0.086699215,1.2014234282\H,0,-1.7039088689,0.1615743074,2.1274552257\O,0,3.0402646219,0.1671780641,-1.0911515856\C,0,-3.3259980648,0.2058845711,-0.0688993581\H,0,-3.7965250717,-0.2629450732,0.8005324844\O,0,3.0567070027,0.5159215981,1.2146906565\H,0,-3.7362859624,-0.2591303802,-0.9699014805\H,0,2.7475040407,1.4252590628,1.1135667479\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-459.8662339\MP4/GTBas1=-459.9812875\CCSD(T)/G3Bas1=-459.9780535\MP2/GTBas2=-459.8997489\MP4/GTBas2=-460.0164137\MP2/GTBas3=-460.2171249\MP4/GTBas3=-460.3507763\HF/GTLargeXP=-458.652461\MP2/GTLargeXP=-460.8670976\HF/GFHFB1=-458.6892444\HF/GFHF

B2=-458.6965758\G4=-461.0698102

H (HO)₂CPF₄

\\0,1\H,0,2.4202095055,0.7642139976,0.2594779681\F,0,-1.4
097451048,1.742617347,-0.5275656722\O,0,1.5190526313,0.8981229675,-0.0
58207542\F,0,-0.7386918559,-0.0444525675,-1.6741780699\P,0,-0.98225016
3,0.3071585926,-0.1088556035\C,0,0.762752874,-0.2369121328,0.279165874
8\O,0,1.134153628,-1.3852623989,-0.4017955249\F,0,-1.2327170964,0.6901
71015,1.4287961921\H,0,0.8184346947,-0.4769629578,1.3445553172\F,0,-2.
1493053618,-0.7193798668,-0.0613742703\H,0,0.9582262484,-1.2324639959,
-1.3401786694\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-929.1967
401\MP4/GTBas1=-929.2546293\CCSD(T)/G3Bas1=-929.2467843\MP2/GTBas2=-92
9.2467985\MP4/GTBas2=-929.3098798\MP2/GTBas3=-929.6314422\MP4/GTBas3=-
929.7185926\HF/GTLargeXP=-928.1922945\MP2/GTLargeXP=-930.6502739\HF/GF
HFB1=-928.2551347\HF/GFHFB2=-928.2735029\G4=-930.9408239

H (HO)₂CGeH₃

\\0,1\H,0,0.4867058998,1.4396545287,-0.601210668\H,0,-1.94
66015281,-0.4310973917,-1.7561434461\O,0,1.2099732077,-0.4383679422,-1
.1224430465\C,0,0.455553076,0.3923952985,-0.2731183568\Ge,0,-1.4117179
68,-0.2976083642,-0.3239694571\H,0,2.1151587488,-0.1006813703,-1.14048
71026\O,0,0.9746074295,0.4243443494,1.039480491\H,0,0.9722305274,-0.48
09236751,1.3745584202\H,0,-2.3178486102,0.6495230034,0.4764016511\H,0,
-1.4040007829,-1.6778484365,0.3578215147\\Version=EM64L-G09RevA.02\Sta
te=1-A\MP2/GTBas1=-2266.8638188\MP4/GTBas1=-2266.9050669\CCSD(T)/G3Bas
1=-2266.902727\MP2/GTBas2=-2266.8833301\MP4/GTBas2=-2266.9259719\MP2/G
TBas3=-2267.0585826\MP4/GTBas3=-2267.1149355\HF/GTLargeXP=-2266.480426
3\MP2/GTLargeXP=-2268.4036114\HF/GFHFB1=-2266.5583786\HF/GFHFB2=-2266.
5623779\G4=-2268.5637618

ALDEHYDE RADICALS

(O)CNH₂

\\0,2\O,0,-1.2171569581,-0.1982450178,-0.0000938906\C,0,
-0.1558585895,0.3521908906,0.000099213\N,0,1.0793567967,-0.1711875517,
0.0000203313\H,0,1.8823426933,0.4308397524,0.0007393778\H,0,1.22800605
76,-1.1742080735,0.0004649684\\Version=EM64L-G09RevA.02\State=2-A\MP2/
GTBas1=-168.751016\MP4/GTBas1=-168.7831909\CCSD(T)/G3Bas1=-168.7803333
\MP2/GTBas2=-168.7664204\MP4/GTBas2=-168.7993658\MP2/GTBas3=-168.86544
83\MP4/GTBas3=-168.9050701\HF/GTLargeXP=-168.3751276\MP2/GTLargeXP=-16
9.0870365\HF/GFHFB1=-168.3887325\HF/GFHFB2=-168.3914853\G4=-169.168704
4

(O)CC(CH₃)₃

\\0,2\O,0,2.1099935592,-0.1320473277,-0.0006680059\C,0,1.0
45461901,-0.6453882773,-0.0008768606\C,0,-0.3431684125,0.0317802469,0.
0000289867\C,0,-0.186727291,1.5607351736,0.0001608366\C,0,-1.077138495
5,-0.4569191466,-1.2623323247\C,0,-1.0754248339,-0.4572817523,1.263271
5117\H,0,0.3603871735,1.8993397692,-0.8839097791\H,0,-1.1708993443,2.0
417477828,0.0009808435\H,0,0.3617344465,1.8990336163,0.8835100623\H,0,
-1.1426181349,-1.548376193,-1.282617557\H,0,-2.093390507,-0.0496275941
, -1.278836641\H,0,-0.5661383105,-0.1287716546,-2.1727339333\H,0,-0.563
1426856,-0.1294599481,2.1730664287\H,0,-2.0916105064,-0.0498951798,1.2
812809997\H,0,-1.1409885585,-1.5487395151,1.2832954323\\Version=EM64L-
G09RevA.02\State=2-A\MP2/GTBas1=-270.2148685\MP4/GTBas1=-270.3007349\C
CSD(T)/G3Bas1=-270.2988514\MP2/GTBas2=-270.2314253\MP4/GTBas2=-270.318
7067\MP2/GTBas3=-270.4367564\MP4/GTBas3=-270.536584\HF/GTLargeXP=-269.

4967805\MP2/GTLargeXP=-270.8226931\HF/GFHFB1=-269.518061\HF/GFHFB2=-269.5223956\G4=-270.9465201

(O) CC≡N

\0,2\O,0,-1.6681614305,-0.2716274029,-0.0000009667\C,0,-0.6261642814,0.273246462,-0.0000110196\C,0,0.7417276109,-0.0539493886,-0.0000136849\N,0,1.908438101,-0.0345596706,0.0000056712\\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-205.5031214\MP4/GTBas1=-205.5509831\CCSD(T)/G3Bas1=-205.5609577\MP2/GTBas2=-205.5156135\MP4/GTBas2=-205.5639858\MP2/GTBas3=-205.6167846\MP4/GTBas3=-205.6718955\HF/GTLargeXP=-205.037607\MP2/GTLargeXP=-205.8855296\HF/GFHFB1=-205.053328\HF/GFHFB2=-205.0562174\G4=-206.0234265

(O) CN(CH₃)₂

\0,2\O,0,1.9548113639,-0.2021848106,-0.0002482061\C,0,0.8389490732,-0.6425379556,-0.0001620145\N,0,-0.3398339895,-0.006627433,-0.0001497854\C,0,-0.4229193217,1.4525598902,0.0001684182\C,0,-1.5804727688,-0.7571593816,0.0003208896\H,0,0.5903863844,1.8540865894,-0.0007197767\H,0,-0.9570624138,1.8085527244,-0.8888689193\H,0,-0.9554036509,1.8083479925,0.8902922538\H,0,-2.1801166978,-0.5231502618,0.8890287242\H,0,-2.1810907369,-0.5225111654,-0.887550219\H,0,-1.3469672421,-1.8225361886,-0.0001813646\\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-247.0731624\MP4/GTBas1=-247.1380703\CCSD(T)/G3Bas1=-247.1353953\MP2/GTBas2=-247.0894085\MP4/GTBas2=-247.1556552\MP2/GTBas3=-247.2596023\MP4/GTBas3=-247.3367301\HF/GTLargeXP=-246.4547539\MP2/GTLargeXP=-247.5974513\HF/GFHFB1=-246.4740126\HF/GFHFB2=-246.4779897\G4=-247.7111365

(O) CF

\0,2\O,0,1.1557847512,0.1584195044,0.\C,0,0.0015608985,0.3625983471,0.\F,0,-0.9776956497,-0.5269378515,0.\\Version=EM64L-G09RevA.02\State=2-A'\MP2/GTBas1=-212.5644987\MP4/GTBas1=-212.5889213\CCSD(T)/G3Bas1=-212.5846643\MP2/GTBas2=-212.5807711\MP4/GTBas2=-212.6063694\MP2/GTBas3=-212.6885883\MP4/GTBas3=-212.7211549\HF/GTLargeXP=-212.1914317\MP2/GTLargeXP=-212.9422714\HF/GFHFB1=-212.2113145\HF/GFHFB2=-212.215189\G4=-213.0477445

(O) CH

\0,2\O,0,0.6685397012,0.00766165,0.\C,0,-0.5076174935,-0.0029196864,0.\H,0,-1.1311822077,-0.9433919636,0.\\Version=EM64L-G09RevA.02\State=2-A'\MP2/GTBas1=-113.5327841\MP4/GTBas1=-113.5553307\CCSD(T)/G3Bas1=-113.552853\MP2/GTBas2=-113.5416908\MP4/GTBas2=-113.5646268\MP2/GTBas3=-113.605095\MP4/GTBas3=-113.6324611\HF/GTLargeXP=-113.2921405\MP2/GTLargeXP=-113.7513532\HF/GFHFB1=-113.3015721\HF/GFHFB2=-113.3033957\G4=-113.8136107

(O) COH

\0,2\C,0,-0.1394411002,0.3628806833,-0.0000120594\O,0,-1.1690266635,-0.2250917411,-0.0000046451\O,0,1.1083788647,-0.0870319668,-0.0000074666\H,0,1.095038899,-1.0642769755,0.0000041711\\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-188.5871526\MP4/GTBas1=-188.6142609\CCSD(T)/G3Bas1=-188.6111392\MP2/GTBas2=-188.6010777\MP4/GTBas2=-188.6291748\MP2/GTBas3=-188.7105243\MP4/GTBas3=-188.7455445\HF/GTLargeXP=-188.2041425\MP2/GTLargeXP=-188.9431916\HF/GFHFB1=-188.2201292\HF/GFHFB2=-188.2233641\G4=-189.03525

(O) CCH₃

\\0,2\\O,0,1.2414275958,-0.2569868487,-0.0008262125\\C,0,0.2
457580317,0.3811511868,0.000833579\\C,0,-1.1823241772,-0.1441818581,-0.
0000007889\\H,0,-1.3260377117,-0.7658919931,0.8905222461\\H,0,-1.9072047
776,0.6690205911,-0.0032658177\\H,0,-1.3237189609,-0.771621078,-0.88686
3006\\Version=EM64L-G09RevA.02\\State=2-A\\MP2/GTBas1=-152.7098084\\MP4/G
TBas1=-152.7486952\\CCSD(T)/G3Bas1=-152.7463716\\MP2/GTBas2=-152.7213195
\\MP4/GTBas2=-152.7609535\\MP2/GTBas3=-152.8186027\\MP4/GTBas3=-152.86482
17\\HF/GTLargeXP=-152.3539324\\MP2/GTLargeXP=-153.0253836\\HF/GFHFB1=-152
.3664148\\HF/GFHFB2=-152.3688926\\G4=-153.1030486

(O) CC₆H₅

\\0,2\\O,0,2.91928,0.25542,-0.00001\\C,0,2.0164,-0.5167,0.\\C
,0,0.56315,-0.23408,0.\\C,0,-0.33845,-1.3012,0.00001\\C,0,-1.70707,-1.05
291,0.00001\\C,0,-2.17218,0.26091,0.\\C,0,-1.27401,1.33064,-0.00001\\C,0,
0.09252,1.08755,-0.00001\\H,0,0.04761,-2.31485,0.00001\\H,0,-2.40976,-1.
879,0.00002\\H,0,-3.23988,0.45481,0.\\H,0,-1.6448,2.35026,-0.00001\\H,0,0
.81045,1.90023,-0.00001\\Version=EM64L-G09RevA.02\\State=2-A\\MP2/GTBas1
=-343.8467898\\MP4/GTBas1=-343.937009\\CCSD(T)/G3Bas1=-343.931366\\MP2/GT
Bas2=-343.8686735\\MP4/GTBas2=-343.9595428\\MP2/GTBas3=-344.0782604\\MP4/
GTBas3=-344.1800793\\HF/GTLargeXP=-342.9217824\\MP2/GTLargeXP=-344.57169
52\\HF/GFHFB1=-342.9487953\\HF/GFHFB2=-342.9537254\\G4=-344.7437049

(O) CCF₃

\\0,2\\O,0,2.0555188134,0.0920537297,-0.0003377428\\C,0,1.08
12345548,-0.5620280605,0.0002329692\\C,0,-0.3800743469,0.0105468865,0.0
00467912\\F,0,-0.4039242389,1.3395349221,-0.0013050546\\F,0,-1.00540872
23,-0.4355018232,-1.0839034975\\F,0,-1.0047160602,-0.4332956547,1.08531
65345\\Version=EM64L-G09RevA.02\\State=2-A\\MP2/GTBas1=-449.7754935\\MP4/
GTBas1=-449.8223809\\CCSD(T)/G3Bas1=-449.8132479\\MP2/GTBas2=-449.809483
7\\MP4/GTBas2=-449.8592903\\MP2/GTBas3=-450.0422674\\MP4/GTBas3=-450.1065
189\\HF/GTLargeXP=-449.026355\\MP2/GTLargeXP=-450.5716763\\HF/GFHFB1=-449
.0679322\\HF/GFHFB2=-449.0765554\\G4=-450.7849941

(O) CSi(CH₃)₃

\\0,2\\O,0,2.358978044,0.7967308725,-0.4059917385\\C,0,1.
3707390958,0.7920265844,0.2443776152\\Si,0,-0.3390771415,-0.0929611361,
0.0282741478\\C,0,-0.5179797209,-1.1304032001,1.584336254\\C,0,-1.581767
6629,1.3152893262,-0.014959437\\C,0,-0.4510212503,-1.1559122428,-1.5226
987491\\H,0,-0.4124622993,-0.5162938398,2.4834550219\\H,0,-1.5024086529,
-1.6098722198,1.6161760738\\H,0,0.2373342775,-1.9215696414,1.6260526907
\\H,0,-1.4426661133,1.9435761787,-0.9004603683\\H,0,-2.6049903357,0.9251
469335,-0.0426482282\\H,0,-1.4876086852,1.9533299864,0.8686260793\\H,0,0
.3054776455,-1.9466862379,-1.517119914\\H,0,-1.4344620594,-1.634636622,
-1.5993721583\\H,0,-0.3004951413,-0.5564347417,-2.4258372892\\Version=E
M64L-G09RevA.02\\State=2-A\\MP2/GTBas1=-521.2404414\\MP4/GTBas1=-521.3278
635\\CCSD(T)/G3Bas1=-521.3270021\\MP2/GTBas2=-521.258934\\MP4/GTBas2=-521
.3476456\\MP2/GTBas3=-521.4730939\\MP4/GTBas3=-521.5768323\\HF/GTLargeXP=
-520.6002847\\MP2/GTLargeXP=-522.1243096\\HF/GFHFB1=-520.6232099\\HF/GFHF
B2=-520.6292578\\G4=-522.2670724

(O) CBr

\\0,2\\O,0,-0.4352656822,-2.1228741165,0.\\C,0,0.3230034178
, -1.2655027984,0.\\Br,0,0.0232722644,0.8292969149,0.\\Version=EM64L-G09
RevA.02\\State=2-A\\MP2/GTBas1=-2685.3397928\\MP4/GTBas1=-2685.366771\\CC
SD(T)/G3Bas1=-2685.3619208\\MP2/GTBas2=-2685.348478\\MP4/GTBas2=-2685.37
60512\\MP2/GTBas3=-2685.4399604\\MP4/GTBas3=-2685.4786226\\HF/GTLargeXP=-

2685.135017\MP2/GTLargeXP=-2686.705506\HF/GFHFB1=-2685.2087163\HF/GFHF
B2=-2685.2106965\G4=-2686.8695817

(O) CCl

\0,2\0,0,1.1131475028,1.2253878994,0.\C,0,0.0383439739,0
.7947958287,0.\Cl,0,-0.5067314767,-0.951013728,0.\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-572.5757264\MP4/GTBas1=-572.6121428\CCSD(T)/G3Bas1=-572.6083825\MP2/GTBas2=-572.5850514\MP4/GTBas2=-572.6221801\MP2/GTBas3=-572.6925674\MP4/GTBas3=-572.7416364\HF/GTLargeXP=-572.2364056\MP2/GTLargeXP=-573.1929611\HF/GFHFB1=-572.2553405\HF/GFHFB2=-572.258068\G4=-573.3142905

(O) CSiCl₃

\0,2\0,0,2.423515807,0.0003754092,-1.4641912378\C,0,1
.2542595478,0.0004729163,-1.4098336191\Si,0,-0.0224603936,-0.0000211015,0.0379069121\Cl,0,0.6729188864,-0.0012983736,1.9761393921\Cl,0,-1.1390966477,-1.6824866984,-0.2911399385\Cl,0,-1.1382571999,1.6833678479,-0.2892515088\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-1780.9478121\MP4/GTBas1=-1781.0202098\CCSD(T)/G3Bas1=-1781.0167205\MP2/GTBas2=-1780.9646241\MP4/GTBas2=-1781.0384054\MP2/GTBas3=-1781.2100259\MP4/GTBas3=-1781.3140549\HF/GTLargeXP=-1780.3804099\MP2/GTLargeXP=-1782.7450739\HF/GFHFB1=-1780.4227042\HF/GFHFB2=-1780.4298122\G4=-1783.0096375

(O) CSiF₃

\0,2\0,0,2.473655881,-0.0527573399,-0.0136113916\C,0,1
.4067808474,-0.5451324139,0.0160964782\Si,0,-0.3791305741,0.074240525,-0.0000076796\F,0,-0.6624648324,1.622606839,-0.0736020679\F,0,-1.0272058771,-0.4843930715,1.31873873\F,0,-1.0480654448,-0.6095845386,-1.2474240692\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-701.0006759\MP4/GTBas1=-701.0406234\CCSD(T)/G3Bas1=-701.0323134\MP2/GTBas2=-701.0344619\MP4/GTBas2=-701.0776923\MP2/GTBas3=-701.2744022\MP4/GTBas3=-701.3336705\HF/GTLargeXP=-700.3235668\MP2/GTLargeXP=-702.075058\HF/GFHFB1=-700.3669953\HF/GFHFB2=-700.3794887\G4=-702.2956965

(O) CSiH₃

\0,2\0,0,-1.8073774373,-0.1671121889,-0.0089398911\C,0
, -0.7761326728,0.3991088426,0.0090295599\Si,0,1.0778630604,-0.1384918932,0.0010573088\H,0,1.4002451723,-1.5922325441,-0.035290918\H,0,1.6184589808,0.4772160759,1.2330318193\H,0,1.6259628965,0.5396117075,-1.1942978789\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-403.6972609\MP4/GTBas1=-403.7384704\CCSD(T)/G3Bas1=-403.7374094\MP2/GTBas2=-403.7085765\MP4/GTBas2=-403.7505341\MP2/GTBas3=-403.812734\MP4/GTBas3=-403.8646156\HF/GTLargeXP=-403.411917\MP2/GTLargeXP=-404.2775648\HF/GFHFB1=-403.426205\HF/GFHFB2=-403.4299227\G4=-404.3773362

(O) CCB₃

\0,2\0,0,1.0711992653,-0.0002556387,2.4865119523\C,0,0.1
360805756,0.0004350221,1.782339765\C,0,0.0169444201,0.0000438829,0.269081103\Br,0,1.7661584191,-0.0014197701,-0.6595513261\Br,0,-0.9874981546,1.6150638157,-0.1729127497\Br,0,-0.9897545256,-1.6137773119,-0.1720587445\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-7868.0371153\MP4/GTBas1=-7868.0799194\CCSD(T)/G3Bas1=-7868.0678928\MP2/GTBas2=-7868.0536732\MP4/GTBas2=-7868.0976531\MP2/GTBas3=-7868.2421724\MP4/GTBas3=-7868.3121382\HF/GTLargeXP=-7867.7667896\MP2/GTLargeXP=-7871.8128021\HF/GFHFB1=-7867.9707111\HF/GFHFB2=-7867.9736952\G4=-7872.1897968

(O) CCl₃

\\0,2\\0,0,-2.0504632118,0.0007537496,-1.2906261285\\C,0,-0.8803673523,0.0007213023,-1.2578003792\\C,0,0.0543655391,-0.0000292702,-0.0234131167\\Cl,0,-0.8404879414,-0.0013014441,1.5290337919\\Cl,0,1.0541865232,1.4712729836,-0.1604341924\\Cl,0,1.0547164432,-1.4707573213,-0.1625199751\\Version=EM64L-G09RevA.02\\State=2-A\\MP2/GTBas1=-1529.7668546\\MP4/GTBas1=-1529.8428564\\CCSD(T)/G3Bas1=-1529.8367409\\MP2/GTBas2=-1529.7842413\\MP4/GTBas2=-1529.8617372\\MP2/GTBas3=-1530.0122923\\MP4/GTBas3=-1530.1182641\\HF/GTLargeXP=-1529.108062\\MP2/GTLargeXP=-1531.2866441\\HF/GFHFB1=-1529.1480494\\HF/GFHFB2=-1529.1535783\\G4=-1531.5433236

(O) CC₆H₄-4-Br

\\0,2\\0,0,-4.43484,-0.52403,0.00001\\C,0,-3.62632,0.34574,0.0000008989\\C,0,-2.15102,0.22709,0.0000008989\\C,0,-1.37166,1.38586,-0.00001\\C,0,0.01589,1.30052,-0.00001\\C,0,0.60971,0.04104,0.0000008989\\C,0,-0.1497,-1.12983,0.00001\\C,0,-1.53324,-1.03207,0.00001\\H,0,-1.86282,2.35289,-0.00001\\H,0,0.62817,2.1935,-0.00001\\Br,0,2.50752,-0.09043,0.0000008989\\H,0,0.33962,-2.09606,0.00001\\H,0,-2.15123,-1.92311,0.00001\\Version=EM64L-G09RevA.02\\State=2-A\\MP2/GTBas1=-2915.6342592\\MP4/GTBas1=-2915.7244012\\CCSD(T)/G3Bas1=-2915.7153072\\MP2/GTBas2=-2915.6574524\\MP4/GTBas2=-2915.7484628\\MP2/GTBas3=-2915.8975909\\MP4/GTBas3=-2916.005872\\HF/GTLargeXP=-2914.7361592\\MP2/GTLargeXP=-2917.511351\\HF/GFHFB1=-2914.8269129\\HF/GFHFB2=-2914.8319814\\G4=-2917.7818972

(O) CC₆H₄-4-Cl

\\0,2\\0,0,-3.722811894,-0.528371402,0.0000295562\\C,0,-2.9054436111,0.3332891682,0.0000285385\\C,0,-1.4319554963,0.2009769372,0.0000182376\\C,0,-0.6419723412,1.3528685783,0.0000120353\\C,0,0.7440038967,1.2549940515,0.000004001\\C,0,1.3270438152,-0.0099293076,0.0000021051\\C,0,0.5567770621,-1.1741910313,0.0000079246\\C,0,-0.8252408912,-1.0638859842,0.0000156452\\H,0,-1.1247532895,2.3240159243,0.0000143549\\H,0,1.3688149181,2.1392464268,-0.0000007104\\Cl,0,3.0673520471,-0.1449844987,-0.0000073382\\H,0,1.0422113987,-2.1425118985,0.0000066462\\H,0,-1.4517456147,-1.9488769641,0.00001999\\Version=EM64L-G09RevA.02\\State=2-A\\MP2/GTBas1=-802.8786229\\MP4/GTBas1=-802.9801716\\CCSD(T)/G3Bas1=-802.9730734\\MP2/GTBas2=-802.9017968\\MP4/GTBas2=-803.0043093\\MP2/GTBas3=-803.1544737\\MP4/GTBas3=-803.2750616\\HF/GTLargeXP=-801.8505308\\MP2/GTLargeXP=-804.0033102\\HF/GFHFB1=-801.8866446\\HF/GFHFB2=-801.892587\\G4=-804.2341305

(O) CC₆H₄-4-F

\\0,2\\0,0,-3.2949964789,-0.4558406451,0.0000231995\\C,0,-2.4498223782,0.3795670266,0.0000206516\\C,0,-0.9837197604,0.205077722,0.0000109747\\C,0,-0.1603027633,1.3348043215,0.00000396\\C,0,1.2215712444,1.1972383011,-0.0000030427\\C,0,1.7597366586,-0.0841237185,-0.0000039897\\C,0,0.9644320039,-1.2276503841,-0.0000003741\\C,0,-0.4131456681,-1.0778354217,0.0000073297\\H,0,-0.6169249222,2.3183774269,0.0000057961\\H,0,1.8841278525,2.0541838429,-0.0000081594\\F,0,3.0838982488,-0.2258550566,-0.0000152116\\H,0,1.4363340411,-2.2031803607,-0.0000031323\\H,0,-1.0665380782,-1.9430230543,0.0000113633\\Version=EM64L-G09RevA.02\\State=2-A\\MP2/GTBas1=-442.8651586\\MP4/GTBas1=-442.9585226\\CCSD(T)/G3Bas1=-442.9503203\\MP2/GTBas2=-442.8960957\\MP4/GTBas2=-442.9909388\\MP2/GTBas3=-443.1494844\\MP4/GTBas3=-443.2579368\\HF/GTLargeXP=-441.8107146\\MP2/GTLargeXP=-443.7518682\\HF/GFHFB1=-441.8472611\\HF/GFHFB2=-441.8541348\\G4=-443.9700532

(O) CC₆H₄-4-CH₃

\\0,2\\O,0,-3.346578315,-0.4814062968,0.0002221345\\C,0,-2.5
086622767,0.3619198479,0.000220891\\C,0,-1.0402445369,0.2018614004,0.00
00350161\\C,0,-0.225667386,1.3349165572,-0.0001063015\\C,0,1.1580854742,
1.1991022271,-0.0003898458\\C,0,1.7537844268,-0.065131538,-0.0004195724
\\C,0,0.925377572,-1.1986995569,-0.0004552847\\C,0,-0.4534104216,-1.0738
401933,-0.0001657486\\H,0,-0.6886152186,2.3159942839,-0.0001502632\\H,0,
1.7863105536,2.084299779,-0.0006399036\\C,0,3.2529604588,-0.2209861096,
0.0005961932\\H,0,1.3767765469,-2.1868025367,-0.0008017956\\H,0,-1.09627
06937,-1.9472905093,-0.0002551418\\H,0,3.7576049856,0.7479915122,-0.012
9314515\\H,0,3.5911738394,-0.7910185144,-0.871853756\\H,0,3.5921549913,-
0.7662303527,0.8885248299\\Version=EM64L-G09RevA.02\\State=2-A\\MP2/GTBa
s1=-383.0181228\\MP4/GTBas1=-383.1236581\\CCSD(T)/G3Bas1=-383.1179023\\MP
2/GTBas2=-383.041339\\MP4/GTBas2=-383.1478349\\MP2/GTBas3=-383.2870378\\M
P4/GTBas3=-383.4064319\\HF/GTLargeXP=-381.9718914\\MP2/GTLargeXP=-383.84
04443\\HF/GFHFB1=-382.0019169\\HF/GFHFB2=-382.0074496\\G4=-384.0285832

(O) CGeH₃

\\0,2\\C,0,-1.6655071112,0.8669428744,-0.1327473348\\O,0,-2
.388887727,1.5790069238,0.4505481509\\Ge,0,0.2628367172,0.3416723106,0.
3962703878\\H,0,0.7710865521,0.9744795752,1.7063721394\\H,0,1.1216617203
,0.7727466697,-0.797691779\\H,0,0.2333803152,-1.1875673239,0.4937877573
\\Version=AM64L-G09RevA.02\\State=2-A\\MP2/GTBas1=-2190.0286549\\MP4/GTBa
s1=-2190.060878\\CCSD(T)/G3Bas1=-2190.0561841\\MP2/GTBas2=-2190.0388414\\
MP4/GTBas2=-2190.0717023\\MP2/GTBas3=-2190.139607\\MP4/GTBas3=-2190.1819
695\\HF/GTLargeXP=-2189.8107518\\MP2/GTLargeXP=-2191.3887797\\HF/GFHFB1=-
2189.8818739\\HF/GFHFB2=-2189.8840558\\G4=-2191.532277

DEPROTONATED ALDEHYDE ANIONS

⁻(O) CC(O) CH₃

\\-1,1\\C,0,-0.3924915776,-0.1258789821,0.0621132242\\C,0,1
.0023264501,-0.1681590256,-0.040404867\\O,0,1.9749482062,-0.3784791763,
-0.7397826701\\C,0,-0.916734561,1.3256085736,0.0608064703\\O,0,-1.155090
383,-1.0506852812,0.4902390299\\H,0,-1.7932969086,1.3727969281,-0.60341
45595\\H,0,-0.172128942,2.0544681356,-0.2879203001\\H,0,-1.2650322841,1.
636628828,1.0585136723\\Version=EM64L-G09RevA.02\\State=1-A\\MP2/GTBas1=
-265.7315741\\MP4/GTBas1=-265.7901298\\CCSD(T)/G3Bas1=-265.7837115\\MP2/G
TBas2=-265.7779223\\MP4/GTBas2=-265.8377705\\MP2/GTBas3=-265.9154106\\MP4
/GTBas3=-265.9862211\\HF/GTLargeXP=-265.1035825\\MP2/GTLargeXP=-266.2935
926\\HF/GFHFB1=-265.1242921\\HF/GFHFB2=-265.128489\\G4=-266.4319445

⁻(O) CC(CH₃)₃

\\-1,1\\O,0,1.9765006872,-0.1350775409,0.5634659444\\C,0,1.
123569172,-0.813471332,0.0085686862\\C,0,-0.406871551,0.0715004635,-0.0
67238972\\C,0,-0.1657785216,1.5694590163,-0.0419885686\\C,0,-1.133693437
6,-0.4395962795,-1.2989134286\\C,0,-1.0877048677,-0.414182889,1.2068278
371\\H,0,0.040755652,1.9583220047,-1.0497796757\\H,0,-0.9903924178,2.178
0307137,0.3714964262\\H,0,0.7382116036,1.7458424777,0.5676133325\\H,0,-0
.9364725378,-1.5200841529,-1.4000436493\\H,0,-2.2288922629,-0.288868227
6,-1.2903195632\\H,0,-0.7508504753,0.0368886919,-2.2132457534\\H,0,-0.57
894502,-0.0104427373,2.0931443191\\H,0,-2.1564410999,-0.1404179046,1.27
89786218\\H,0,-1.0166649233,-1.5117723038,1.2750544435\\Version=EM64L-G
09RevA.02\\State=1-A\\MP2/GTBas1=-270.1839924\\MP4/GTBas1=-270.272022\\CCS
D(T)/G3Bas1=-270.2699237\\MP2/GTBas2=-270.2304226\\MP4/GTBas2=-270.31985
52\\MP2/GTBas3=-270.4150174\\MP4/GTBas3=-270.5173266\\HF/GTLargeXP=-269.4
566551\\MP2/GTLargeXP=-270.8308694\\HF/GFHFB1=-269.4776746\\HF/GFHFB2=-26

9.4819827\G4=-270.9623812

⁻(O) CN(CH₃)₂

\\-1,1\O,0,1.9026895638,-0.0284828376,-0.0007445808\C,0
,0.9224016743,-0.7837400189,-0.0006276222\N,0,-0.379326263,-0.00211216
1,-0.0001898722\C,0,-0.4238863568,1.4265602075,0.000262694\C,0,-1.5928
828709,-0.7360664247,0.0003998334\H,0,0.6323577075,1.7397370527,0.0000
269121\H,0,-0.9297257951,1.8642806748,-0.8864572599\H,0,-0.9292117117,
1.8636841579,0.8875681901\H,0,-2.2401432724,-0.5496580187,0.8864719311
\H,0,-2.241046287,-0.5496085571,-0.8849975806\H,0,-1.3009463888,-1.797
7540749,0.000217355\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-24
7.0524752\MP4/GTBas1=-247.1195354\CCSD(T)/G3Bas1=-247.1168658\MP2/GTBa
s2=-247.0980462\MP4/GTBas2=-247.1666349\MP2/GTBas3=-247.2470295\MP4/GT
Bas3=-247.3267892\HF/GTLargeXP=-246.4267431\MP2/GTLargeXP=-247.6134203
\HF/GFHFB1=-246.4455499\HF/GFHFB2=-246.449493\G4=-247.735696

⁻(O) CCH=CH₂

\\-1,1\O,0,1.7714621533,-0.2296277315,0.0000195482\C,0,0.
759831767,0.5007463405,0.0000018351\C,0,-0.5579622741,-0.4234916934,0.
0000015157\C,0,-1.7806373639,0.1124458063,-0.0000176855\H,0,-0.4464883
059,-1.5237285608,0.0000177311\H,0,-1.8630389645,1.2023481368,-0.00003
35336\H,0,-2.7169770119,-0.448222298,-0.000019411\\Version=EM64L-G09Re
vA.02\State=1-A\MP2/GTBas1=-190.6400441\MP4/GTBas1=-190.6934918\CCSD(T
MP2/GTBas3=-190.777327\MP4/GTBas3=-190.8393838\HF/GTLargeXP=-190.18154
88\MP2/GTLargeXP=-191.076889\HF/GFHFB1=-190.1963392\HF/GFHFB2=-190.199
2504\G4=-191.1885408

⁻(O) CF

\\-1,1\O,0,1.1534572074,0.0966639881,0.\C,0,0.0659547008,
0.5778872192,0.\F,0,-1.0397619082,-0.6804712073,0.\\Version=EM64L-G09R
evA.02\State=1-A'\MP2/GTBas1=-212.5988188\MP4/GTBas1=-212.6259566\CCSD
(T)/G3Bas1=-212.6199602\MP2/GTBas2=-212.6619998\MP4/GTBas2=-212.691642
3\MP2/GTBas3=-212.7248909\MP4/GTBas3=-212.7612002\HF/GTLargeXP=-212.22
86646\MP2/GTLargeXP=-213.0213151\HF/GFHFB1=-212.2483447\HF/GFHFB2=-212
.2519538\G4=-213.1345376

⁻(O) CH

\\-1,1\O,0,0.6874249651,-0.0367291987,0.\C,0,-0.530742899
5,0.1395628247,0.\H,0,-1.1269420656,-1.0414836261,0.\\Version=EM64L-G0
9RevA.02\State=1-A'\MP2/GTBas1=-113.4905583\MP4/GTBas1=-113.5165485\CC
SD(T)/G3Bas1=-113.5149372\MP2/GTBas2=-113.5325009\MP4/GTBas2=-113.5591
16\MP2/GTBas3=-113.5694501\MP4/GTBas3=-113.6011695\HF/GTLargeXP=-113.2
578742\MP2/GTLargeXP=-113.7511846\HF/GFHFB1=-113.2668456\HF/GFHFB2=-11
3.2687789\G4=-113.8257231

⁻(O) COH

\\-1,1\C,0,-0.1719388631,0.5167550791,-0.0000656259\O,0,-
1.040820087,-0.3616070319,0.0000321671\O,0,1.1663157892,-0.1078377231,
0.0000505986\H,0,0.9413931608,-1.0608303241,-0.0000371398\\Version=EM6
4L-G09RevA.02\State=1-A\MP2/GTBas1=-188.5942347\MP4/GTBas1=-188.623249
6\CCSD(T)/G3Bas1=-188.6200623\MP2/GTBas2=-188.6467622\MP4/GTBas2=-188.
6771832\MP2/GTBas3=-188.7219304\MP4/GTBas3=-188.7598044\HF/GTLargeXP=-
188.2087598\MP2/GTLargeXP=-188.9920795\HF/GFHFB1=-188.2242905\HF/GFHFB
2=-188.2274403\G4=-189.0916928

⁻(O) CCH₃

```
\\-1,1\O,0,1.1743485079,-0.1442152422,-0.4231631635\C,0,0
.3734708434,0.3655537784,0.3751624463\C,0,-1.163610711,-0.1899842301,0
.0527388324\H,0,-1.5834222662,-0.679528315,0.9502448241\H,0,-1.8357125
878,0.6615691235,-0.1582714876\H,0,-1.2171737863,-0.9019051147,-0.7963
114517\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-152.6677318\MP4
/GTBas1=-152.7091703\CCSD(T)/G3Bas1=-152.7075711\MP2/GTBas2=-152.71852
74\MP4/GTBas2=-152.7610953\MP2/GTBas3=-152.7851891\MP4/GTBas3=-152.834
7461\HF/GTLargeXP=-152.3172231\MP2/GTLargeXP=-153.0306085\HF/GFHFB1=-1
52.3293012\HF/GFHFB2=-152.3317988\G4=-153.1187105
```

⁻(O) CC₆H₅

```
\\-1,1\O,0,2.7829646375,-0.5166658569,-0.0000852547\C,0,2
.1648840536,0.5550084085,0.0001086939\C,0,0.5345528097,0.2299808395,-0
.000005358\C,0,-0.3770644637,1.2823237734,-0.0000088661\C,0,-1.7541965
617,1.0524853985,-0.0000278639\C,0,-2.2366684537,-0.2575423052,-0.0000
063094\C,0,-1.3333773962,-1.3263100458,0.0000191763\C,0,0.0349057463,-
1.0724364212,0.0000069698\H,0,0.0276928789,2.2976967727,0.0000097779\H
,0,-2.4584703945,1.884939509,-0.0000556194\H,0,-3.3084536186,-0.446754
0822,-0.0000006407\H,0,-1.7154974275,-2.348848705,0.0000434226\H,0,0.7
8409819,-1.8686072851,-0.0000081283\\Version=EM64L-G09RevA.02\State=1-
A\MP2/GTBas1=-343.8259268\MP4/GTBas1=-343.9189081\CCSD(T)/G3Bas1=-343.
9130857\MP2/GTBas2=-343.8789093\MP4/GTBas2=-343.9723902\MP2/GTBas3=-34
4.0658863\MP4/GTBas3=-344.1709821\HF/GTLargeXP=-342.897371\MP2/GTLarge
XP=-344.5890368\HF/GFHFB1=-342.9237497\HF/GFHFB2=-342.9286776\G4=-344.
7683937
```

⁻(O) CC₆H₄-4-Br

```
\\-1,1\O,0,4.2640408492,-0.7549182866,0.0006246564\C,0
,3.7645706264,0.3743205108,-0.0007414522\C,0,2.1157806616,0.2270057291
,0.0000209584\C,0,1.3251359343,1.3717688468,-0.0000102277\C,0,-0.06814
14823,1.2976315806,0.0001628083\C,0,-0.6479912603,0.0337727472,0.00005
85648\C,0,0.103504272,-1.1404895538,-0.0001052546\C,0,1.4880244876,-1.
0185767725,0.0000008111\H,0,1.8368448773,2.3377714518,-0.0001994874\H
,0,-0.6963167961,2.184257528,0.0003487509\Br,0,-2.5876632478,-0.1030983
348,-0.0000681996\H,0,-0.4002518811,-2.1047257238,-0.0002624974\H,0,2.
1554429592,-1.8852697226,0.0001678724\\Version=EM64L-G09RevA.02\State=
1-A\MP2/GTBas1=-2915.6257475\MP4/GTBas1=-2915.7186581\CCSD(T)/G3Bas1=-
2915.7094934\MP2/GTBas2=-2915.6774739\MP4/GTBas2=-2915.7711758\MP2/GTB
as3=-2915.8971949\MP4/GTBas3=-2916.0089181\HF/GTLargeXP=-2914.7226512\
MP2/GTLargeXP=-2917.5377966\HF/GFHFB1=-2914.8127941\HF/GFHFB2=-2914.81
78212\G4=-2917.8154934
```

⁻(O) CC₆H₄-4-Cl

```
\\-1,1\O,0,-3.6082106491,-0.713762592,0.0006243085\C,0
,-3.093261764,0.4082279488,-0.0006668843\C,0,-1.4379140427,0.230331088
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⁻(O) CC₆H₄-4-F

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⁻(O) CC₆H₄-4-CH₃

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END OF SUPPORTING INFORMATION