Structures and Energetic Properties of 4-Halo-Benzamides

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Synopsis The crystal structures and energetic parameters of 4-halo-benzamides (R = I, Br, Cl, F) have been determined. To our knowledge, the results present the first systematic investigation of the effect of para-halogen substitution on the properties of the amide bond in N,N-disubstituted benzamides.

Abstract The amide bond represents one of the most fundamental functional groups in chemistry. Properties of amides are defined by amidic resonance ($n_N \rightarrow \pi^*_{C=O}$ conjugation), which enforces planarity of the six atoms comprising the amide bond. Despite the importance of 4-halo-substituted benzamides in organic synthesis, molecular interactions and medicinal chemistry, the effect of 4-halo-substitution on the properties of the amide bond in N,N-disubstituted benzamides has not been studied. Herein, we report the crystal structures and energetic properties of a full series of 4-halo-benzamides. The structures of four 4-halo-benzamides (R = I, Br, Cl, F) in the N-morpholinyl series have been determined. Computations have been used to determine the effect of halogen substitution on structures and resonance energies. The 4-iodo-N-morpholinyl-benzamide crystallized with a significant distortion of the amide bond ($\tau+\chi_N$ = 33°). The present study supports the correlation between Ar–C(O) axis twist angle and twist angle of the amide N–C(O) bond. Comparison of resonance energies in synthetically-valuable N-morpholinyl and N-piperidinyl amides demonstrates that oxygen atom of the morpholinyl ring has a negligible effect on amidic resonance in the series.

Keywords: crystal structure; amide bonds; morpholinyl amides; resonance energies; twisted amides

1. Introduction

The amide bond represents a textbook example of the most fundamental functional groups in chemistry (Greenberg *et al*., 2000). Properties of amides are defined by amidic resonance ($n_N \rightarrow \pi^*_{C=O}$ conjugation, 15-20 kcal/mol in typical amides), which enforces planarity of the six atoms comprising the amide bond (Kemnitz *et al*., 2007; Glover *et al*., 2012). Despite the fact that the majority of amides are planar, distortions of amides from planarity by twisting, pyramidalization or a combined effect have a major impact on the properties and application of amides in synthetic chemistry, biochemistry and structural chemistry, among other areas of science (Adachi *et al*., 2018; Szostak *et al*., 2013). The effect of diminution of amidic resonance on the properties of amides caused by steric and electronic destabilization has been investigated by us (Meng *et al*., 2016; Liu *et al*., 2017) and others (Tani *et al*., 2006; Sliter *et al*., 2011; Komarov *et al*., 2015). These destabilized amides are useful because of the unusual reactivity of the amide bond triggered by switching-off Nlp to C=O delocalization (Nlp = lone pair at nitrogen) by sterics or electronics that can be rationally tuned across a full reactivity scale ranging from 0 to 20 kcal/mol (Szostak *et al*., 2018).

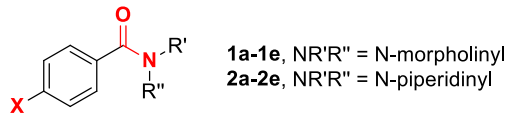
In contrast, few studies exist on the effect of steric and electronic properties of the amide bond in synthetically valuable planar acyclic amides (Stewart *et al*., 1970; Wiberg *et al*., 1995). We have been interested in the properties of 4-halo-substituted benzamides because of their utility in selective cross-coupling reactions (Molander *et al*., 2013; Bisz *et al*., 2018; Bisz *et al*., 2017) that can be controlled by electronic properties of the amide bond (Hammett σ^* of 1.94, $CONMe_2$) (Hansch *et al*., 1991; Piontek *et al*., 2017). In particular, we recognized that despite the importance of 4-halo-substituted benzamides (Larock, 1999; Montalbetti *et al*., 2005; Marchildon, 2011), effect of 4-halo-substitution on the properties of the amide bond in N,N-disubstituted benzamides has not been studied.

Herein, we report the crystal structures and energetic properties of a full series of 4-halo-benzamides. Specifically, the structures of four 4-halo-benzamides (R = I, Br, Cl, F) in the N-morpholinyl series have been determined. Computations have been used to determine the effect of halogen substitution on structures and resonance energies. The 4-iodo-N-morpholinyl-benzamide crystallized with a significant distortion of the amide bond ($\tau+\chi_N$ = 33°, additive Winkler-Dunitz distortion parameter) (Winkler *et al*., 1971; Szostak *et al*., 2015). The present study supports the correlation between Ar–C(O) axis twist angle and twist angle of the amide N–C(O) bond. Comparison of resonance energies in synthetically-valuable N-morpholinyl (Martin *et al*., 1997; Nahm *et al*., 1981) and N-piperidinyl amides demonstrates that oxygen atom of the morpholinyl ring has a negligible effect on amidic resonance in the series.

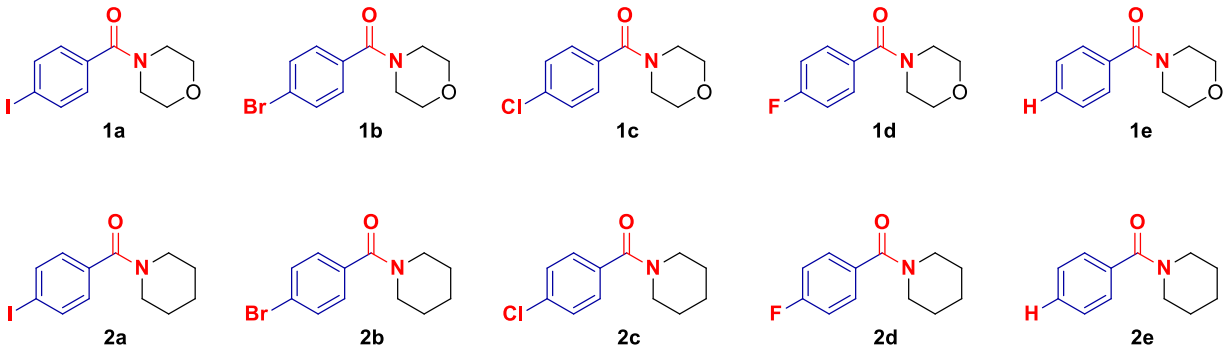
Structures of amides selected for the present study are shown in Scheme 1. Our investigation started by obtaining X-ray structures of a full set of 4-halo-substituted benzamides in a single series. Note that for reliable comparison of crystallographic and computational data, all compounds must be

obtained in a single, well-defined series, which in our experience is often far from trivial. After initial unsuccessful tries with other amides, morpholinyl amides were selected for the crystallographic study due to high crystallinity. We recognized that these amides are further synthetically useful because of the stable tetrahedral intermediates formed in nucleophilic addition reactions (cf. Weinreb amides).

A: General structure of amides



B: Amides selected for the present study



Scheme 1 Structures of amides employed in the present study.

2. Experimental

B3LYP/6-311++G(d,p) was selected to conduct geometry optimization as a result of good reproducibility of literature data and method practicality (Greenberg *et al*., 1993; Greenberg *et al*., 1996; Morgan *et al*., 2014; Glover *et al*., 2012; Meng *et al*., 2018; Szostak *et al*., 2017). Extensive studies have showed that this level is accurate in predicting properties and resonance energies of amides. B3LYP/6-311++G(d,p)+QZVP was selected to conduct geometry optimization of iodoamides selected for this study. The COSNAR method was used to calculate resonance energies of amides selected for the study (Greenberg *et al*., 1993; Greenberg *et al*., 1996). The structure of (4-chlorophenyl)(morpholino)methanone (**1c**) has been previously published (Bisz *et al*., 2018).

2.1. Synthesis and crystallization

The compounds were synthesized according to the procedure described by Rushworth et al. (Rushworth *et al*., 2013). The crystallization was performed from a diethyl ether solution. Diethyl ether (0.60 mL) was placed in storage reaction vials (8 mL) equipped with silicone septa. The title compounds were added in small portions until saturated solutions were obtained. The solutions were warmed, and then, left to stand in a refrigerator at -20 °C. After 24 h, hexane (0.40 mL, 50 °C) was added to the cold solutions, and the samples were left to stand in a refrigerator at -20 °C.

2.2. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1 in the manuscript. Hydrogen-bond geometry is summarized in Table 2. Selected geometric parameters are summarized in the Supporting Information.

Table 1 Experimental details for **1a-1d**.

	1a	**1b**	**1c**	**1d**
Crystal data				
Chemical formula	$C_{11}H_{12}INO_2$	$C_{11}H_{12}BrNO_2$	$C_{11}H_{12}ClNO_2$	$C_{11}H_{12}FNO_2$
M_r	317.12	270.13	225.67	209.22
Crystal system, space group	Monoclinic, $P2_1/c$	Trigonal, $P3_1$	Trigonal, $P3_1$	Orthorhombic, *Pbca*
a, b, c (Å)	10.5193 (3), 12.2078 (4), 8.8674 (3)	9.9577 (2), 9.9577 (2), 9.8213 (2)	9.9808 (3), 9.9808 (3), 9.5853 (3)	7.3584 (5), 7.2979 (5), 37.576 (2)
α, β, γ (°)	90, 93.763 (3), 90	90, 90, 120	90, 90, 120	90, 90, 90
V (Å^3)	1136.27 (6)	843.37 (4)	826.93 (6)	2017.9 (2)
Z	4	3	3	8
μ (mm^{-1})	2.80	3.64	0.33	0.11
Crystal size (mm)	0.5 × 0.4 × 0.3	0.5 × 0.5 × 0.4	0.5 × 0.5 × 0.4	0.2 × 0.2 × 0.1
Data collection				
Absorption correction	–	–	–	–
No. of measured, independent and observed [I> 2σ(I)] reflections	7452, 2207, 2019	5805, 2180, 2129	5673, 1680, 1590	12441, 1977, 1193
R_{int}	0.019	0.046	0.017	0.092
(sin θ/λ)$_{max}$ (Å^{-1})	0.617	0.617	0.616	0.617
Refinement				
$R[F^2> 2\sigma(F^2)]$, $wR(F^2)$, S	0.017, 0.044, 1.07	0.023, 0.057, 1.05	0.028, 0.068, 1.09	0.047, 0.087, 0.98
No. of reflections	2207	2180	1680	1977
No. of parameters	136	136	181	136
No. of restraints	0	1	1	0
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.42, −0.52	0.32, −0.37	0.27, −0.45	0.19, −0.24

Experiments were carried out at 100 K with Mo $K\alpha$ radiation using aXcalibur. H-atom parameters were constrained. Computer programs: *CrysAlis CCD* (Oxford Diffraction Ltd., 2008), *SHELXS2014* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *SHELXTL* (Sheldrick, 2008).

Table 2 Summary of hydrogen-bond geometry (Å, °) for **1a-1d**

D—H···*A*	*D*—H (Å)	H···*A* (Å)	*D*···*A* (Å)	*D*—H···*A* (°)
1a				
C14—H14A···O8^{i}	0.97	2.51	3.479 (3)	172.9
C14—H14B···O8^{ii}	0.97	2.39	3.068 (2)	127.0
1b				
C3—H3A···O2^{iii}	0.97	2.57	3.257 (4)	127.8
C2—H2B···O1^{iv}	0.97	2.48	3.322 (5)	144.6
C3P—H3P···O2^{v}	0.93	2.49	3.418 (5)	177.3
1c				
C5—H5···O12^{v}	0.93	2.42	3.353 (4)	178.7
C10A—H10A···O8^{vi}	0.97	2.43	3.240 (4)	140.3
C10A—H10B···Cl15^{vii}	0.97	2.92	3.382 (4)	110.1
C14A—H14B···O12^{viii}	0.97	2.55	3.281 (4)	132.6
C10B—H10D···O8^{vi}	0.97	2.48	3.307 (7)	143.2
C11B—H11C···O8^{ix}	0.97	2.65	3.601 (8)	166.1
C14B—H14C···O12^{viii}	0.97	2.54	3.250 (7)	130.2
1d				
C11—H11A···O12^{x}	0.97	2.56	3.265 (2)	129.7
C13—H13A···O8^{xi}	0.97	2.64	3.576 (2)	161.8
C13—H13B···O8^{xii}	0.97	2.49	3.244 (2)	134.4
C14—H14A···O8^{xiii}	0.97	2.58	3.395 (2)	141.6

Symmetry code(s): (i) −*x*+1, −*y*+1, −*z*; (ii) −*x*+1, *y*−1/2, −*z*+1/2; (iii) −*x*+*y*, −*x*, *z*−1/3; (iv) −*y*+1, *x*−*y*+1, *z*+1/3; (v) *x*, *y*, *z*−1; (vi) −*y*+1, *x*−*y*, *z*+1/3; (vii) −*x*+*y*, −*x*, *z*+2/3; (viii) −*x*+*y*, −*x*+1, *z*−1/3; (ix) −*x*+*y*+1, −*x*+1, *z*+2/3; (x) −*x*+1, *y*+1/2, −*z*+1/2; (xi) −*x*+3/2, *y*−1/2, *z*; (xii) *x*, *y*−1, *z*; (xiii) −*x*+1/2, *y*−1/2, *z*.

3. Results and discussion

Selected structural parameters relevant to the amide bond geometry in **1a-1d** along with representative non-planar and planar amides are presented in Table 3. Structures of amides **1a-1d** (50% ellipsoids) along with Newman projections along N–C(O) bonds and crystal packing of amides **1a-1d** are shown in Figures 1-8.

Table 3 Selected Crystallographic Structural Parameters of 4-Halo-Benzamides **1a–1d**[a]

entry	amide	N–C(O) [Å]	C=O [Å]	NC(O) τ [deg]	NC(O) χ_N [deg]	CC(O) τ [deg]
1	**1a (R = I)**	1.357	1.234	12.90	19.99	43.77
2	**1b (R = Br)**	1.345	1.230	0.18	8.28	74.30
3	**1c (R = Cl)**	1.389	1.224	1.35	0.89	62.54
4	**1d (R = F)**	1.354	1.236	6.69	7.81	57.28
5	**benzamide**	1.342	1.265	0.02	0.07	25.66
6	**formamide**	1.349	1.193	0.0	0.0	0.0

[a]Entries 1-4: this study, X-ray structures. Entry 5: Johansson *et al*., 2016, X-ray structure. Entry 6: Greenberg *et al*., 1993, calculated values.

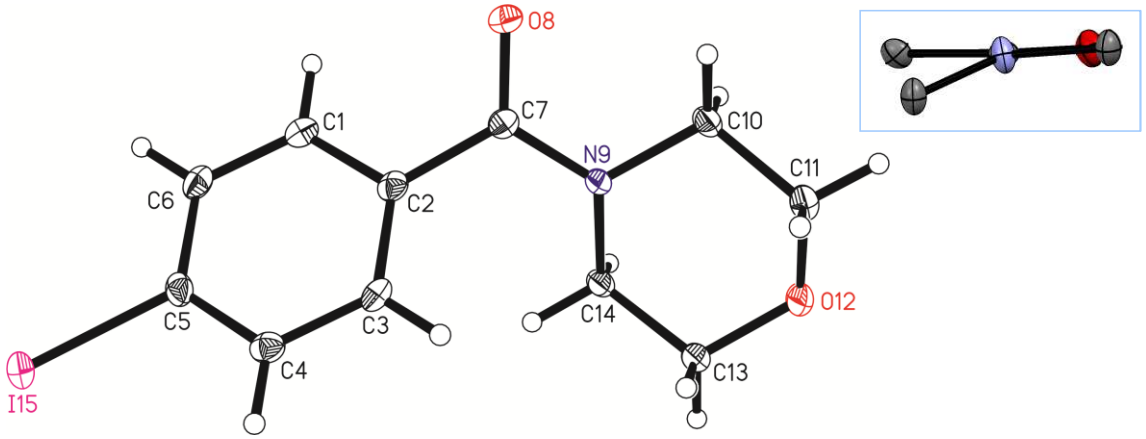


Figure 1 Crystal structure of **1a**. Ellipsoids are drawn at the 50% probability level. Inset shows Newman projection along the N–C(O) bond.

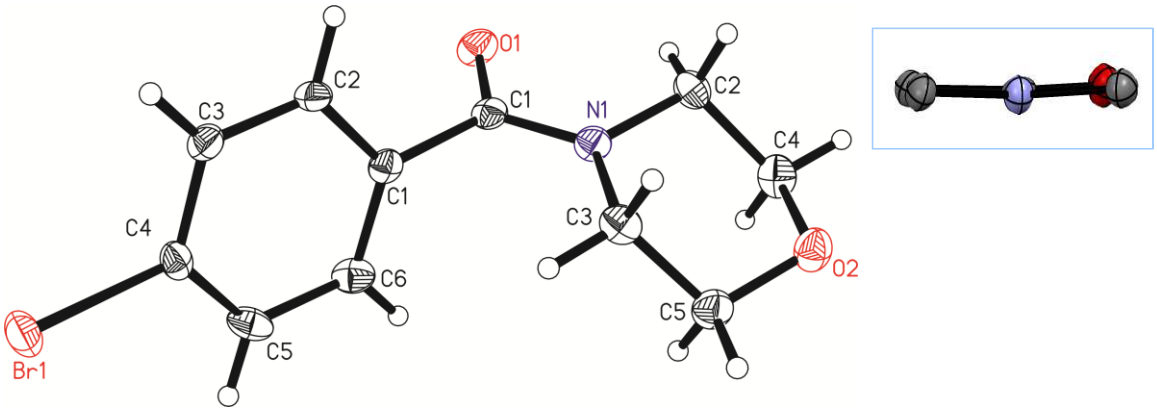


Figure 2 Crystal structure of **1b**. Ellipsoids are drawn at the 50% probability level. Inset shows Newman projection along the N–C(O) bond.

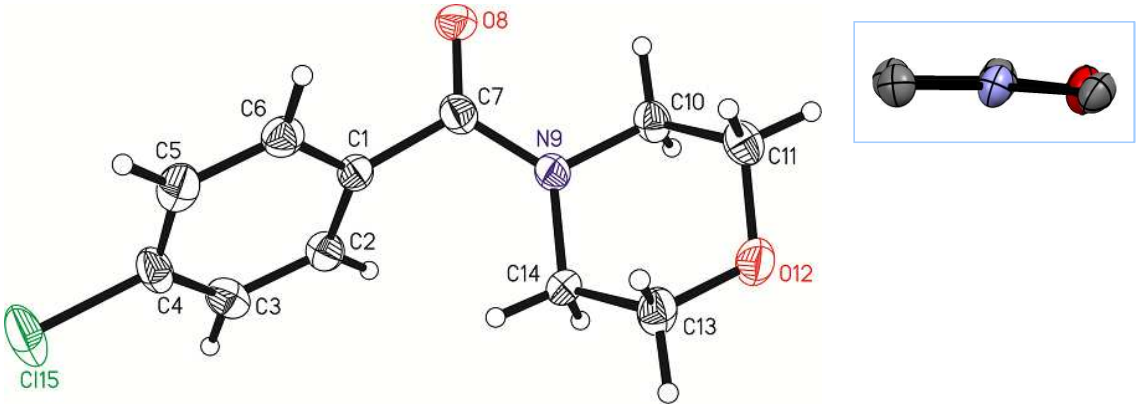


Figure 3 Crystal structure of **1c**. Ellipsoids are drawn at the 50% probability level. Inset shows Newman projection along the N–C(O) bond. Disorder of the morpholinyl ring in **1c** is omitted for clarity.

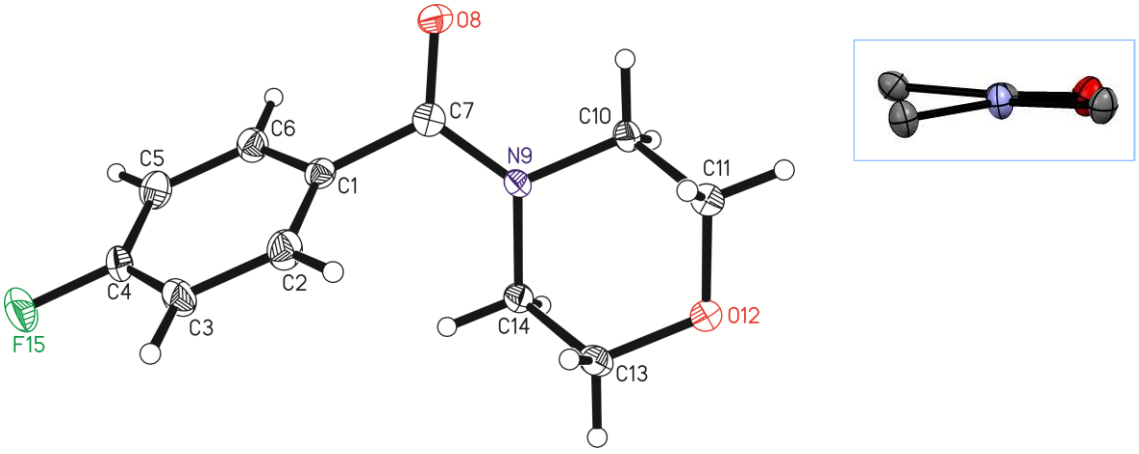


Figure 4 Crystal structure of **1d**. Ellipsoids are drawn at the 50% probability level. Inset shows Newman projection along the N–C(O) bond.

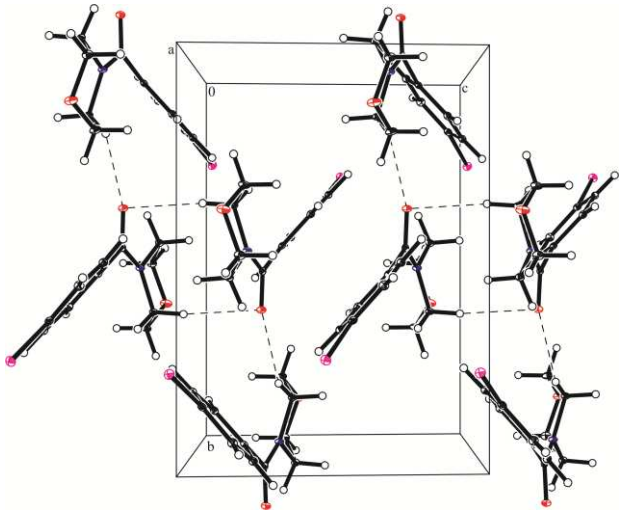


Figure 5 The crystal packing of **1a**, viewed along the *c* axis. Ellipsoids are drawn at the 50% probability level.

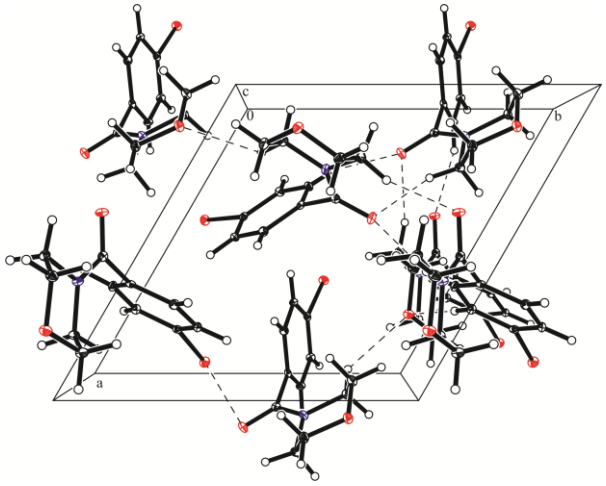


Figure 6 The crystal packing of **1b**, viewed along the *c* axis. Ellipsoids are drawn at the 50% probability level.

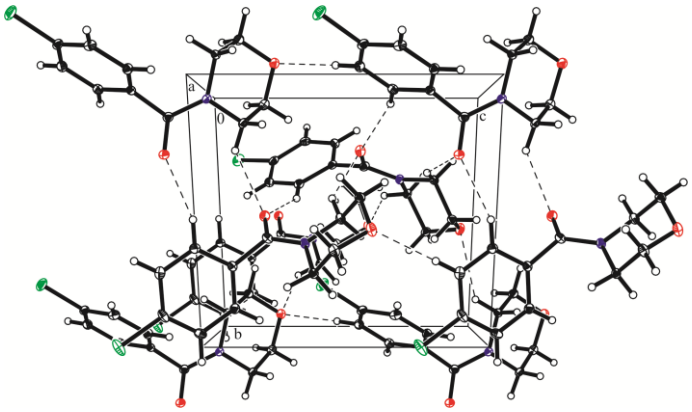


Figure 7 The crystal packing of **1c**, viewed along the *c* axis. Ellipsoids are drawn at the 50% probability level.

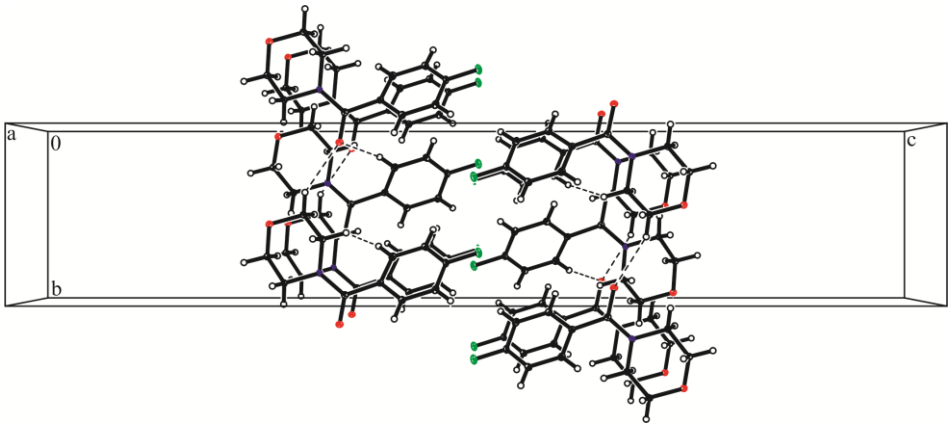


Figure 8 The crystal packing of **1d**, viewed along the *c* axis. Ellipsoids are drawn at the 50% probability level.

Interestingly, we found that 4-iodo-N-morpholinyl-benzamide (**1a**) crystallized with a significant distortion of the amide bond (τ = 12.9°; χ_N = 20.0°; $\tau+\chi_N$ = 32.9°, additive Winkler-Dunitz distortion parameter; the N–C(O) amide bond length of 1.357 Å; the N–C(O) amide bond length of 1.234 Å). This corresponds to a significant 22% of maximum theoretical amide bond distortion (Tani *et al*., 2006; Yamada, 1999). The amide bond distortion in the remaining compounds in the series ranges from $\Sigma(\tau+\chi_N)$ = 2.2° for **1c** to $\Sigma(\tau+\chi_N)$ = 8.5° for **1b**, and $\Sigma(\tau+\chi_N)$ = 14.5° for **1d**. The amide N–C(O) bond length show values between 1.345 Å (**1b**) and 1.354 Å (**1d**) to 1.389 Å (**1c**) and the amide C=O bond length ranges from 1.224 Å (**1c**) and 1.230 Å (**1b**) to 1.236 Å (**1d**). The correlation of N–C(O) bond length to C=O bond length gives an inverse relationship in the series (Y = –0.524X + 2.002, R^2 = 0.920, outlier analysis, **1c**, not shown), indicating that elongation of the N–C(O) bond correlates with shortening of the C=O bond, as expected from the resonance model (Greenberg *et al*., 2000). Correlations involving twist and N pyramidalization give scattered results. Interestingly, the C–C(O) bond twist angle changes from moderately planar to almost twisted in the series (**1a**, τ = 43.8°; **1d**, τ = 57.3°; **1c**, τ = 62.5°; **1b**, τ = 74.3°), indicating a gradual increase of π_{Ar} to $\pi^*_{C=O}$ conjugation in the series. Most importantly, there is an excellent inverse correlation between twist angle of the amide N–C(O) bond and the Ar–C(O) axis twist angle (Chart 1, Y = -0.437X + 31.31, R^2 = 0.907) in the series. The highest the C–C(O) bond twist (**1b**, τ = 74.3°) corresponds to the strongest amide N–C(O) bond (**1b**, 1.345 Å) (Pace *et al*., 2016).

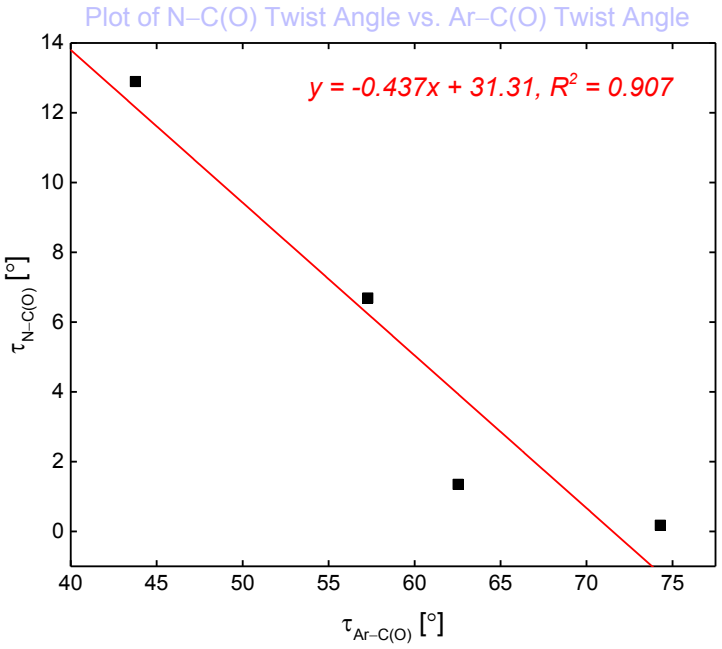


Chart 1 Plot of N–C(O) Twist Angle [°] vs. Ar–C(O) Twist Angle [°] in 4-Halo-Benzamides **1a–1d**.

Calculations were employed to gain further insight into the structural and energetic properties of the amide bond in the series of 4-halo-benzamides. Unsubstituted morpholino(phenyl)methanone (**1e**) and a full set of the corresponding 4-halo-subsituted N-piperidinyl amides (**2a-e**) were selected for comparison. Cartesian coordinates and energies of all compounds with zero-point energies and thermal corrections are listed in the Supporting Information. Computational methods and a full reference for Gaussian 09 are presented in the Supporting Information. Most importantly, computations confirm the findings from the X-ray data and show that there is an excellent correlation between twist angle of the amide N–C(O) bond and the Ar–C(O) axis twist angle in both series (Charts 2-3, **1**: Y = –0.468X + 36.60, R^2 = 0.991; **2**: Y = –0.448X + 35.52, R^2 = 0.982). Furthermore, there is an inverse correlation between the N–C(O) bond length and twist of the Ar–C(O) axis in **1a-d** series (Y = –0.001X + 1.430, R^2 = 0.933, not shown); **2a-d** series (Y = –0.001X + 1.481, R^2 = 0.931, not shown).

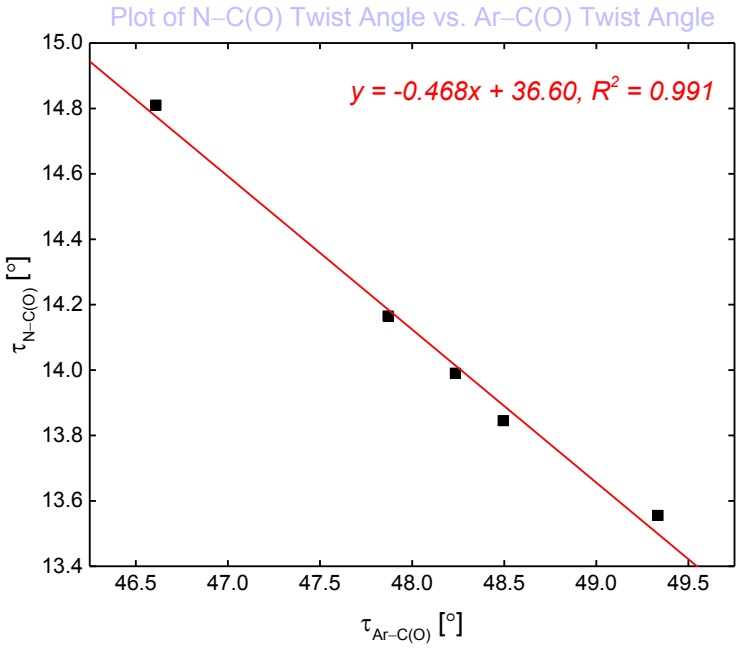


Chart 2 Plot of N–C(O) Twist Angle [°] vs. Ar–C(O) Twist Angle [°] in 4-Halo-Benzamides **1a–1e**.

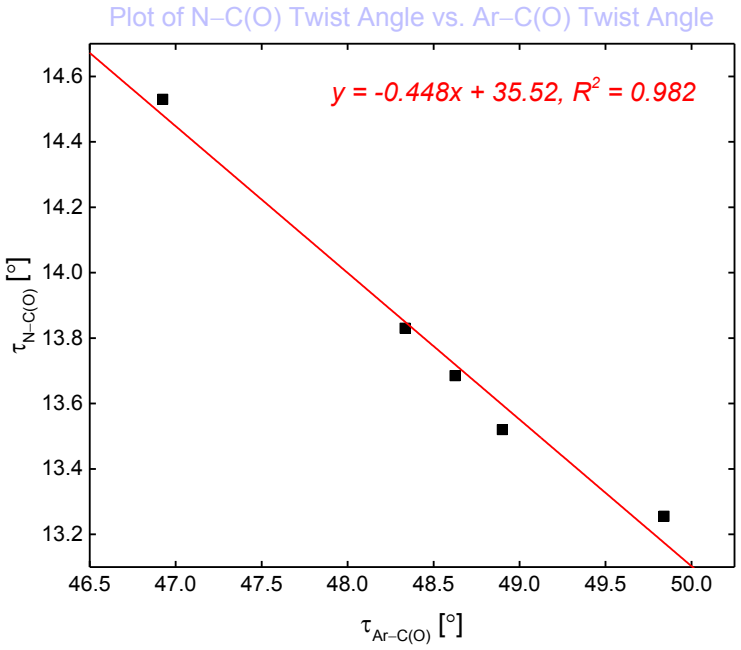


Chart 3 Plot of N–C(O) Twist Angle [°] vs. Ar–C(O) Twist Angle [°] in 4-Halo-Benzamides **2a–2e**.

Overall, the highest twist of the amide bond corresponds to the lowest C–C(O) bond twist, which indicates that switching-off amidic resonance is compensated by an increased delocalization into the C=O bond from the aryl ring (Pace *et al*., 2016; Szostak *et al*., 2016). Future studies will exploit the C–C(O) to N–C(O) communication to further develop our understanding of the properties of various classes of important acyclic benzamides.

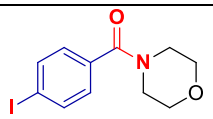
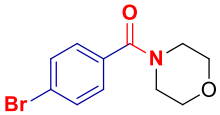
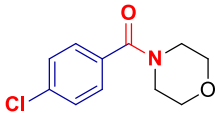
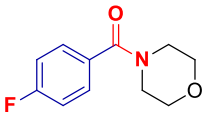
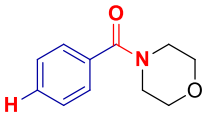
To gain insight into the energetic properties of the amide bond in 4-halo-susbtituted benzamides, resonance energies of amides **1a-e** were calculated using the COSNAR method (eq 1, Table 4).

$$-RE = E_{T(amide)} - [E_{T(amine)} + E_{T(ketone)} - E_{T(hydrocarbon)}] \quad \text{(eq. 1)}$$

As shown in Table 4, we found that resonance in these amides is relatively unchanged with respect to the parent unsubstituted amide in the series (**1a-1d**: 15.0-15.3 kcal/mol, **1e**: 15.3 kcal/mol), which can be compared with resonance for N,N-dimethylacetamide (18.3 kcal/mol) calculated at the same level. More interesting data is gained from calculating the energetic properties of amides in the piperidinyl series (Table 5). Morpholinyl amides are synthetically-valuable because of their Weinreb amide-type reactivity (Martin *et al*., 1997; Nahm *et al*., 1981). This chelation effect has been uniquely exploited in organic synthesis to furnish stable tetrahedral intermediates that collapse with no overaddition in organometallic addition reactions (Balasubramaniam *et al*., 2008). However, it is a common misconception that morpholinyl amides are more reactive than typical N,N-dialkyl amides due to inductive effect of the oxygen atom. The data in Table 5 confirms that amidic resonance in piperidinyl

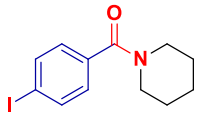
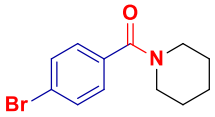
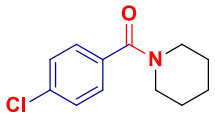
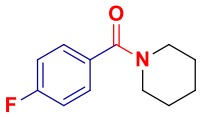
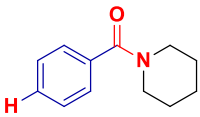
amides is practically the same as in morpholinyl amides (**2a-2d**: 15.1-15.5 kcal/mol, **2e**: 15.5 kcal/mol, ΔE = 0.20 kcal/mol). A plot of resonance energy in **2a-2e** vs. resonance energy in **1a-1e** gives an excellent linear correlation (Y = 1.083X – 1.081, R^2 = 0.991, Chart 4). Thus, our data verifies that the inductive effect of the oxygen atom in morpholinyl amides is negligible at best, and the unusual reactivity of these amides results from chelation effect rather than increased electrophilicity of the amide bond.

Table 4 Resonance Energies of Amides **1a–e** Calculated using COSNAR Method[a]

entry	amide	**1**	E_R [kcal/mol]
1		**1a (R = I)**	15.3
2		**1b (R = Br)**	15.2
3		**1c (R = Cl)**	15.2
4		**1d (R = F)**	15.0
5		**1e (R = H)**	15.3

[a]Representative data on twisted amides: Szostak *et al*., 2016. Representative data on bridged lactams: Greenberg *et al*., 1996; Szostak *et al*., 2015.

Table 5 Resonance Energies of Amides **2a–e** Calculated using COSNAR Method[a]

entry	amide	**2**	E_R [kcal/mol]
1		**2a (R = I)**	15.5
2		**2b (R = Br)**	15.4
3		**2c (R = Cl)**	15.5
4		**2d (R = F)**	15.1
5		**2e (R = H)**	15.5

[a]Representative data on twisted amides: Szostak *et al*., 2016. Representative data on bridged lactams: Greenberg *et al*., 1996; Szostak *et al*., 2015.

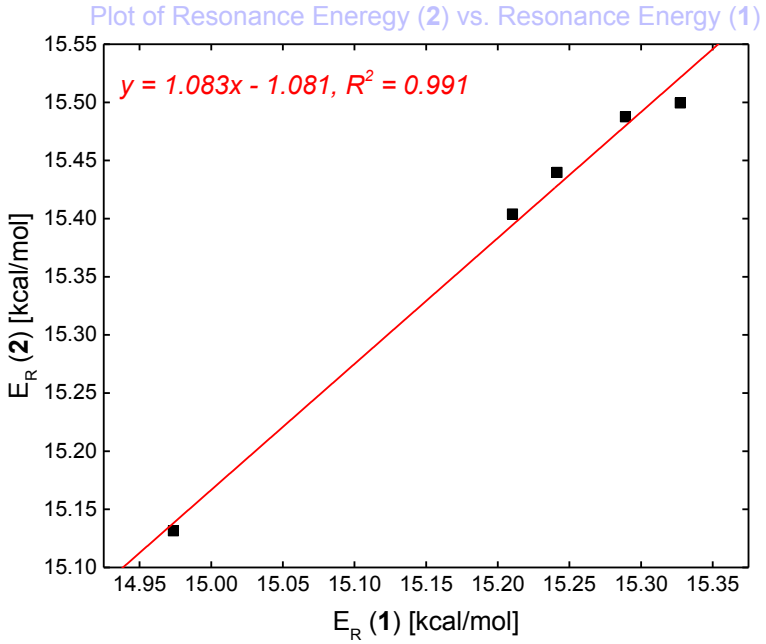


Chart 4 Correlation of Resonance Energy [kcal/mol] in 4-Halobenzamides **2a-e** with Resonance Energy [kcal/mol] in 2-Halobenzamides **1a-e**.

4. Conclusion

In summary, we have reported the crystal structures and energetic properties of a full series of 4-halo-benzamides. Morpholinyl amides were selected for the study to obtain the x-ray structures of a full set of 4-halo-benzamides (R = I, Br, Cl, F). These amides are additionally useful in organic synthesis due to the formation of stable tetrahedral intermediates in nucleophilic addition reactions. The presented results describe the first systematic investigation of the effect of para-halogen substitution on the properties of the amide bond in N,N-disubstituted benzamides. The 4-iodo-N-morpholinyl-benzamide crystallized with a significant distortion of the amide bond ($\tau+\chi_N$ = 33°). The effect of halogen substitution on structures and resonance energies was determined by computations. Resonance energies in 4-halo-benzamides are relatively unchanged as compared with the parent unsubstituted amide. However, comparison of resonance energies in N-morpholinyl amides with N-piperidinyl amides demonstrated that, in contrast to the common assumption, oxygen atom of the morpholinyl does not significantly contribute to the electrophilicity of the amide bond. Furthermore, the present study demonstrated the correlation between Ar–C(O) axis twist angle and twist angle of the amide N–C(O) bond, which in principle could be utilized to gauge structural properties amides. Future work will be focused on elucidation of structural and energetic properties of acyclic amides of relevance to organic synthesis.

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Supporting information

(4-Iodophenyl)(morpholino)methanone (1a)

Crystal data	
Chemical formula	$C_{11}H_{12}INO_2$
M_r	317.12
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	10.5193 (3), 12.2078 (4), 8.8674 (3)
β (°)	93.763 (3)
V (Å^3)	1136.27 (6)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	2.80
Crystal size (mm)	0.5 × 0.4 × 0.3
Data collection	
Diffractometer	Xcalibur
Absorption correction	–
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7452, 2207, 2019
R_{int}	0.019
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.017, 0.044, 1.07
No. of reflections	2207
No. of parameters	144
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.42, −0.52

Computer programs: *CrysAlis CCD* (Oxford Diffraction Ltd., 2008), *SHELXS2014*/7 (Sheldrick, 2014), *SHELXL2014*/7 (Sheldrick, 2014), *SHELXTL* (Sheldrick, 2008).

(4-Bromophenyl)(morpholino)methanone (1b)

Crystal data	
Chemical formula	$C_{11}H_{12}BrNO_2$
M_r	270.13
Crystal system, space group	Trigonal, $P3_1$

Temperature (K)	100
a, *c* (Å)	9.9577 (2), 9.8213 (2)
V (Å^3)	843.37 (4)
Z	3
Radiation type	Mo *K*α
μ (mm^{-1})	3.64
Crystal size (mm)	0.5 × 0.45 × 0.4
Data collection	
Diffractometer	Xcalibur
Absorption correction	–
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	5805, 2180, 2129
R_{int}	0.046
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.023, 0.057, 1.05
No. of reflections	2180
No. of parameters	150
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.32, −0.37
Absolute structure	Flack x determined using 1007 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
Absolute structure parameter	−0.007 (9)

Computer programs: *CrysAlis CCD* (Oxford Diffraction Ltd., 2008), *SHELXS2014*/7 (Sheldrick, 2014), *SHELXL2014*/7 (Sheldrick, 2014), *SHELXTL* (Sheldrick, 2008).

(4-Chlorophenyl)(morpholino)methanone (1c)

Crystal data	
Chemical formula	$C_{11}H_{12}ClNO_2$
M_r	225.67
Crystal system, space group	Trigonal, $P3_1$
Temperature (K)	100
a, *c* (Å)	9.9808 (3), 9.5853 (3)
V (Å^3)	826.93 (6)
Z	3

Radiation type	Mo *K*α
μ (mm^{-1})	0.33
Crystal size (mm)	0.5 × 0.45 × 0.4
Data collection	
Diffractometer	Xcalibur
Absorption correction	–
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	5673, 1680, 1590
R_{int}	0.017
$(\sin \theta/\lambda)_{max}$ ($Å^{-1}$)	0.616
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.028, 0.068, 1.09
No. of reflections	1680
No. of parameters	185
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e $Å^{-3}$)	0.27, −0.45
Absolute structure	Flack x determined using 505 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
Absolute structure parameter	0.00 (2)

Computer programs: *CrysAlis CCD* (Oxford Diffraction Ltd., 2008), *SHELXS2014*/7 (Sheldrick, 2014), *SHELXL2014*/7 (Sheldrick, 2014), *SHELXTL* (Sheldrick, 2008).

(4-Fluorophenyl)(morpholino)methanone (1d)

Crystal data	
Chemical formula	$C_{11}H_{12}FNO_2$
M_r	209.22
Crystal system, space group	Orthorhombic, *Pbca*
Temperature (K)	100
a, *b*, *c* (Å)	7.3584 (5), 7.2979 (5), 37.576 (2)
V ($Å^3$)	2017.9 (2)
Z	8
Radiation type	Mo *K*α
μ (mm^{-1})	0.11
Crystal size (mm)	0.2 × 0.15 × 0.1
Data collection	

Diffractometer	Xcalibur
Absorption correction	–
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	12441, 1977, 1193
R_{int}	0.092
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.047, 0.087, 0.98
No. of reflections	1977
No. of parameters	152
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.19, −0.23

Computer programs: *CrysAlis CCD* (Oxford Diffraction Ltd., 2008), *SHELXS2014*/7 (Sheldrick, 2014), *SHELXL2014*/7 (Sheldrick, 2014), *SHELXTL* (Sheldrick, 2008).

Summary of selected geometric parameters (Å, °) for ***1a-1d****.*

1a			
C1—C6	1.384 (3)	N9—C10	1.470 (3)
C1—C2	1.397 (3)	O8—C7	1.234 (2)
C1—H1	0.9300	C10—C11	1.515 (3)
C2—C3	1.394 (3)	C10—H10A	0.9700
C2—C7	1.496 (3)	C10—H10B	0.9700
C3—C4	1.386 (3)	C11—O12	1.426 (2)
C3—H3	0.9300	C11—H11A	0.9700
C4—C5	1.390 (3)	C11—H11B	0.9700
C4—H4	0.9300	O12—C13	1.430 (2)
C5—C6	1.391 (3)	C13—C14	1.509 (3)
C5—I15	2.098 (2)	C13—H13A	0.9700
C6—H6	0.9300	C13—H13B	0.9700
N9—C7	1.357 (2)	C14—H14A	0.9700
N9—C14	1.469 (2)	C14—H14B	0.9700
C6—C1—C2	120.56 (19)	N9—C10—H10A	109.9
C6—C1—H1	119.7	C11—C10—H10A	109.9
C2—C1—H1	119.7	N9—C10—H10B	109.9

C3—C2—C1	119.1 (2)	C11—C10—H10B	109.9
C3—C2—C7	123.02 (18)	H10A—C10—H10B	108.3
C1—C2—C7	117.72 (18)	O12—C11—C10	111.76 (17)
C4—C3—C2	120.71 (19)	O12—C11—H11A	109.3
C4—C3—H3	119.6	C10—C11—H11A	109.3
C2—C3—H3	119.6	O12—C11—H11B	109.3
C3—C4—C5	119.52 (19)	C10—C11—H11B	109.3
C3—C4—H4	120.2	H11A—C11—H11B	107.9
C5—C4—H4	120.2	C11—O12—C13	110.29 (16)
C4—C5—C6	120.44 (19)	O12—C13—C14	111.01 (17)
C4—C5—I15	119.49 (15)	O12—C13—H13A	109.4
C6—C5—I15	120.07 (16)	C14—C13—H13A	109.4
C1—C6—C5	119.64 (19)	O12—C13—H13B	109.4
C1—C6—H6	120.2	C14—C13—H13B	109.4
C5—C6—H6	120.2	H13A—C13—H13B	108.0
C7—N9—C14	126.04 (17)	N9—C14—C13	109.70 (17)
C7—N9—C10	118.35 (17)	N9—C14—H14A	109.7
C14—N9—C10	112.91 (16)	C13—C14—H14A	109.7
O8—C7—N9	122.03 (18)	N9—C14—H14B	109.7
O8—C7—C2	119.18 (18)	C13—C14—H14B	109.7
N9—C7—C2	118.77 (17)	H14A—C14—H14B	108.2
N9—C10—C11	109.13 (16)		
C6—C1—C2—C3	−2.0 (3)	C10—N9—C7—C2	−176.19 (17)
C6—C1—C2—C7	−177.07 (18)	C3—C2—C7—O8	−132.8 (2)
C1—C2—C3—C4	1.1 (3)	C1—C2—C7—O8	42.1 (3)
C7—C2—C3—C4	175.87 (18)	C3—C2—C7—N9	45.5 (3)
C2—C3—C4—C5	1.2 (3)	C1—C2—C7—N9	−139.69 (19)
C3—C4—C5—C6	−2.6 (3)	C7—N9—C10—C11	144.61 (18)
C3—C4—C5—I15	177.17 (14)	C14—N9—C10—C11	−52.9 (2)
C2—C1—C6—C5	0.7 (3)	N9—C10—C11—O12	55.7 (2)
C4—C5—C6—C1	1.7 (3)	C10—C11—O12—C13	−60.2 (2)
I15—C5—C6—C1	−178.08 (15)	C11—O12—C13—C14	60.2 (2)
C14—N9—C7—O8	−158.01 (19)	C7—N9—C14—C13	−145.45 (19)
C10—N9—C7—O8	2.0 (3)	C10—N9—C14—C13	53.6 (2)

C14—N9—C7—C2	23.8 (3)	O12—C13—C14—N9	−56.4 (2)
1b			
Br1—C4P	1.902 (4)	C5—H5A	0.9700
N1—C1	1.345 (5)	C5—H5B	0.9700
N1—C2	1.467 (5)	C4—H4A	0.9700
N1—C3	1.468 (5)	C4—H4B	0.9700
O1—C1	1.231 (4)	C1P—C6P	1.386 (5)
C1—C1P	1.506 (5)	C1P—C2P	1.394 (5)
C3—C5	1.506 (5)	C2P—C3P	1.383 (5)
C3—H3A	0.9700	C2P—H2P	0.9300
C3—H3B	0.9700	C3P—C4P	1.392 (5)
C2—C4	1.513 (6)	C3P—H3P	0.9300
C2—H2A	0.9700	C4P—C5P	1.367 (5)
C2—H2B	0.9700	C5P—C6P	1.394 (6)
O2—C5	1.427 (5)	C5P—H5P	0.9300
O2—C4	1.432 (4)	C6P—H6P	0.9300
C1—N1—C2	120.5 (3)	O2—C4—C2	111.9 (3)
C1—N1—C3	125.8 (3)	O2—C4—H4A	109.2
C2—N1—C3	113.2 (3)	C2—C4—H4A	109.2
O1—C1—N1	122.7 (3)	O2—C4—H4B	109.2
O1—C1—C1P	119.4 (3)	C2—C4—H4B	109.2
N1—C1—C1P	117.9 (3)	H4A—C4—H4B	107.9
N1—C3—C5	108.9 (3)	C6P—C1P—C2P	120.0 (3)
N1—C3—H3A	109.9	C6P—C1P—C1	122.2 (3)
C5—C3—H3A	109.9	C2P—C1P—C1	117.7 (3)
N1—C3—H3B	109.9	C3P—C2P—C1P	120.0 (3)
C5—C3—H3B	109.9	C3P—C2P—H2P	120.0
H3A—C3—H3B	108.3	C1P—C2P—H2P	120.0
N1—C2—C4	110.1 (3)	C2P—C3P—C4P	118.9 (3)
N1—C2—H2A	109.6	C2P—C3P—H3P	120.6
C4—C2—H2A	109.6	C4P—C3P—H3P	120.6
N1—C2—H2B	109.6	C5P—C4P—C3P	121.8 (3)
C4—C2—H2B	109.6	C5P—C4P—Br1	119.9 (3)
H2A—C2—H2B	108.2	C3P—C4P—Br1	118.2 (3)

C5—O2—C4	109.8 (3)	C4P—C5P—C6P	119.1 (3)
O2—C5—C3	111.9 (3)	C4P—C5P—H5P	120.4
O2—C5—H5A	109.2	C6P—C5P—H5P	120.4
C3—C5—H5A	109.2	C1P—C6P—C5P	120.0 (3)
O2—C5—H5B	109.2	C1P—C6P—H6P	120.0
C3—C5—H5B	109.2	C5P—C6P—H6P	120.0
H5A—C5—H5B	107.9		
C2—N1—C1—O1	3.2 (5)	N1—C1—C1P—C6P	−76.7 (4)
C3—N1—C1—O1	175.0 (3)	O1—C1—C1P—C2P	−72.0 (4)
C2—N1—C1—C1P	−175.4 (3)	N1—C1—C1P—C2P	106.7 (4)
C3—N1—C1—C1P	−3.5 (5)	C6P—C1P—C2P—C3P	2.7 (5)
C1—N1—C3—C5	134.5 (4)	C1—C1P—C2P—C3P	179.5 (3)
C2—N1—C3—C5	−53.1 (4)	C1P—C2P—C3P—C4P	−1.8 (5)
C1—N1—C2—C4	−135.4 (3)	C2P—C3P—C4P—C5P	−0.7 (5)
C3—N1—C2—C4	51.8 (4)	C2P—C3P—C4P—Br1	176.4 (3)
C4—O2—C5—C3	−60.9 (4)	C3P—C4P—C5P—C6P	2.1 (6)
N1—C3—C5—O2	57.4 (4)	Br1—C4P—C5P—C6P	−174.9 (3)
C5—O2—C4—C2	58.8 (4)	C2P—C1P—C6P—C5P	−1.3 (6)
N1—C2—C4—O2	−54.0 (4)	C1—C1P—C6P—C5P	−177.9 (3)
O1—C1—C1P—C6P	104.7 (4)	C4P—C5P—C6P—C1P	−1.1 (6)
1c			
C1—C6	1.388 (4)	C10A—H10A	0.9700
C1—C2	1.391 (3)	C10A—H10B	0.9700
C1—C7	1.503 (3)	C11A—H11A	0.9700
C2—C3	1.387 (4)	C11A—H11B	0.9700
C2—H2	0.9300	C13A—C14A	1.518 (6)
C3—C4	1.375 (4)	C13A—H13A	0.9700
C3—H3	0.9300	C13A—H13B	0.9700
C4—C5	1.388 (4)	C14A—H14A	0.9700
C4—Cl15	1.741 (3)	C14A—H14B	0.9700
C5—C6	1.381 (4)	N9A—C14B	1.466 (10)
C5—H5	0.9300	N9A—C10B	1.482 (10)
C6—H6	0.9300	C10B—C11B	1.489 (12)
C7—O8	1.224 (3)	C10B—H10C	0.9700

C7—N9A	1.334 (8)	C10B—H10D	0.9700
C7—N9B	1.389 (5)	C11B—H11C	0.9700
O12—C13A	1.418 (6)	C11B—H11D	0.9700
O12—C11A	1.444 (5)	C13B—C14B	1.474 (14)
O12—C11B	1.490 (8)	C13B—H13C	0.9700
O12—C13B	1.516 (10)	C13B—H13D	0.9700
N9B—C10A	1.463 (5)	C14B—H14C	0.9700
N9B—C14A	1.465 (6)	C14B—H14D	0.9700
C10A—C11A	1.501 (6)		
C6—C1—C2	119.7 (2)	O12—C13A—C14A	108.8 (4)
C6—C1—C7	117.9 (2)	O12—C13A—H13A	109.9
C2—C1—C7	122.2 (2)	C14A—C13A—H13A	109.9
C3—C2—C1	120.1 (3)	O12—C13A—H13B	109.9
C3—C2—H2	119.9	C14A—C13A—H13B	109.9
C1—C2—H2	119.9	H13A—C13A—H13B	108.3
C4—C3—C2	119.0 (2)	N9B—C14A—C13A	109.7 (4)
C4—C3—H3	120.5	N9B—C14A—H14A	109.7
C2—C3—H3	120.5	C13A—C14A—H14A	109.7
C3—C4—C5	121.8 (3)	N9B—C14A—H14B	109.7
C3—C4—Cl15	120.0 (2)	C13A—C14A—H14B	109.7
C5—C4—Cl15	118.2 (2)	H14A—C14A—H14B	108.2
C6—C5—C4	118.6 (3)	C7—N9A—C14B	126.4 (6)
C6—C5—H5	120.7	C7—N9A—C10B	120.2 (6)
C4—C5—H5	120.7	C14B—N9A—C10B	113.2 (6)
C5—C6—C1	120.6 (2)	N9A—C10B—C11B	109.8 (6)
C5—C6—H6	119.7	N9A—C10B—H10C	109.7
C1—C6—H6	119.7	C11B—C10B—H10C	109.7
O8—C7—N9A	120.0 (4)	N9A—C10B—H10D	109.7
O8—C7—N9B	121.6 (3)	C11B—C10B—H10D	109.7
O8—C7—C1	119.5 (2)	H10C—C10B—H10D	108.2
N9A—C7—C1	116.1 (4)	C10B—C11B—O12	109.4 (6)
N9B—C7—C1	118.1 (2)	C10B—C11B—H11C	109.8
C13A—O12—C11A	110.6 (3)	O12—C11B—H11C	109.8
C11B—O12—C13B	102.8 (5)	C10B—C11B—H11D	109.8

C7—N9B—C10A	121.0 (3)	O12—C11B—H11D	109.8
C7—N9B—C14A	126.0 (3)	H11C—C11B—H11D	108.2
C10A—N9B—C14A	113.0 (4)	C14B—C13B—O12	108.7 (7)
N9B—C10A—C11A	110.7 (3)	C14B—C13B—H13C	110.0
N9B—C10A—H10A	109.5	O12—C13B—H13C	110.0
C11A—C10A—H10A	109.5	C14B—C13B—H13D	110.0
N9B—C10A—H10B	109.5	O12—C13B—H13D	110.0
C11A—C10A—H10B	109.5	H13C—C13B—H13D	108.3
H10A—C10A—H10B	108.1	N9A—C14B—C13B	109.8 (7)
O12—C11A—C10A	108.3 (3)	N9A—C14B—H14C	109.7
O12—C11A—H11A	110.0	C13B—C14B—H14C	109.7
C10A—C11A—H11A	110.0	N9A—C14B—H14D	109.7
O12—C11A—H11B	110.0	C13B—C14B—H14D	109.7
C10A—C11A—H11B	110.0	H14C—C14B—H14D	108.2
H11A—C11A—H11B	108.4		
C6—C1—C2—C3	−0.9 (4)	C7—N9B—C10A—C11A	126.8 (4)
C7—C1—C2—C3	−175.8 (2)	C14A—N9B—C10A—C11A	−52.4 (5)
C1—C2—C3—C4	−1.2 (4)	C13A—O12—C11A—C10A	−64.4 (5)
C2—C3—C4—C5	1.8 (4)	N9B—C10A—C11A—O12	56.5 (5)
C2—C3—C4—Cl15	−177.10 (19)	C11A—O12—C13A—C14A	64.7 (5)
C3—C4—C5—C6	−0.3 (4)	C7—N9B—C14A—C13A	−127.2 (4)
Cl15—C4—C5—C6	178.56 (19)	C10A—N9B—C14A—C13A	52.0 (5)
C4—C5—C6—C1	−1.7 (3)	O12—C13A—C14A—N9B	−57.1 (5)
C2—C1—C6—C5	2.3 (4)	O8—C7—N9A—C14B	169.4 (6)
C7—C1—C6—C5	177.5 (2)	C1—C7—N9A—C14B	13.0 (10)
C6—C1—C7—O8	−64.8 (3)	O8—C7—N9A—C10B	−16.7 (9)
C2—C1—C7—O8	110.2 (3)	C1—C7—N9A—C10B	−173.1 (6)
C6—C1—C7—N9A	91.7 (5)	C7—N9A—C10B—C11B	−123.5 (8)
C2—C1—C7—N9A	−93.3 (5)	C14B—N9A—C10B—C11B	51.1 (9)
C6—C1—C7—N9B	124.7 (3)	N9A—C10B—C11B—O12	−60.1 (8)
C2—C1—C7—N9B	−60.2 (3)	C13B—O12—C11B—C10B	67.7 (8)
O8—C7—N9B—C10A	6.7 (5)	C11B—O12—C13B—C14B	−68.8 (8)
C1—C7—N9B—C10A	176.9 (3)	C7—N9A—C14B—C13B	121.7 (9)
O8—C7—N9B—C14A	−174.2 (3)	C10B—N9A—C14B—C13B	−52.6 (9)

C1—C7—N9B—C14A	−3.9 (5)	O12—C13B—C14B—N9A	62.1 (9)
1d			
C1—C6	1.385 (3)	N9—C14	1.463 (2)
C1—C2	1.391 (3)	N9—C10	1.470 (2)
C1—C7	1.501 (3)	C10—C11	1.513 (3)
C2—C3	1.381 (3)	C10—H10A	0.9700
C2—H2	0.9300	C10—H10B	0.9700
C3—C4	1.370 (3)	C11—O12	1.430 (2)
C3—H3	0.9300	C11—H11A	0.9700
C4—C5	1.366 (3)	C11—H11B	0.9700
C4—F15	1.366 (2)	O12—C13	1.429 (2)
C5—C6	1.386 (3)	C13—C14	1.508 (3)
C5—H5	0.9300	C13—H13A	0.9700
C6—H6	0.9300	C13—H13B	0.9700
O8—C7	1.236 (2)	C14—H14A	0.9700
C7—N9	1.354 (2)	C14—H14B	0.9700
C6—C1—C2	119.18 (18)	N9—C10—H10A	109.8
C6—C1—C7	118.88 (18)	C11—C10—H10A	109.8
C2—C1—C7	121.81 (18)	N9—C10—H10B	109.8
C3—C2—C1	120.6 (2)	C11—C10—H10B	109.8
C3—C2—H2	119.7	H10A—C10—H10B	108.2
C1—C2—H2	119.7	O12—C11—C10	111.61 (16)
C4—C3—C2	118.4 (2)	O12—C11—H11A	109.3
C4—C3—H3	120.8	C10—C11—H11A	109.3
C2—C3—H3	120.8	O12—C11—H11B	109.3
C5—C4—F15	118.32 (19)	C10—C11—H11B	109.3
C5—C4—C3	122.83 (19)	H11A—C11—H11B	108.0
F15—C4—C3	118.85 (19)	C13—O12—C11	110.17 (15)
C4—C5—C6	118.4 (2)	O12—C13—C14	111.15 (16)
C4—C5—H5	120.8	O12—C13—H13A	109.4
C6—C5—H5	120.8	C14—C13—H13A	109.4
C5—C6—C1	120.6 (2)	O12—C13—H13B	109.4
C5—C6—H6	119.7	C14—C13—H13B	109.4
C1—C6—H6	119.7	H13A—C13—H13B	108.0

O8—C7—N9	122.10 (17)	N9—C14—C13	109.49 (16)
O8—C7—C1	119.77 (18)	N9—C14—H14A	109.8
N9—C7—C1	118.13 (17)	C13—C14—H14A	109.8
C7—N9—C14	126.54 (16)	N9—C14—H14B	109.8
C7—N9—C10	120.76 (16)	C13—C14—H14B	109.8
C14—N9—C10	112.30 (15)	H14A—C14—H14B	108.2
N9—C10—C11	109.50 (16)		
C6—C1—C2—C3	2.3 (3)	C2—C1—C7—N9	59.3 (3)
C7—C1—C2—C3	178.2 (2)	O8—C7—N9—C14	−169.42 (18)
C1—C2—C3—C4	0.0 (3)	C1—C7—N9—C14	10.6 (3)
C2—C3—C4—C5	−1.4 (3)	O8—C7—N9—C10	2.7 (3)
C2—C3—C4—F15	178.62 (19)	C1—C7—N9—C10	−177.21 (17)
F15—C4—C5—C6	−179.58 (19)	C7—N9—C10—C11	133.13 (19)
C3—C4—C5—C6	0.5 (3)	C14—N9—C10—C11	−53.7 (2)
C4—C5—C6—C1	1.9 (3)	N9—C10—C11—O12	55.6 (2)
C2—C1—C6—C5	−3.2 (3)	C10—C11—O12—C13	−59.3 (2)
C7—C1—C6—C5	−179.27 (19)	C11—O12—C13—C14	60.1 (2)
C6—C1—C7—O8	55.3 (3)	C7—N9—C14—C13	−132.6 (2)
C2—C1—C7—O8	−120.7 (2)	C10—N9—C14—C13	54.7 (2)
C6—C1—C7—N9	−124.8 (2)	O12—C13—C14—N9	−57.4 (2)

Computational Methods

Computational Methods. All of the calculations were performed using Gaussian 09 suite of programs. All of the geometry optimizations were performed at the B3LYP/6-311++G(d,p**)** level of theory in the gas phase. Extensive studies have showed that this level is accurate in predicting properties and resonance energies of amides. This method was further verified by obtaining good correlations between the calculated structures and X-ray structures in the series. All conformations within 3 kcal/mol from the lowest energy conformer were explored. The absence of imaginary frequencies was used to characterize the structures as minima on

the potential energy surface. All of the optimized geometries were verified as minima (no imaginary frequencies). Electronic and thermal energies were calculated for all structures. Energetic parameters were calculated under standard conditions (298.15 K and 1 atm). For geometry optimizations, we employed the X-ray structures of (4-iodophenyl)(morpholino)methanone, (4-bromophenyl)(morpholino)methanone, (4-chlorophenyl)(morpholino)methanone, (4-fluorophenyl)(morpholino)methanone as the starting geometry and performed full optimization for all structures. Optimized amide conformations were used as starting geometries for isodesmic calculations for the aza, keto, and hydrocarbon derivatives. Optimization of all of the protonated structures started with the optimized geometries of the amides. Structural representations were generated using CYLview software (Legault, C. Y. CYLview version 1.0 BETA, University of Sherbrooke). All other representations were generated using GaussView (GaussView, version 5, Dennington, R.; Keith, T.; Millam, J. Semichem Inc., Shawnee Mission, KS, 2009).

Full Reference for Gaussian 09

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Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

Cartesian Coordinates with Zero-Point Energies and Thermal Corrections

1a
Energy: -929.566516 au
Sum of electronic and thermal Energies: -929.338722 au
Geometry:

C	0.13468700	1.62619200	0.61496800
H	-0.21672000	2.51880000	1.11872200
C	-0.78026100	0.82663500	-0.07579600
C	-0.31297300	-0.29466700	-0.76764600
H	-1.00215900	-0.90471000	-1.34087600
C	1.04092600	-0.62477700	-0.75909700
H	1.39241600	-1.48629300	-1.31245000
C	1.93289500	0.16744400	-0.03869400
C	1.48606800	1.29453700	0.65045700
H	2.18206700	1.91505900	1.20035900
N	-3.20346900	0.35077800	0.06989700
O	-2.46674900	2.44280800	-0.44439500
C	-2.21389400	1.28165400	-0.15022500
C	-4.59988700	0.77684700	-0.06982600
H	-4.63764000	1.61752900	-0.76099100
H	-4.98470900	1.11770200	0.90063500
C	-5.43694400	-0.39229500	-0.57845300
H	-6.49638700	-0.13184500	-0.57675300
H	-5.13761400	-0.64552400	-1.60616300
O	-5.30433700	-1.54007200	0.25634700
C	-3.95077700	-1.96453700	0.34238900
H	-3.59326700	-2.27889100	-0.64998100
H	-3.93827500	-2.82829900	1.00933400
C	-3.05487200	-0.85651600	0.89050800
H	-3.35778000	-0.63103600	1.92263400
H	-2.01615700	-1.17940100	0.90715500
I	3.97980000	-0.33591600	-0.00279300

1a amine
Energy: -855.506664 au
Sum of electronic and thermal Energies: -855.261414 au
Geometry:

C	0.05145500	1.57341600	0.81232500
H	-0.30671600	2.31401900	1.52050000
C	-0.83328700	1.01600700	-0.11207300
C	-0.34498500	0.05667600	-1.00559600
H	-1.02470900	-0.39463400	-1.71947500
C	0.99085500	-0.33489200	-0.98100900
H	1.35141200	-1.07878100	-1.68036500
C	1.85718700	0.24062000	-0.05126700
C	1.39460000	1.19563400	0.84902800
H	2.06375000	1.63938200	1.57529700
N	-3.22863400	0.35819500	-0.25321300
C	-2.27948300	1.46672000	-0.17731700
C	-4.56902700	0.80247500	-0.63879200
H	-4.50940300	1.32164400	-1.60069200
H	-4.99107600	1.50844200	0.10085900
C	-5.50007100	-0.39846200	-0.76723000

H	-6.52134900	-0.07396800	-0.97451100
H	-5.15881200	-1.04391700	-1.58991000
O	-5.55184300	-1.14615600	0.44213400
C	-4.25353700	-1.58850000	0.82457800
H	-3.86199800	-2.28716400	0.07089400
H	-4.37521100	-2.12156000	1.76901600
C	-3.29154100	-0.41768500	0.98824200
H	-3.62629600	0.21249600	1.83361800
H	-2.29408000	-0.79570500	1.22732400
I	3.88393600	-0.34743000	-0.00655400
H	-2.49234400	2.12789100	0.68280300
H	-2.41957700	2.07548400	-1.07790900

1a ketone

Energy: -913.514868 au

Sum of electronic and thermal Energies: -913.275713 au

Geometry:

C	0.28280900	1.69394500	0.38175200
H	-0.06384700	2.67176000	0.69316000
C	-0.66895300	0.74590000	-0.02047500
C	-0.22242800	-0.51775900	-0.42711200
H	-0.92439100	-1.27626300	-0.74957500
C	1.13497500	-0.83120000	-0.43343300
H	1.46348600	-1.81171200	-0.75338100
C	2.06019800	0.12808400	-0.02697200
C	1.63893600	1.39481300	0.38276400
H	2.36004300	2.13823700	0.69787000
O	-2.42100400	2.29700900	0.27946800
C	-2.11793200	1.15116300	0.00238400
C	-4.51473600	0.74577100	-0.74483000
H	-4.37463700	1.26371700	-1.69915600
H	-4.83049900	1.49557200	-0.01619700
C	-5.59908900	-0.32044600	-0.89362100
H	-6.56365300	0.13159900	-1.13017700
H	-5.34286600	-1.01840700	-1.70778200
O	-5.79602200	-1.05434300	0.31212400
C	-4.61423600	-1.71919200	0.73417200
H	-4.31739900	-2.46376600	-0.02324800
H	-4.87673500	-2.25461700	1.64851400
C	-3.46359500	-0.74274900	0.98611500
H	-3.73151800	-0.07714200	1.81297100
H	-2.57049500	-1.29904700	1.28725600
I	4.11384200	-0.33758700	-0.03169200
C	-3.19666800	0.10772300	-0.28124600
H	-2.84056600	-0.56548800	-1.07029000

1a hydrocarbon

Energy: -839.479374 au

Sum of electronic and thermal Energies: -839.222303 au

Geometry:

C	-0.08286900	0.41182500	1.45984400
H	-0.57102400	0.24171400	2.41407000
C	-0.79659200	1.00821400	0.41624000
C	-0.12736500	1.22069900	-0.79511600
H	-0.64951100	1.69281700	-1.62171400
C	1.20374000	0.84818300	-0.96717300
H	1.69982900	1.02757800	-1.91274200
C	1.88844300	0.25090800	0.09001600
C	1.25081000	0.03169200	1.30785100
H	1.78127900	-0.42657100	2.13304600
C	-2.24833400	1.40286300	0.57505500

C	-4.67991300	1.01992200	-0.07109000
H	-4.73779700	1.98502300	-0.58778400
H	-4.96381900	1.19335000	0.97395900
C	-5.67732600	0.04568600	-0.69921900
H	-6.70479700	0.39090600	-0.56976700
H	-5.48380200	-0.04755000	-1.78046900
O	-5.61488200	-1.24054300	-0.09341500
C	-4.32136400	-1.82490400	-0.21268300
H	-4.08466800	-1.97763900	-1.27830300
H	-4.38987400	-2.80595700	0.26075900
C	-3.24240800	-0.96499500	0.44598600
H	-3.43405700	-0.92354300	1.52542100
H	-2.26496300	-1.43767200	0.30680800
I	3.90677800	-0.31531600	-0.15584800
H	-2.49938100	1.45137700	1.64028500
H	-2.39014300	2.41427500	0.17685300
C	-3.24844800	0.46040600	-0.13043100
H	-2.95770100	0.39498600	-1.18881600

1b

Energy: -3205.911298 au

Sum of electronic and thermal Energies: -3205.683290 au

Geometry:

Br	4.35201100	-0.46762400	0.00506500
N	-2.61714300	0.36714000	-0.06865400
O	-1.82160400	2.43853400	0.44164000
C	-1.60165200	1.27026700	0.14933900
C	-2.50395600	-0.84274900	-0.89124800
H	-1.47495700	-1.19525000	-0.90967900
H	-2.80134200	-0.60708500	-1.92269900
C	-4.00081200	0.83275800	0.07254400
H	-4.37639700	1.18576300	-0.89718500
H	-4.01416000	1.67328700	0.76479700
O	-4.77144000	-1.46259500	-0.25616300
C	-3.43070100	-1.92547100	-0.34387100
H	-3.44337700	-2.78831300	-1.01199500
H	-3.08155400	-2.25129000	0.64779200
C	-4.87053200	-0.31266400	0.58029000
H	-4.57781100	-0.57575100	1.60743100
H	-5.92208000	-0.02199200	0.57978700
C	-0.18144000	0.77500400	0.07509100
C	0.75582700	1.55085600	-0.61308400
H	0.42953600	2.45424000	-1.11418700
C	2.09720300	1.18239200	-0.64923800
H	2.81642400	1.77970200	-1.19443100
C	2.50467900	0.04186500	0.03767600
C	1.59678700	-0.72972000	0.75630900
H	1.93097700	-1.60069600	1.30503600
C	0.25326200	-0.36100300	0.76438800
H	-0.45326200	-0.95248000	1.33563900

1b amine

Energy: -3131.851480 au

Sum of electronic and thermal Energies: -3131.606034 au

Geometry:

Br	-4.26988400	-0.47525500	-0.01088100
N	2.62944900	0.36962300	-0.25284000
C	1.65094400	1.45223700	-0.17425700
C	2.71140100	-0.40881200	0.98591800
H	1.72412500	-0.81441700	1.22205100
H	3.02778900	0.22707800	1.83409000

C	3.95802800	0.85118600	-0.63480300
H	4.35976700	1.56567000	0.10796200
H	3.88584900	1.37195100	-1.59498700
O	4.99132700	-1.07396100	0.44101400
C	3.70487100	-1.55265400	0.81964000
H	3.83936800	-2.08568800	1.76234800
H	3.33358300	-2.25888900	0.06276100
C	4.92125300	-0.32382600	-0.76586400
H	4.59869000	-0.97539700	-1.59126300
H	5.93371700	0.02876600	-0.97046100
C	0.21757400	0.96208500	-0.11076800
C	-0.67954000	1.48499000	0.82192900
H	-0.34010600	2.22790000	1.53661900
C	-2.01128000	1.06976400	0.85883400
H	-2.69612500	1.48219200	1.58853900
C	-2.44248600	0.11254600	-0.05113400
C	-1.56933300	-0.43124800	-0.99016100
H	-1.91783200	-1.17722700	-1.69299900
C	-0.24565100	-0.00146500	-1.01328600
H	0.44468000	-0.42591200	-1.73322800
H	1.84566800	2.11632900	0.68789000
H	1.77530500	2.06705900	-1.07299200

1b ketone
Energy: -3189.859682 au
Sum of electronic and thermal Energies: -3189.620301 au
Geometry:

Br	-4.50406100	-0.46382000	-0.04613000
O	1.76754600	2.28427600	0.28924700
C	1.49432300	1.13232600	0.00666000
C	2.88886800	-0.72812600	0.98615300
H	2.01064600	-1.30830900	1.28603100
H	3.13926300	-0.05762700	1.81453300
C	3.90084400	0.79149300	-0.74108100
H	4.19687500	1.54736900	-0.01046500
H	3.74731500	1.30800900	-1.69411500
O	5.22860600	-0.97714200	0.31147300
C	4.06462900	-1.67359300	0.73190800
H	4.34101800	-2.20413600	1.64499400
H	3.78727400	-2.42387100	-0.02726500
C	5.01260500	-0.24571500	-0.89247900
H	4.77468100	-0.94805800	-1.70841200
H	5.96502100	0.23195800	-1.12786200
C	0.05616700	0.69066200	-0.02115000
C	-0.92011800	1.61486200	0.37830200
H	-0.59866000	2.60073700	0.69087200
C	-2.26810000	1.28272200	0.37528300
H	-3.01426300	2.00229200	0.68657000
C	-2.64891300	0.00622900	-0.03613200
C	-1.70495300	-0.93249500	-0.44010100
H	-2.01517400	-1.91885100	-0.75947500
C	-0.35657700	-0.58407100	-0.42929800
H	0.36556400	-1.32423800	-0.74925600
C	2.59982400	0.11799700	-0.27927800
H	2.26178600	-0.56239400	-1.07010100

1b hydrocarbon
Energy: -3115.824145 au
Sum of electronic and thermal Energies: -3115.566859 au
Geometry:

Br	4.29773800	0.41787000	-0.23149400

C	-1.61535700	-1.35708000	0.63278100
C	-2.66940800	0.97686400	0.40205600
H	-1.70564100	1.46565700	0.22757800
H	-2.84744800	0.98353000	1.48460200
C	-4.06323800	-1.06515400	0.00101600
H	-4.33026900	-1.19381600	1.05692700
H	-4.10334700	-2.05559400	-0.46712900
O	-5.05412200	1.16819500	-0.11927200
C	-3.77701700	1.77716000	-0.28366300
H	-3.86424900	2.77829400	0.14226600
H	-3.55671600	1.88312500	-1.35843200
C	-5.09189600	-0.14734300	-0.66076400
H	-4.91367200	-0.10267400	-1.74772400
H	-6.10887600	-0.51051200	-0.50113500
C	-0.17577300	-0.93537700	0.43648700
C	0.53430600	-0.27102700	1.44095300
H	0.05285000	-0.06645700	2.39161600
C	1.85581900	0.13427100	1.25449400
H	2.39027700	0.64576600	2.04475700
C	2.47809200	-0.13108000	0.04051800
C	1.80311500	-0.79483800	-0.97958000
H	2.29908900	-1.00478100	-1.91860100
C	0.48422200	-1.19072400	-0.77177300
H	-0.03552300	-1.71552000	-1.56730100
H	-1.85267000	-1.35985100	1.70223600
H	-1.73668000	-2.38985600	0.28601300
C	-2.64691700	-0.47472200	-0.10432400
H	-2.37067300	-0.45403600	-1.16841900

1c

Energy: -1091.991668 au

Sum of electronic and thermal Energies: -1091.763290 au

Geometry:

N	1.91335500	0.38821300	0.06712000
O	1.01175300	2.41727800	-0.43645100
C	0.85209100	1.23833600	-0.14770400
C	1.86428600	-0.82509000	0.89106400
H	0.85522300	-1.23106200	0.91055400
H	2.14942200	-0.57304000	1.92213400
C	3.27065800	0.92575600	-0.07451500
H	3.62735800	1.29901300	0.89478600
H	3.23988300	1.76521400	-0.76751400
O	4.16099100	-1.32565800	0.25603200
C	2.84642400	-1.85821100	0.34448300
H	2.90452500	-2.71854700	1.01344400
H	2.51471900	-2.20289300	-0.64679600
C	4.19930300	-0.17280500	-0.58141400
H	3.92060400	-0.45185500	-1.60824500
H	5.23412200	0.17273000	-0.58142000
C	-0.54032900	0.67019400	-0.07464100
C	-1.51787200	1.39861600	0.60971600
H	-1.23920200	2.31900700	1.10841700
C	-2.83779600	0.96137100	0.64477600
H	-3.59153500	1.51918200	1.18549500
C	-3.18485000	-0.20057200	-0.03912100
C	-2.23695500	-0.92609700	-0.75383200
H	-2.52962000	-1.81421900	-1.29909000
C	-0.91476100	-0.48885600	-0.76123500
H	-0.17765600	-1.04438100	-1.32975100
Cl	-4.85202800	-0.75443800	-0.01023300

1c amine
Energy: -1017.931705 au
Sum of electronic and thermal Energies: -1017.685922 au
Geometry:

N	1.90440600	0.37920500	-0.25143200
C	0.87409900	1.41251500	-0.16916900
C	2.02339000	-0.39975100	0.98397700
H	1.05697200	-0.85437400	1.21708800
H	2.30721100	0.24718200	1.83534500
C	3.20800900	0.92709100	-0.62996600
H	3.57347500	1.65743400	0.11613600
H	3.11109400	1.44768000	-1.58807000
O	4.33387100	-0.94924200	0.43911400
C	3.07220800	-1.49247100	0.81400400
H	3.23183000	-2.02236700	1.75456700
H	2.73708500	-2.21285500	0.05357100
C	4.22809100	-0.19845900	-0.76474400
H	3.93884100	-0.86176000	-1.59314700
H	5.22215900	0.20441600	-0.96672000
C	-0.53381300	0.85323600	-0.10866900
C	-1.45551600	1.32723400	0.82631900
H	-1.15235300	2.08181900	1.54494400
C	-2.76509700	0.84799300	0.85998600
H	-3.47281800	1.22007000	1.58981200
C	-3.14979900	-0.12388300	-0.05501500
C	-2.25095400	-0.61952500	-0.99620500
H	-2.56744900	-1.37775900	-1.70134900
C	-0.94999600	-0.12664300	-1.01672800
H	-0.23980500	-0.51318100	-1.73858800
Cl	-4.79748500	-0.74346200	-0.02177000
H	1.03601200	2.08150000	0.69598700
H	0.96944700	2.03653300	-1.06511300

1c ketone
Energy: -1075.940131 au
Sum of electronic and thermal Energies: -1075.700374 au
Geometry:

O	0.95508400	2.25097100	0.30276800
C	0.73532000	1.08977500	0.01111300
C	2.21206200	-0.71016200	0.98367800
H	1.36092500	-1.33222400	1.27769300
H	2.42889000	-0.03368800	1.81665600
C	3.15676200	0.86473400	-0.73213600
H	3.41557900	1.62935800	0.00347700
H	2.98175500	1.37900300	-1.68268800
O	4.56257100	-0.84630100	0.31411800
C	3.43108800	-1.59847400	0.72719800
H	3.72951200	-2.12117000	1.63787600
H	3.19076800	-2.35616100	-0.03722400
C	4.31592400	-0.11878200	-0.88629400
H	4.11302900	-0.82674000	-1.70683000
H	5.24571400	0.40398200	-1.11626800
C	-0.68061200	0.58330100	-0.02548100
C	-1.70028000	1.46077800	0.37175700
H	-1.42539700	2.45897500	0.68931100
C	-3.03098700	1.06757900	0.35984400
H	-3.81440800	1.74792000	0.66838100
C	-3.35133300	-0.22331600	-0.05767900
C	-2.36338400	-1.11648800	-0.45939600
H	-2.63159100	-2.11394000	-0.78285300
C	-1.03288600	-0.70757100	-0.44008300

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 H                -0.27592000   -1.41270500   -0.75839600
 Cl               -5.03036400   -0.73063000   -0.07765600
 C                 1.88718600    0.12902400   -0.27765000
 H                 1.58294200   -0.56165400   -1.07328500

1c hydrocarbon
Energy: -1001.904400 au
Sum of electronic and thermal Energies: -1001.646755 au
Geometry:
 C                 0.83418600    1.26221600    0.72168400
 C                 1.98834800   -0.99953100    0.31698400
 H                 1.04985000   -1.50797500    0.07425100
 H                 2.14062300   -1.09488900    1.39929000
 C                 3.30615400    1.12253000    0.13339500
 H                 3.54250900    1.16800900    1.20338500
 H                 3.31664400    2.15115600   -0.24550600
 O                 4.39061800   -1.05135500   -0.15385900
 C                 3.14384700   -1.69256200   -0.40544800
 H                 3.26202300   -2.72325400   -0.06630400
 H                 2.95368200   -1.71164800   -1.49097400
 C                 4.38713300    0.30727300   -0.57745900
 H                 4.23681700    0.35168900   -1.66864700
 H                 5.38425000    0.69418700   -0.35908800
 C                -0.58192500    0.80207600    0.45355800
 C                -1.28568800    0.02633800    1.37969600
 H                -0.81686500   -0.23963700    2.32134400
 C                -2.58427500   -0.41319500    1.12584400
 H                -3.11815800   -1.01162300    1.85316900
 C                -3.19054000   -0.06995600   -0.07645000
 C                -2.52139100    0.70502800   -1.01871800
 H                -3.00912200    0.97241000   -1.94759800
 C                -1.22547100    1.13368600   -0.74512200
 H                -0.71060500    1.74489600   -1.47968400
 Cl               -4.83079400   -0.61641200   -0.41022000
 H                 1.04752500    1.18178900    1.79319800
 H                 0.91992600    2.32522800    0.46812200
 C                 1.91817000    0.48909400   -0.06131200
 H                 1.66817100    0.55152900   -1.13027400

1d
Energy: -731.637720 au
Sum of electronic and thermal Energies: -731.408379 au
Geometry:
 C                 0.96197800    0.54660100   -0.07091300
 C                 1.26200100   -0.64034000   -0.74787300
 H                 0.48866200   -1.15512800   -1.30613500
 C                 2.55615700   -1.15539800   -0.74394100
 H                 2.80938300   -2.06332000   -1.27683600
 C                 3.53625600   -0.47099100   -0.04227200
 C                 3.27751600    0.71260100    0.63280300
 H                 4.07769900    1.21932600    1.15752400
 C                 1.98478600    1.22511800    0.60045900
 H                 1.76095100    2.16536500    1.08926300
 O                -0.48434200    2.38537800   -0.42097300
 C                -0.39338300    1.19659300   -0.14258900
 N                -1.50486500    0.40837300    0.06096700
 C                -2.82620000    1.02801000   -0.08500300
 H                -2.74326200    1.86044300   -0.78220200
 H                -3.16058400    1.42807000    0.88164300
 C                -3.82040300   -0.01339600   -0.58797300
 H                -4.83176500    0.39576100   -0.59191200
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H	-3.55783400	-0.31469600	-1.61278200
O	-3.85551900	-1.16213900	0.25532700
C	-2.57644600	-1.77414600	0.35011600
H	-2.26476300	-2.14484500	-0.63829800
H	-2.68891000	-2.62511800	1.02414600
C	-1.53343000	-0.80040800	0.89270100
H	-1.80496700	-0.52474300	1.92151700
H	-0.55167700	-1.26822800	0.91773200
F	4.79411300	-0.97143200	-0.02426100

1d amine

Energy: -657.577422 au

Sum of electronic and thermal Energies: -657.330676 au

Geometry:

C	0.97692100	0.73545300	-0.10210700
C	1.34783400	-0.23660200	-1.03887500
H	0.62297400	-0.56170500	-1.77612200
C	2.62126600	-0.79798000	-1.02607600
H	2.91893300	-1.55077600	-1.74565000
C	3.52394600	-0.37164500	-0.06264700
C	3.19724900	0.58548000	0.88200700
H	3.92896000	0.88682000	1.62122800
C	1.91377900	1.13260600	0.85418500
H	1.64237400	1.87971700	1.59279600
C	-0.40007100	1.36803000	-0.15449000
N	-1.48331400	0.39053300	-0.24750600
C	-2.75787200	1.01108900	-0.61185100
H	-2.63734700	1.54144000	-1.56191000
H	-3.08249100	1.74736700	0.14730000
C	-3.83551200	-0.05763600	-0.76049000
H	-4.80805200	0.39941500	-0.95176300
H	-3.58388300	-0.72147000	-1.60068400
O	-3.97628700	-0.82160500	0.43151900
C	-2.74296000	-1.43452200	0.79331800
H	-2.44740100	-2.15913400	0.02059500
H	-2.92699900	-1.97018200	1.72615800
C	-1.63881500	-0.40000400	0.97621400
H	-1.88666200	0.24747900	1.83843400
H	-0.69637700	-0.90710000	1.19887200
F	4.76746400	-0.91545300	-0.04457500
H	-0.52662500	2.03338400	0.71939400
H	-0.46566900	2.00730000	-1.04222000

1d ketone

Energy: -715.586408 au

Sum of electronic and thermal Energies: -715.345686 au

Geometry:

C	1.10488900	0.46521100	-0.03218800
C	1.38973800	-0.84069500	-0.45463100
H	0.59567800	-1.50463700	-0.77049900
C	2.69809200	-1.31532700	-0.48337600
H	2.93245400	-2.32070200	-0.80965700
C	3.71705600	-0.46532400	-0.08326900
C	3.47860900	0.83506100	0.34166500
H	4.30765800	1.46242200	0.64447000
C	2.16852000	1.29178700	0.36296700
H	1.94181700	2.30013200	0.68594200
O	-0.44618000	2.20698900	0.32186400
C	-0.28319400	1.03943500	0.01730500
C	-2.71395000	0.94093500	-0.72368300
H	-2.51428000	1.44999000	-1.67220300

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 H                 -2.93210300    1.71435800    0.01587800
 C                 -3.92225300    0.01888900   -0.88044400
 H                 -4.82441600    0.58971800   -1.10620500
 H                 -3.75726000   -0.69460900   -1.70469900
 O                 -4.20399000   -0.70098000    0.31686100
 C                 -3.11178300   -1.51215900    0.72404600
 H                 -2.91187800   -2.27720200   -0.04470000
 H                 -3.43518000   -2.02362600    1.63259300
 C                 -1.84852500   -0.68872900    0.98264600
 H                 -2.02898900   -0.00641100    1.81950600
 H                 -1.02986400   -1.35511300    1.27189200
 F                  4.98967100   -0.91897000   -0.10833800
 C                 -1.48281900    0.13926600   -0.27478900
 H                 -1.21558700   -0.56176100   -1.07457900

1d hydrocarbon
Energy: -641.549964 au
Sum of electronic and thermal Energies: -641.291370 au
Geometry:
 C                  1.03023200    0.65081900    0.46512000
 C                  1.65560300    1.09555300   -0.70690400
 H                  1.14721500    1.80858100   -1.34804000
 C                  2.92478400    0.65067600   -1.06872300
 H                  3.41331700    0.99613300   -1.97146500
 C                  3.57010200   -0.25176100   -0.23770000
 C                  2.99429700   -0.71510200    0.93276100
 H                  3.53349500   -1.41514000    1.55893900
 C                  1.72230400   -0.25602600    1.27451200
 H                  1.26482100   -0.61000200    2.19228900
 C                 -0.35795200    1.13267400    0.82812800
 C                 -2.84945200    1.15848400    0.30836700
 H                 -2.82691300    2.22391200    0.05114600
 H                 -3.05414700    1.08824200    1.38354600
 C                 -3.98322300    0.47424100   -0.45636300
 H                 -4.95674000    0.87135400   -0.16270000
 H                 -3.86140900    0.63969200   -1.53945500
 O                 -4.03248000   -0.92343600   -0.19258200
 C                 -2.82109500   -1.57865900   -0.55620300
 H                 -2.66172600   -1.47849800   -1.64226100
 H                 -2.97344200   -2.63651100   -0.33459200
 C                 -1.61804700   -1.01977800    0.20376000
 H                 -1.74445700   -1.23453100    1.27222800
 H                 -0.70876100   -1.53235300   -0.12585400
 F                  4.80869700   -0.68967100   -0.58054000
 H                 -0.54558800    0.93788800    1.88979300
 H                 -0.40544300    2.22050600    0.70128100
 C                 -1.49523600    0.49888200   -0.00250500
 H                 -1.27256600    0.67523600   -1.06483400

1e
Energy: -632.369172 au
Sum of electronic and thermal Energies: -632.132416 au
Geometry:
 C                  1.37057500    0.36835600   -0.08221800
 C                  1.58205700   -0.82136500   -0.78728900
 H                  0.77532200   -1.25480800   -1.36799600
 C                  2.83349700   -1.43418100   -0.77370100
 H                  2.99291300   -2.34680700   -1.33699000
 C                  3.87896200   -0.87163900   -0.04319600
 C                  3.67500800    0.31757800    0.65647700
 H                  4.48834300    0.76412200    1.21726000
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C	2.43162800	0.94269600	0.62485300
H	2.27462500	1.88415800	1.13763700
O	0.06790000	2.31127700	-0.44763700
C	0.06923900	1.12258300	-0.15398300
N	-1.09796300	0.42638900	0.07037400
C	-2.37014100	1.14311800	-0.06019300
H	-2.22910300	1.97563300	-0.74792700
H	-2.66903800	1.55428800	0.91348700
C	-3.44156400	0.18415200	-0.56870200
H	-4.42036000	0.66614000	-0.56015700
H	-3.20822000	-0.12237400	-1.59903300
O	-3.55539700	-0.96978500	0.26061300
C	-2.32363100	-1.67518800	0.33836800
H	-2.04621700	-2.05419300	-0.65699600
H	-2.49444000	-2.52463100	1.00205300
C	-1.20820300	-0.78805900	0.88549100
H	-1.45071700	-0.50844000	1.92051600
H	-0.26267400	-1.32592400	0.89385200
H	4.85072900	-1.35213300	-0.02756100

1e amine

Energy: -558.308678 au

Sum of electronic and thermal Energies: -558.054539 au

Geometry:

C	-1.41613700	-0.56656000	-0.09853300
C	-1.71539100	0.41387100	-1.05180900
H	-0.96427500	0.67818300	-1.78763800
C	-2.95257900	1.05231000	-1.04868400
H	-3.16988000	1.81004500	-1.79370500
C	-3.91327600	0.71925800	-0.09243200
C	-3.62494800	-0.25380900	0.86098000
H	-4.36255400	-0.51633900	1.61136900
C	-2.38230100	-0.88891000	0.85714800
H	-2.16142200	-1.64212400	1.60710700
C	-0.08373800	-1.29028100	-0.13009000
N	1.06422600	-0.39149500	-0.24081200
C	2.29586300	-1.10650200	-0.57624300
H	2.14617100	-1.65477400	-1.51192500
H	2.56534100	-1.84103400	0.20611300
C	3.44429500	-0.11767100	-0.74614500
H	4.38512700	-0.64444700	-0.91586800
H	3.24345200	0.53673500	-1.60717800
O	3.62873900	0.66988000	0.42454800
C	2.43649100	1.37362300	0.75905500
H	2.19511900	2.09401900	-0.03609700
H	2.65034300	1.92210100	1.67804800
C	1.26424300	0.42099900	0.96146700
H	1.46234600	-0.21670300	1.84377400
H	0.35638800	0.99595500	1.16152900
H	-4.87665000	1.21682400	-0.09065700
H	-0.00414000	-1.94243300	0.75927800
H	-0.06000000	-1.95254700	-1.00313100

1e ketone

Energy: -616.317473 au

Sum of electronic and thermal Energies: -616.069339 au

Geometry:

C	1.51961700	0.29800400	-0.05049900
C	1.71339600	-1.01406800	-0.50376500
H	0.87445400	-1.61246000	-0.83555300
C	2.99082400	-1.56912900	-0.54129200

H	3.12714200	-2.58414100	-0.89681100
C	4.08982000	-0.82099100	-0.12481200
C	3.90870900	0.48690500	0.32873600
H	4.76204200	1.07170400	0.65316000
C	2.63535600	1.04089800	0.36388600
H	2.47632400	2.05476300	0.70976700
O	0.08697100	2.13834700	0.32106800
C	0.17146000	0.96426000	0.01038400
C	-2.27215400	1.03151200	-0.69413400
H	-2.05437100	1.54566800	-1.63590200
H	-2.43206400	1.80275200	0.06247600
C	-3.53717700	0.18882300	-0.85007200
H	-4.40555900	0.81808000	-1.05205900
H	-3.42746300	-0.51737500	-1.68973200
O	-3.84706700	-0.53576900	0.33756000
C	-2.80095300	-1.41959800	0.71445500
H	-2.65873700	-2.18089600	-0.07067300
H	-3.14328400	-1.92724600	1.61825900
C	-1.48617900	-0.68015300	0.96913100
H	-1.61329500	-0.00391600	1.82071500
H	-0.70596500	-1.40036400	1.23398300
H	5.08353700	-1.25390600	-0.15403200
C	-1.08721900	0.14707300	-0.27845600
H	-0.87500800	-0.55450900	-1.09399100

1e hydrocarbon
Energy: -542.281399 au
Sum of electronic and thermal Energies: -542.015431 au
Geometry:

C	-1.47421800	-0.47002000	0.42711600
C	-2.07142700	-1.03946300	-0.70502600
H	-1.57009600	-1.85273400	-1.22122400
C	-3.30206100	-0.58588400	-1.17381900
H	-3.74773800	-1.04464000	-2.04975500
C	-3.96386300	0.45034300	-0.51524200
C	-3.38518000	1.02328700	0.61490400
H	-3.89356800	1.82562300	1.13844100
C	-2.15236700	0.56500100	1.07942300
H	-1.71266700	1.01505000	1.96387900
C	-0.12687900	-0.95869700	0.91361100
C	2.37891900	-1.16089400	0.51097600
H	2.31428000	-2.24908100	0.39461000
H	2.54672700	-0.95758600	1.57559500
C	3.57214400	-0.63407700	-0.28714400
H	4.51386600	-1.03027800	0.09758600
H	3.48243600	-0.93673200	-1.34344000
O	3.67981900	0.78291800	-0.20744800
C	2.51515300	1.43591600	-0.70452300
H	2.39106000	1.19970600	-1.77402900
H	2.71070500	2.50623100	-0.61676000
C	1.25955900	1.03515900	0.06976600
H	1.35690000	1.38347600	1.10557400
H	0.38842100	1.53799500	-0.36183600
H	-4.92330000	0.80273200	-0.87680000
H	0.02907300	-0.63214600	1.94781900
H	-0.12755200	-2.05488500	0.93155900
C	1.07077300	-0.49065700	0.05812900
H	0.87960100	-0.79616500	-0.98066200

2a
Energy: -893.663822 au

Sum of electronic and thermal Energies: -893.411853 au
Geometry:

C	0.14461000	1.64841700	0.60126900
H	-0.19787700	2.55512000	1.08563600
C	-0.78148900	0.83554200	-0.05827700
C	-0.32547700	-0.30416500	-0.72685000
H	-1.02379500	-0.92796300	-1.27350100
C	1.02739200	-0.63908500	-0.72595600
H	1.36929300	-1.51602100	-1.26083500
C	1.93023400	0.16771300	-0.03630600
C	1.49537000	1.31309100	0.62970500
H	2.19980000	1.94467400	1.15582500
N	-3.20897000	0.38706000	0.12622500
O	-2.45100100	2.45491900	-0.46380900
C	-2.21463000	1.29847700	-0.13322200
C	-4.60493600	0.80638700	-0.04964500
H	-4.60902700	1.69648600	-0.67486000
H	-5.02219000	1.08924000	0.92813100
C	-5.43107600	-0.32748700	-0.66486500
H	-6.47712800	-0.01201200	-0.72814000
H	-5.08564000	-0.50006500	-1.69058400
C	-3.83182400	-1.99490800	0.35403800
H	-3.38401900	-2.27882200	-0.60541300
H	-3.74036700	-2.85818000	1.02075300
C	-3.04733500	-0.81993500	0.94598400
H	-3.42533900	-0.60561600	1.95742300
H	-1.99125400	-1.05876800	1.04264400
I	3.97647500	-0.34201100	-0.01172700
C	-5.30616200	-1.62221100	0.14878100
H	-5.84129900	-2.43876900	-0.34482900
H	-5.78158400	-1.48247400	1.12826000

2a amine
Energy: -819.602728 au
Sum of electronic and thermal Energies: -819.333441 au
Geometry:

C	0.07550100	1.59971700	0.80433000
H	-0.27080800	2.36033700	1.49713100
C	-0.82423900	1.01961200	-0.09137200
C	-0.35100500	0.03445100	-0.96445600
H	-1.04337400	-0.43442200	-1.65437300
C	0.98416300	-0.36037000	-0.94801500
H	1.33260700	-1.12498800	-1.63102000
C	1.86515600	0.23842800	-0.04752200
C	1.41811700	1.21951300	0.83236700
H	2.09877900	1.68110000	1.53653000
N	-3.22669800	0.37727600	-0.23550300
C	-2.26927700	1.47699300	-0.15131800
C	-4.55245800	0.83782400	-0.65579600
H	-4.43910200	1.40632500	-1.58367100
H	-4.98900400	1.52772700	0.09470300
C	-5.50540000	-0.33944500	-0.87362900
H	-6.49164500	0.04137900	-1.15794200
H	-5.13553300	-0.94134400	-1.71115400
C	-4.20170600	-1.61671000	0.85789100
H	-3.75024600	-2.30128000	0.13125900
H	-4.25481300	-2.14796500	1.81355000
C	-3.29637600	-0.39293300	1.01051700
H	-3.67232600	0.24315700	1.83763800
H	-2.28504400	-0.70423200	1.28189900
I	3.89138200	-0.35436000	-0.01498100

C	-5.60199600	-1.21005300	0.38476700
H	-6.21731600	-2.09477200	0.19419200
H	-6.10321300	-0.64331500	1.18010600
H	-2.47565900	2.13517200	0.71356600
H	-2.40252700	2.09513800	-1.04648800

2a ketone

Energy: -877.610687 au

Sum of electronic and thermal Energies: -877.347428 au

Geometry:

C	0.29765500	1.69892100	0.37440200
H	-0.04545900	2.68271600	0.67060500
C	-0.65934300	0.74376900	0.00286400
C	-0.21792200	-0.52843200	-0.38164700
H	-0.92458700	-1.29344400	-0.67709700
C	1.13926800	-0.84333200	-0.39617000
H	1.46341900	-1.83136100	-0.69694500
C	2.06947800	0.12415500	-0.02247700
C	1.65384300	1.39971100	0.36460900
H	2.37902900	2.14949000	0.65436500
O	-2.40689400	2.29133200	0.34001600
C	-2.10957100	1.14955100	0.03817300
C	-4.47921900	0.77031200	-0.78832200
H	-4.26348300	1.31818500	-1.71089300
H	-4.81853200	1.51449300	-0.06178700
C	-5.57988200	-0.27154000	-1.03050400
H	-6.49159500	0.22812900	-1.37310900
H	-5.27455700	-0.94676500	-1.84107000
C	-4.59223600	-1.74418200	0.78022200
H	-4.23261300	-2.49793000	0.06737200
H	-4.80521300	-2.27626800	1.71311800
C	-3.48641400	-0.70693600	1.02150400
H	-3.79896400	-0.01279300	1.81073900
H	-2.57699500	-1.19975000	1.37861200
I	4.12344700	-0.34259100	-0.04245300
C	-5.86980800	-1.09545900	0.23142600
H	-6.62161900	-1.86279700	0.02040200
H	-6.29925900	-0.43970100	0.99957800
C	-3.19188300	0.11541400	-0.26057200
H	-2.82092400	-0.57725100	-1.02507100

2a hydrocarbon

Energy: -803.574265 au

Sum of electronic and thermal Energies: -803.293187 au

Geometry:

C	-0.06448100	0.44253200	1.46475600
H	-0.54643900	0.29543000	2.42594000
C	-0.78683800	1.01029400	0.41112600
C	-0.12549200	1.19228100	-0.80961900
H	-0.65437800	1.64106300	-1.64484300
C	1.20516200	0.81781000	-0.98096900
H	1.69451100	0.97308900	-1.93431200
C	1.89800800	0.24975000	0.08686600
C	1.26902300	0.06109900	1.31414700
H	1.80575500	-0.37489700	2.14735100
C	-2.23734900	1.40949600	0.56941400
C	-4.66696000	1.05639300	-0.07772600
H	-4.67149900	2.04285400	-0.55524800
H	-4.95379900	1.21790400	0.97075100
C	-5.70031100	0.14077900	-0.74962400
H	-6.70059800	0.57769700	-0.66241200

H	-5.48165700	0.07800100	-1.82365800
C	-4.26938300	-1.87234800	-0.18655100
H	-3.97571800	-2.03820500	-1.23130300
H	-4.26193700	-2.85517100	0.29604500
C	-3.24089200	-0.95116700	0.48590500
H	-3.47041000	-0.87653300	1.55848700
H	-2.24086300	-1.38873700	0.41168800
I	3.91629800	-0.31905300	-0.15764700
C	-5.68060300	-1.27076000	-0.14757500
H	-6.38533700	-1.91923700	-0.67839800
H	-6.02434200	-1.22366800	0.89418400
H	-2.48309100	1.47331300	1.63537100
H	-2.37537300	2.41679200	0.15959600
C	-3.24731700	0.46298700	-0.11981200
H	-2.95402000	0.37522000	-1.17599200

2b

Energy: -3170.008628 au

Sum of electronic and thermal Energies: -3169.756444 au

Geometry:

Br	-4.34801400	-0.47666500	-0.01762000
N	2.62185200	0.40399400	0.12504500
O	1.80499200	2.45113300	-0.45873000
C	1.60179500	1.28745300	-0.13163500
C	2.49566700	-0.80659400	0.94586600
H	1.44706000	-1.07608900	1.04317600
H	2.86746000	-0.58048300	1.95704300
C	4.00508600	0.86378200	-0.05080000
H	4.41369600	1.15946400	0.92683100
H	3.98342200	1.75318800	-0.67663500
C	3.31397700	-1.95859700	0.35471100
H	3.24762700	-2.82374700	1.02194900
H	2.87472600	-2.25601800	-0.60461300
C	4.86408300	-0.24591700	-0.66508900
H	4.52413900	-0.42913500	-1.69080300
H	5.90048000	0.09994400	-0.72829500
C	0.18256200	0.78336700	-0.05827000
C	-0.76708400	1.57081400	0.59894100
H	-0.45093600	2.48763700	1.08182100
C	-2.10753600	1.19780000	0.62681700
H	-2.83610200	1.80477600	1.14848400
C	-2.50147900	0.03991900	-0.03832400
C	-1.58138000	-0.74453200	-0.72648200
H	-1.90472200	-1.63019200	-1.25798300
C	-0.23925600	-0.37019300	-0.72574400
H	0.47750000	-0.97406800	-1.27055300
C	4.77685700	-1.54325400	0.14931300
H	5.24790400	-1.38915300	1.12874500
H	5.33559000	-2.34416500	-0.34376700

2b amine

Energy: -3095.947556 au

Sum of electronic and thermal Energies: -3095.678072 au

Geometry:

Br	-4.27859900	-0.48445100	-0.02309500
N	2.62624800	0.38865200	-0.23414800
C	1.63893100	1.46145000	-0.14691700
C	2.71499200	-0.38484200	1.00859900
H	1.71217400	-0.72503500	1.27687300
H	3.07200000	0.25769000	1.83912300
C	3.93960800	0.88750900	-0.64968400

H	4.35560100	1.58548500	0.10499500
H	3.81233200	1.45721400	-1.57501100
C	3.65386500	-1.58264500	0.85208700
H	3.72005100	-2.11651500	1.80546500
H	3.22240900	-2.27606500	0.12170200
C	4.92489600	-0.26199500	-0.87136400
H	4.57316100	-0.86978400	-1.71243500
H	5.90079200	0.14713100	-1.15203000
C	0.20712900	0.96384200	-0.09007500
C	-0.70712300	1.50999000	0.81235400
H	-0.38135100	2.27358800	1.51153700
C	-2.03823200	1.09212300	0.83908400
H	-2.73620000	1.52279100	1.54549400
C	-2.45157800	0.10795100	-0.05017700
C	-1.56152300	-0.45980700	-0.95831600
H	-1.89610000	-1.22716700	-1.64476700
C	-0.23867100	-0.02650200	-0.97190700
H	0.46599800	-0.46892900	-1.66660300
C	5.04326400	-1.13567800	0.38309300
H	5.52761100	-0.55925800	1.18191800
H	5.68278100	-2.00236600	0.18939200
H	1.82631000	2.12175700	0.72064800
H	1.75630600	2.08632100	-1.03959900

2b ketone

Energy: -3153.955524 au

Sum of electronic and thermal Energies: -3153.692050 au

Geometry:

Br	-4.51457900	-0.47017500	-0.06036400
O	1.75187300	2.27767500	0.34969100
C	1.48474600	1.13021400	0.04136100
C	2.90689900	-0.69418100	1.01999000
H	2.00980000	-1.21198000	1.37292700
H	3.19943000	0.00453900	1.81283500
C	3.86505700	0.81608800	-0.78135400
H	4.18319100	1.56581600	-0.05096900
H	3.63720800	1.36195800	-1.70219600
C	4.03987100	-1.70129700	0.77710300
H	4.26449100	-2.23151300	1.70831800
H	3.70166200	-2.46119400	0.06030700
C	4.99294900	-0.19579900	-1.02515200
H	4.70715700	-0.87528800	-1.83926800
H	5.89212800	0.32883800	-1.36350600
C	0.04550700	0.68782400	-0.00008900
C	-0.93618800	1.61755900	0.37204200
H	-0.61848900	2.60838100	0.67265800
C	-2.28413400	1.28509300	0.35750400
H	-3.03447400	2.00973300	0.64626100
C	-2.65906200	0.00122200	-0.03555100
C	-1.70990800	-0.94406500	-0.41034500
H	-2.01554600	-1.93676600	-0.71417300
C	-0.36184800	-0.59405100	-0.39041900
H	0.36511700	-1.33942500	-0.68623200
C	5.30134600	-1.01720200	0.23401700
H	5.71191200	-0.35380300	1.00592100
H	6.07331700	-1.76383400	0.02154500
C	2.59399900	0.12565100	-0.25935200
H	2.24298800	-0.57307500	-1.02775500

2b hydrocarbon

Energy: -3079.919047 au

Sum of electronic and thermal Energies: -3079.637751 au
Geometry:

Br	-4.30865100	-0.42283000	-0.23348200
C	1.60291600	1.36390600	0.62543400
C	2.66564400	-0.96505600	0.44252800
H	1.67788000	-1.42279200	0.33372900
H	2.87980100	-0.93659400	1.52050000
C	4.04810000	1.10136700	-0.00538600
H	4.31794600	1.21949100	1.05334200
H	4.03391800	2.10936300	-0.43537700
C	3.72516300	-1.82755600	-0.25900800
H	3.73617500	-2.83231700	0.17598400
H	3.44883200	-1.95010700	-1.31441200
C	5.11222900	0.24439800	-0.70599900
H	4.90853000	0.22770800	-1.78466800
H	6.10011500	0.70090800	-0.58457300
C	0.16466200	0.93743400	0.42994000
C	-0.55496600	0.30257300	1.44663800
H	-0.08041100	0.12201200	2.40560600
C	-1.87626800	-0.10441000	1.26199800
H	-2.41765700	-0.59308200	2.06195800
C	-2.48890200	0.12908900	0.03677100
C	-1.80480500	0.76275400	-0.99620300
H	-2.29326100	0.94771700	-1.94440000
C	-0.48644000	1.16102400	-0.78951700
H	0.04081000	1.66183000	-1.59546000
C	5.12031200	-1.19434500	-0.17201000
H	5.44955800	-1.18874800	0.87546300
H	5.84767300	-1.79932800	-0.72325700
H	1.83453000	1.38276200	1.69627300
H	1.72066400	2.39272700	0.26587500
C	2.64428500	0.47634600	-0.09469400
H	2.36609500	0.43235300	-1.15768700

2c
Energy: -1056.088984 au
Sum of electronic and thermal Energies: -1055.836436 au
Geometry:

N	1.91626000	0.42644000	0.12512400
O	0.99334700	2.42999900	-0.45149000
C	0.85098800	1.25591000	-0.12934900
C	1.85400500	-0.78971400	0.94498400
H	0.82109500	-1.11438400	1.04161100
H	2.21281600	-0.54498300	1.95655000
C	3.27325100	0.95925700	-0.04846700
H	3.66468800	1.27494000	0.92996100
H	3.20516500	1.84711500	-0.67316800
C	2.73249900	-1.89623600	0.35344100
H	2.71172900	-2.76430100	1.01988600
H	2.31018800	-2.21566500	-0.60642400
C	4.19054300	-0.10251900	-0.66324400
H	3.86179800	-0.30213000	-1.68955300
H	5.20722200	0.29786300	-0.72492300
C	-0.53942900	0.67723900	-0.05981300
C	-1.53146300	1.41368700	0.59427700
H	-1.26532300	2.34621900	1.07703200
C	-2.84962700	0.96999400	0.61890600
H	-3.61438200	1.53466200	1.13662400
C	-3.18010600	-0.20756400	-0.04594000
C	-2.21774900	-0.94231200	-0.73090200
H	-2.49709700	-1.84377100	-1.26111000

C	-0.89787000	-0.49766600	-0.72738400
H	-0.14861100	-1.06278400	-1.26985700
Cl	-4.84555800	-0.77034100	-0.03064200
C	4.17150500	-1.40380500	0.14939000
H	4.77210700	-2.17339100	-0.34436600
H	4.63320900	-1.22630400	1.12931500

2c amine

Energy: -982.027773 au

Sum of electronic and thermal Energies: -981.757960 au

Geometry:

N	1.89904500	0.39948400	-0.23057800
C	0.85995000	1.42178200	-0.13621000
C	2.02236900	-0.38091200	1.00481300
H	1.03662800	-0.77204600	1.26683700
H	2.34571400	0.26999700	1.84259800
C	3.18741500	0.96623800	-0.63689400
H	3.56664700	1.67611800	0.12603700
H	3.03495200	1.53836000	-1.55690400
C	3.01876100	-1.52994700	0.83920900
H	3.10853600	-2.06963100	1.78738200
H	2.62333300	-2.23606200	0.10063900
C	4.22854100	-0.13129200	-0.86693700
H	3.90943000	-0.74680400	-1.71537000
H	5.18404500	0.32799700	-1.14008400
C	-0.54575200	0.85403200	-0.08700400
C	-1.48635500	1.34326200	0.82109000
H	-1.19867600	2.11313900	1.52989800
C	-2.79470400	0.85996500	0.84092300
H	-3.51687100	1.24394800	1.55019600
C	-3.15915400	-0.13207000	-0.06061300
C	-2.24156200	-0.64358200	-0.97451300
H	-2.54224400	-1.41795500	-1.66902000
C	-0.94209400	-0.14593800	-0.98172800
H	-0.21616300	-0.54435000	-1.68103800
Cl	-4.80577100	-0.75763000	-0.04421800
C	4.38598700	-1.01117300	0.37891100
H	5.06743700	-1.84367400	0.17834400
H	4.83963800	-0.42015000	1.18506100
H	1.01318800	2.08244400	0.73778100
H	0.94878000	2.05979100	-1.02287700

2c ketone

Energy: -1040.035962 au

Sum of electronic and thermal Energies: -1039.772116 au

Geometry:

O	0.93706500	2.23903300	0.37172600
C	0.72355900	1.08394700	0.04991200
C	2.22982200	-0.67751200	1.01867700
H	1.35815300	-1.24010500	1.36684200
H	2.48739300	0.02923800	1.81650000
C	3.11644100	0.88841100	-0.77188700
H	3.39734300	1.64807600	-0.03654600
H	2.86350300	1.42828600	-1.68973000
C	3.41025800	-1.62734400	0.77098000
H	3.65910400	-2.15217300	1.69909300
H	3.10988700	-2.39797900	0.04881500
C	4.29198700	-0.06641100	-1.02040500
H	4.04019800	-0.75379600	-1.83910800
H	5.16528700	0.50299400	-1.35414800
C	-0.69334300	0.57730800	-0.00437000

C	-1.71924100	1.46079300	0.36204200
H	-1.44873800	2.46383400	0.66795400
C	-3.04992600	1.06788900	0.33476000
H	-3.83816900	1.75374800	0.61785400
C	-3.36355400	-0.23029200	-0.06448900
C	-2.36950400	-1.13053900	-0.43338700
H	-2.63243900	-2.13429200	-0.74139400
C	-1.03935300	-0.72060200	-0.40142200
H	-0.27688500	-1.43131000	-0.69284300
Cl	-5.04300800	-0.73807000	-0.10294100
C	4.63798000	-0.87979100	0.23417000
H	5.44538600	-1.58698000	0.01844400
H	5.01494000	-0.20215800	1.01083900
C	1.87933700	0.13457700	-0.25578800
H	1.56285500	-0.57505200	-1.02915500

2c hydrocarbon

Energy: -965.999290 au

Sum of electronic and thermal Energies: -965.717636 au

Geometry:

C	0.81973100	1.26730400	0.71624100
C	1.98259100	-0.99246700	0.35858900
H	1.01734200	-1.47730700	0.18463600
H	2.17118100	-1.05084800	1.44013700
C	3.28744400	1.15834100	0.12936500
H	3.52814100	1.19239600	1.20108400
H	3.24104600	2.19921600	-0.21061500
C	3.09255300	-1.74704200	-0.38786800
H	3.13564600	-2.78516400	-0.04240300
H	2.84533600	-1.78639200	-1.45679400
C	4.40182900	0.40955800	-0.61563800
H	4.22332600	0.48037900	-1.69657200
H	5.36689300	0.89215700	-0.42900800
C	-0.59483500	0.80262500	0.44797600
C	-1.30885700	0.05149300	1.38651900
H	-0.84766600	-0.19432000	2.33738100
C	-2.60708300	-0.38974600	1.13347600
H	-3.14837500	-0.96929000	1.87059100
C	-3.20289200	-0.07337300	-0.08120800
C	-2.52392500	0.67660700	-1.03647100
H	-3.00347700	0.92307500	-1.97537300
C	-1.22869100	1.10749800	-0.76302900
H	-0.70578400	1.69876100	-1.50811500
Cl	-4.84311200	-0.62253200	-0.41463100
C	4.45784700	-1.06941600	-0.20960900
H	5.22191600	-1.59401500	-0.79265300
H	4.76310500	-1.14356100	0.84251300
H	1.02680100	1.20137900	1.79026900
H	0.90228300	2.32763100	0.45065200
C	1.91326500	0.48879100	-0.05104900
H	1.66133400	0.52791000	-1.12078100

2d

Energy: -695.734940 au

Sum of electronic and thermal Energies: -695.481428 au

Geometry:

C	0.96180900	0.55117600	-0.05713900
C	1.24157500	-0.65049000	-0.71620600
H	0.45368200	-1.17228200	-1.24684100
C	2.53205100	-1.17505100	-0.72647800
H	2.76853100	-2.09541600	-1.24561600

C	3.52986500	-0.48461600	-0.05678900
C	3.29177300	0.71314400	0.60037200
H	4.10503600	1.22410400	1.10038400
C	2.00207200	1.23439700	0.58162300
H	1.79404400	2.18587200	1.05546600
O	-0.46202800	2.39844000	-0.43026100
C	-0.38986800	1.21418900	-0.12188700
N	-1.50545200	0.44776900	0.12029300
C	-2.82582300	1.06496500	-0.05577400
H	-2.70154100	1.94474200	-0.68324900
H	-3.19752200	1.40861500	0.92104100
C	-3.80815000	0.06154800	-0.66800800
H	-4.79723400	0.52559500	-0.73255100
H	-3.49154000	-0.16229500	-1.69313800
C	-2.46851600	-1.81745700	0.35685600
H	-2.06639000	-2.16694700	-0.60122700
H	-2.50371900	-2.68244100	1.02674300
C	-1.52234400	-0.76651600	0.94531200
H	-1.86689100	-0.49538300	1.95524500
H	-0.51240600	-1.15576400	1.04558600
F	4.78519900	-0.99411400	-0.05242000
C	-3.87309000	-1.23542100	0.14900000
H	-4.32373900	-1.02548000	1.12766300
H	-4.52083000	-1.96701200	-0.34297700

2d amine

Energy: -621.673427 au

Sum of electronic and thermal Energies: -621.402664 au

Geometry:

C	0.98946800	0.73516500	-0.07780200
C	1.34039200	-0.24202000	-1.01674700
H	0.60015700	-0.56721900	-1.73844300
C	2.61182200	-0.80844600	-1.02401200
H	2.89359200	-1.56575400	-1.74531800
C	3.53300500	-0.38187700	-0.07862800
C	3.22660500	0.58027200	0.86767500
H	3.97220200	0.88134300	1.59306600
C	1.94483200	1.13214000	0.86014600
H	1.68898200	1.88271900	1.60088900
C	-0.38484800	1.37649500	-0.11095500
N	-1.47642500	0.41151900	-0.22374500
C	-2.73577500	1.05485100	-0.60604500
H	-2.55917800	1.64163900	-1.51242400
H	-3.07260400	1.76397200	0.17733400
C	-3.83477500	0.01965800	-0.85583900
H	-4.76649700	0.53530400	-1.10998800
H	-3.55389000	-0.58985200	-1.72195400
C	-2.68940400	-1.48397500	0.80417600
H	-2.33649500	-2.18994700	0.04421700
H	-2.80123500	-2.04320300	1.73861800
C	-1.63311200	-0.39336800	0.99185200
H	-1.91706100	0.25126100	1.84869000
H	-0.66755700	-0.84185700	1.23631900
F	4.77520100	-0.93096100	-0.07989400
C	-4.03033800	-0.88238100	0.36844100
H	-4.44659700	-0.28915200	1.19295000
H	-4.75629000	-1.67233500	0.15236000
H	-0.50210800	2.02429300	0.77818500
H	-0.44449000	2.03772800	-0.98280700

2d ketone
Energy: -679.682210 au
Sum of electronic and thermal Energies: -679.417390 au
Geometry:

C	1.11836500	0.45760600	-0.01226000
C	1.39612300	-0.85450100	-0.41948900
H	0.59588400	-1.52385800	-0.70682700
C	2.70410700	-1.32942900	-0.46522500
H	2.93247300	-2.34045200	-0.77813700
C	3.73013000	-0.47260000	-0.09981900
C	3.49910800	0.83423400	0.30882000
H	4.33353100	1.46699400	0.58454000
C	2.18902100	1.29002500	0.34995600
H	1.96733600	2.30255300	0.66325500
O	-0.42729800	2.19089100	0.39812700
C	-0.27058100	1.03121300	0.05935400
C	-2.67142900	0.96350100	-0.76007000
H	-2.39213500	1.49605000	-1.67457900
H	-2.91208100	1.73140300	-0.01905700
C	-3.89481000	0.07220600	-1.01362600
H	-4.73805700	0.68805900	-1.34218900
H	-3.67957800	-0.62159100	-1.83735100
C	-3.09240800	-1.54423400	0.76573300
H	-2.83276100	-2.32420000	0.03779600
H	-3.36697700	-2.06216500	1.69049300
C	-1.86450300	-0.65801100	1.01825900
H	-2.08442700	0.05549200	1.82129900
H	-1.02250800	-1.26710500	1.36130200
F	5.00312000	-0.92600200	-0.14323100
C	-4.28076700	-0.73101400	0.23585600
H	-4.62146600	-0.04025300	1.01769800
H	-5.12369600	-1.39431500	0.01655000
C	-1.47393200	0.14368100	-0.25096400
H	-1.19578200	-0.57578600	-1.02986700

2d hydrocarbon
Energy: -605.644804 au
Sum of electronic and thermal Energies: -605.362205 au
Geometry:

C	1.04381300	0.65257900	0.45689900
C	1.65825300	1.06908300	-0.73127300
H	1.14086900	1.76201300	-1.38703200
C	2.92667200	0.62074400	-1.09168500
H	3.40604300	0.94436300	-2.00737800
C	3.58312900	-0.25631200	-0.24254600
C	3.01892000	-0.69126000	0.94420900
H	3.56627500	-1.37240500	1.58405500
C	1.74730200	-0.22931300	1.28384400
H	1.29833800	-0.56192700	2.21375200
C	-0.34273300	1.13992400	0.81887400
C	-2.82867700	1.19399700	0.30424600
H	-2.74811100	2.26423400	0.08218000
H	-3.03774700	1.11542600	1.38027100
C	-3.99406800	0.57851600	-0.48358400
H	-4.93250900	1.07333400	-0.21226000
H	-3.84323600	0.76529300	-1.55489200
C	-2.77040500	-1.63882900	-0.54321700
H	-2.55492900	-1.56556300	-1.61722700
H	-2.84753600	-2.70717100	-0.31589000
C	-1.60954700	-1.01754900	0.24730700
H	-1.77042000	-1.19163900	1.32090100

H	-0.67054600	-1.51602500	-0.01110800
F	4.82165600	-0.69762600	-0.58399100
C	-4.10057200	-0.93392200	-0.24547600
H	-4.37903100	-1.11569400	0.80098500
H	-4.90204200	-1.35885100	-0.85873000
H	-0.52353500	0.96204400	1.88499300
H	-0.38749700	2.22596300	0.67658200
C	-1.48930200	0.49695700	0.00534200
H	-1.26599800	0.64757200	-1.06092800

2e

Energy: -596.466223 au

Sum of electronic and thermal Energies: -596.205303 au

Geometry:

C	1.37076300	0.36783500	-0.07294900
C	1.55865600	-0.83237600	-0.76651300
H	0.73576500	-1.26810300	-1.32220500
C	2.80494500	-1.45590100	-0.77048400
H	2.94478700	-2.37744500	-1.32452000
C	3.87001100	-0.89343000	-0.06885700
C	3.68979000	0.30617800	0.61959000
H	4.51796700	0.75290900	1.15822400
C	2.45114300	0.94139800	0.60479300
H	2.31265100	1.89106100	1.10773700
O	0.09341500	2.31976300	-0.45521500
C	0.07528300	1.13676000	-0.13406500
N	-1.09465500	0.46442400	0.12934800
C	-2.36480800	1.18276000	-0.02623500
H	-2.17819900	2.05913000	-0.64300400
H	-2.70102800	1.53943400	0.95882500
C	-3.42690300	0.26650300	-0.64217500
H	-4.37837600	0.80536200	-0.69002500
H	-3.13782800	0.03385600	-1.67346200
C	-2.22482700	-1.72388400	0.34277100
H	-1.85934900	-2.08835200	-0.62428000
H	-2.31990800	-2.59373000	1.00054100
C	-1.19479500	-0.75746700	0.93579300
H	-1.50618200	-0.47772600	1.95417600
H	-0.21622700	-1.22393300	1.01569600
H	4.83791800	-1.38201500	-0.06674700
C	-3.58272000	-1.03336300	0.15796900
H	-4.28950900	-1.70625600	-0.33668900
H	-4.00644500	-0.80334200	1.14420000

2e amine

Energy: -522.404499 au

Sum of electronic and thermal Energies: -522.126331 au

Geometry:

C	-1.42930700	-0.56431000	-0.07073400
C	-1.70807300	0.39947700	-1.04680100
H	-0.94165800	0.64791100	-1.77224300
C	-2.94293800	1.04185100	-1.07791000
H	-3.14370800	1.78689500	-1.84028000
C	-3.92232000	0.72960300	-0.13371700
C	-3.65454100	-0.22684300	0.84237100
H	-4.40643600	-0.47296300	1.58420700
C	-2.41422000	-0.86569800	0.87271600
H	-2.20931200	-1.60526500	1.64067700
C	-0.10031000	-1.29622000	-0.06691900
N	1.05586800	-0.41375000	-0.21043100
C	2.27140400	-1.15803500	-0.54624600

H	2.06380200	-1.77362800	-1.42661700
H	2.55183600	-1.85100500	0.27331500
C	3.44115700	-0.21289300	-0.82986000
H	4.33801000	-0.80192000	-1.04772300
H	3.21080100	0.37265600	-1.72688100
C	2.38503300	1.44140900	0.74394800
H	2.08810500	2.13295400	-0.05234600
H	2.52595400	2.03517300	1.65288200
C	1.25512700	0.43461800	0.96832200
H	1.48637400	-0.18658200	1.85790800
H	0.31997800	0.95815600	1.17912200
H	-4.88376600	1.23039100	-0.15844700
C	3.68609800	0.73082800	0.35348400
H	4.46628200	1.45884000	0.11010100
H	4.05315600	0.15036600	1.20988900
H	-0.03085900	-1.91352900	0.84866200
H	-0.08228500	-1.99493300	-0.91113700

2e ketone
Energy: -580.413101 au
Sum of electronic and thermal Energies: -580.140875 au
Geometry:

C	1.53393400	0.28907400	-0.03392700
C	1.71896200	-1.02873800	-0.47366300
H	0.87234000	-1.63347000	-0.77260300
C	2.99608400	-1.58274100	-0.53504200
H	3.12482200	-2.60325200	-0.87758900
C	4.10427100	-0.82682400	-0.15907700
C	3.93212100	0.48714900	0.28028100
H	4.79247300	1.07832400	0.57332100
C	2.65867000	1.03871900	0.34211100
H	2.50593400	2.05631700	0.67983600
O	0.10607000	2.11611000	0.41057100
C	0.18474700	0.95314700	0.05675200
C	-2.22862400	1.05425800	-0.72491300
H	-1.93002600	1.59069500	-1.63101300
H	-2.41119100	1.81758900	0.03717800
C	-3.50818000	0.24601700	-0.97996800
H	-4.31661600	0.91980200	-1.28147300
H	-3.34742600	-0.44003900	-1.82241600
C	-2.78212500	-1.45828200	0.74955000
H	-2.58105000	-2.23520200	0.00012700
H	-3.07528000	-1.98021100	1.66640900
C	-1.49853900	-0.65508800	1.00289700
H	-1.66316900	0.05157100	1.82513000
H	-0.69080000	-1.32218100	1.31876500
H	5.09785200	-1.25836000	-0.20829500
C	-3.92555400	-0.56173000	0.25654600
H	-4.81074500	-1.16679200	0.03496200
H	-4.21229700	0.12991800	1.05904600
C	-1.07714500	0.15054100	-0.25379400
H	-0.85511300	-0.56660600	-1.05245800

2e hydrocarbon
Energy: -506.376068 au
Sum of electronic and thermal Energies: -506.086102 au
Geometry:

C	-1.48852500	-0.47289200	0.41573300
C	-2.07047000	-1.00808300	-0.74096100
H	-1.55640700	-1.79800300	-1.28031300
C	-3.30079100	-0.54968800	-1.20579900

H	-3.73372900	-0.98176900	-2.10154400
C	-3.97871100	0.45707600	-0.51844100
C	-3.41574400	0.99571000	0.63623900
H	-3.93620100	1.77521000	1.18207700
C	-2.18295000	0.53279900	1.09627100
H	-1.75504400	0.95677300	1.99923100
C	-0.14293500	-0.96896100	0.89957700
C	2.35572400	-1.19674800	0.50573900
H	2.23182900	-2.28223200	0.41840500
H	2.52743600	-0.98898500	1.57116400
C	3.57880500	-0.73931200	-0.30209300
H	4.48133400	-1.23494500	0.07087600
H	3.45982500	-1.05623400	-1.34651900
C	2.46698900	1.50235100	-0.69723500
H	2.28900000	1.29988000	-1.76152100
H	2.58734100	2.58687200	-0.60505000
C	1.24829200	1.03931400	0.11447100
H	1.37661300	1.34346100	1.16319100
H	0.34462400	1.53978600	-0.24563800
H	-4.93794400	0.81318300	-0.87702200
C	3.74940500	0.78520600	-0.25431100
H	4.59326900	1.09228000	-0.88104600
H	3.99648700	1.08855000	0.77168800
H	0.00527800	-0.66228300	1.94129800
H	-0.14575900	-2.06532000	0.89777200
C	1.06392200	-0.48709700	0.06212200
H	0.87398000	-0.76427900	-0.98492000