STRUCTURAL CHEMISTRY

Volume 74 (2018)

Supporting information for article:

Structures and energetic properties of 4-halobenzamides

Aleksandra Piontek, Elwira Bisz, Błażej Dziuk, Roman Szostak and Michal Szostak

(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*α
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

Gaussian 09, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, M. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; 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
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
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
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
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