Supporting Information

Ring Splitting of Azetidin-2-ones *via* Radical Anions

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S1:^{1}H-NMR spectrum of *trans*-3-cyclopropyl-*N*,4-diphenylazetidin-2-one (*t*-**1b**).

S2:^{13}C-NMR spectrum of *trans*-3-cyclopropyl-*N*,4-diphenylazetidin-2-one (*t*-**1b**).

S3: DEPT spectrum of *trans*-3-cyclopropyl-*N*,4-diphenylazetidin-2-one (*t*-**1b**).

S4:^{1}H-NMR spectrum of *cis*-3-cyclopropyl-*N*,4-diphenylazetidin-2-one (*c*-**1b**).

S5:^{13}C-NMR spectrum of *cis*-3-cyclopropyl-*N*,4-diphenylazetidin-2-one (*c*-**1b**).

S6: DEPT spectrum of *cis*-3-cyclopropyl-*N*,4-diphenylazetidin-2-one (*c*-**1b**).

S7:^{1}H-NMR spectrum of *trans*-*N*,3-diphenyl-4-methylazetidin-2-one (*t*-**1c**).

S8:^{13}C-NMR spectrum of *trans*-*N*,3-diphenyl-4-methylazetidin-2-one (*t*-**1c**).

S9: ^{1}H-NMR spectrum of *cis*-*N*,3-diphenyl-4-methylazetidin-2-one (*c*-**1c**).

S10: ^{13}C-NMR spectrum of *cis*-*N*,3-diphenyl-4-methylazetidin-2-one (*c*-**1c**).

S11:^{1}H-NMR spectrum of 2-cyclopropyl-*N*,3-diphenylpropanamide (**2b**).

S12:^{13}C-NMR spectrum of 2-cyclopropyl-*N*,3-diphenylpropanamide (**2b**).

S13: X-Ray structure of 2-cyclopropyl-*N*,3-diphenylpropanamide (**2b**).

S14-**S22**: X-Ray data of **2b** (Tables).

S23-**S78**: Geometries of the stationary points (Cartesian coordinates).

^{1}H-NMR spectrum of *trans*-3-cyclopropyl-*N*,4-diphenylazetidin-2-one (*t*-**1b**)
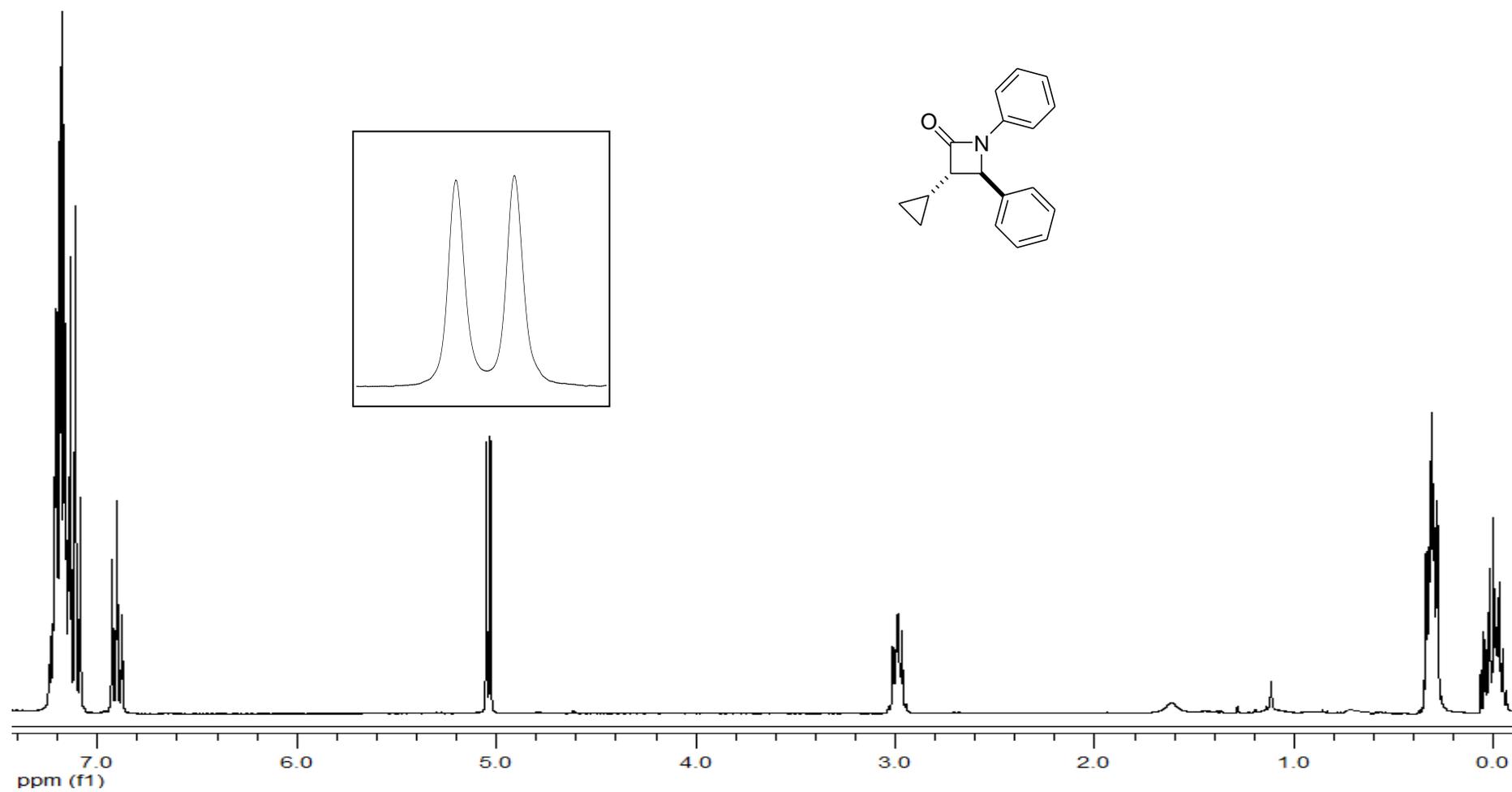
^{13}C-NMR spectrum of *trans*-3-cyclopropyl-*N*,4-diphenylazetidin-2-one (*t*-**1b**)
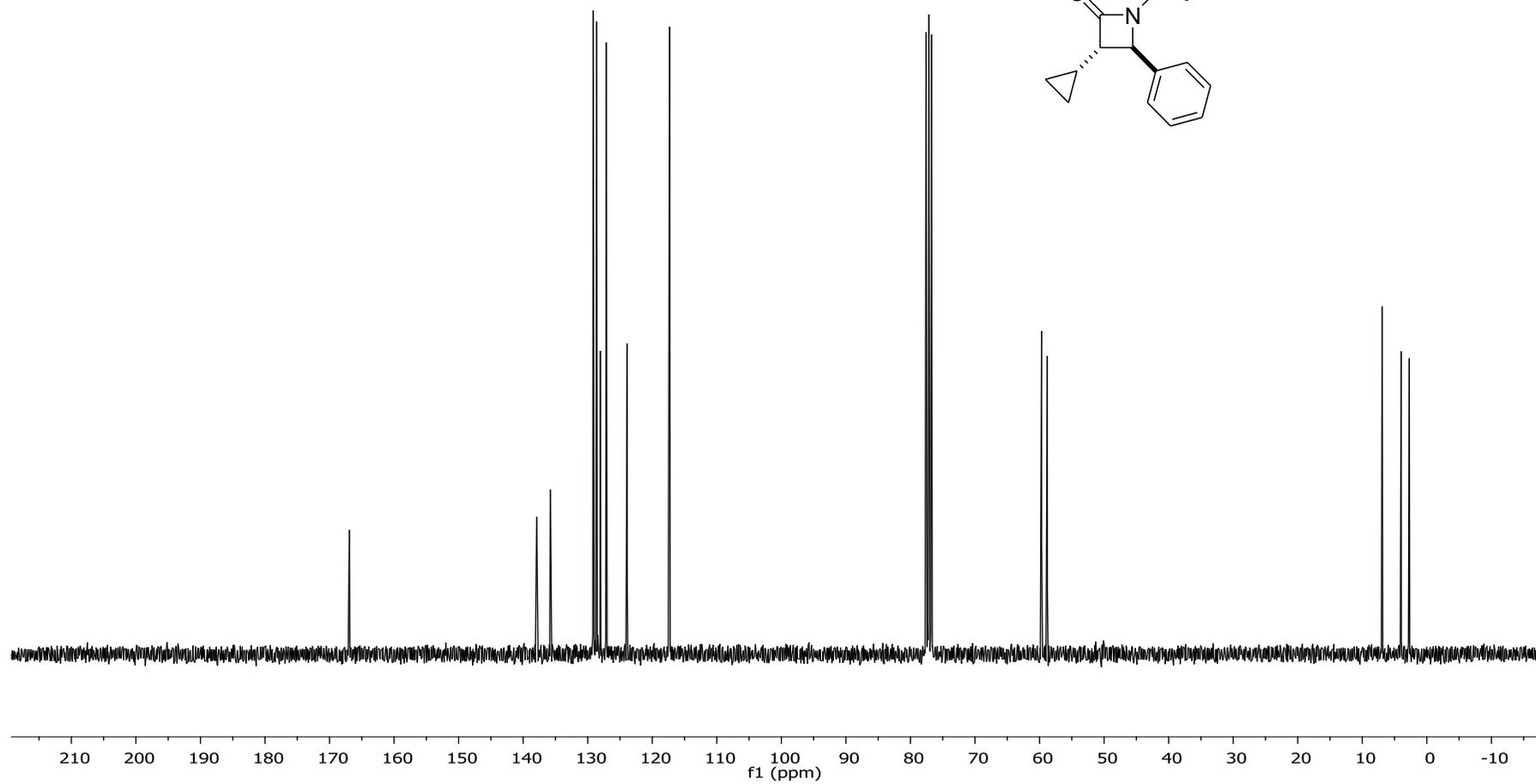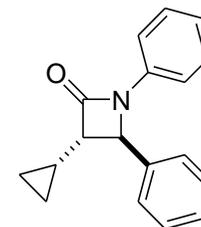
DEPT spectrum of *trans*-3-cyclopropyl-*N*,4-diphenylazetidin-2-one (*t*-**1b**)
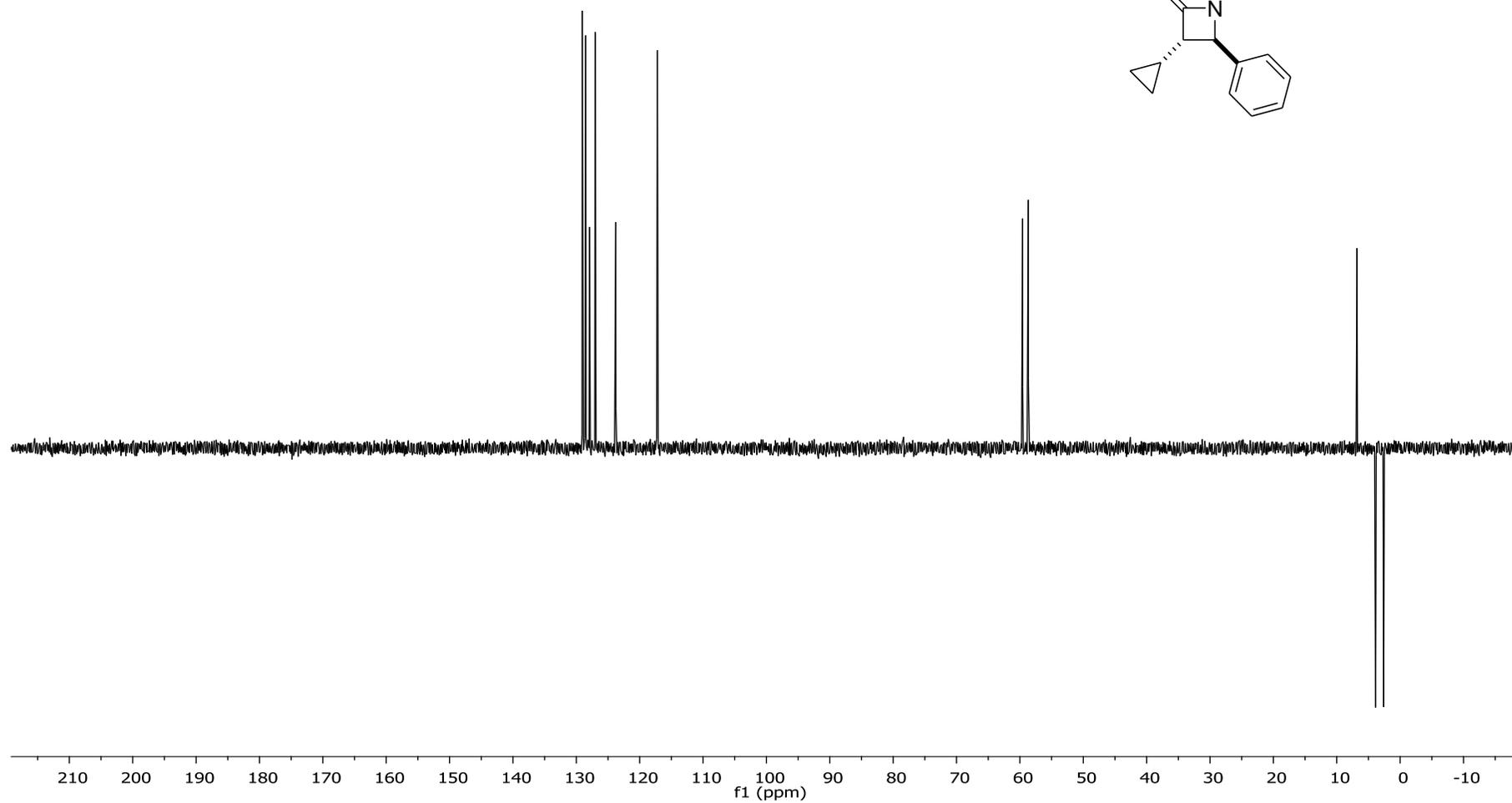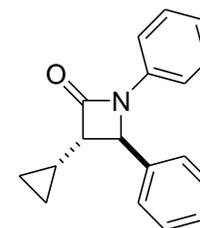
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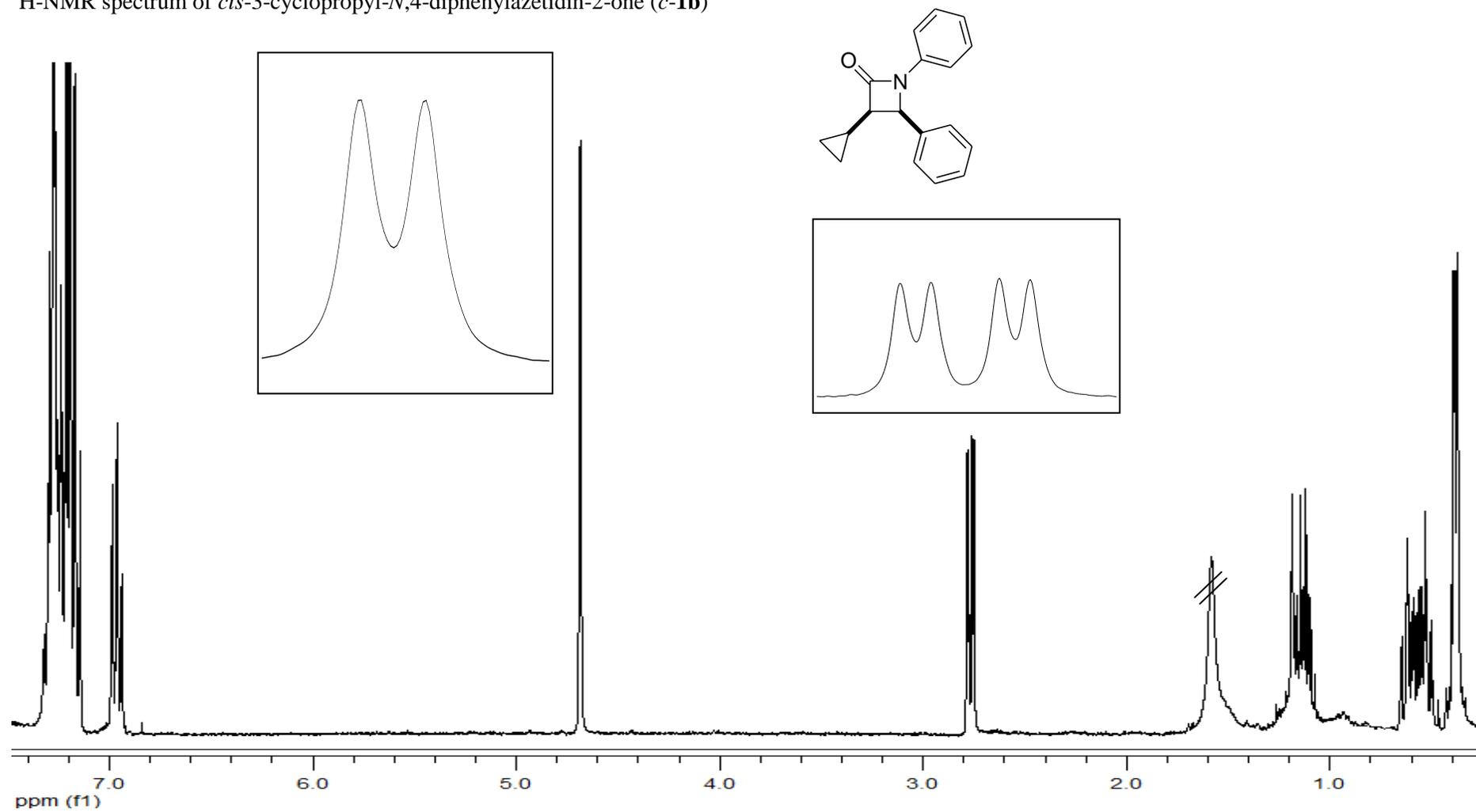
^{13}C-NMR spectrum of *cis*-3-cyclopropyl-*N*,4-diphenylazetidin-2-one (*c*-**1b**)
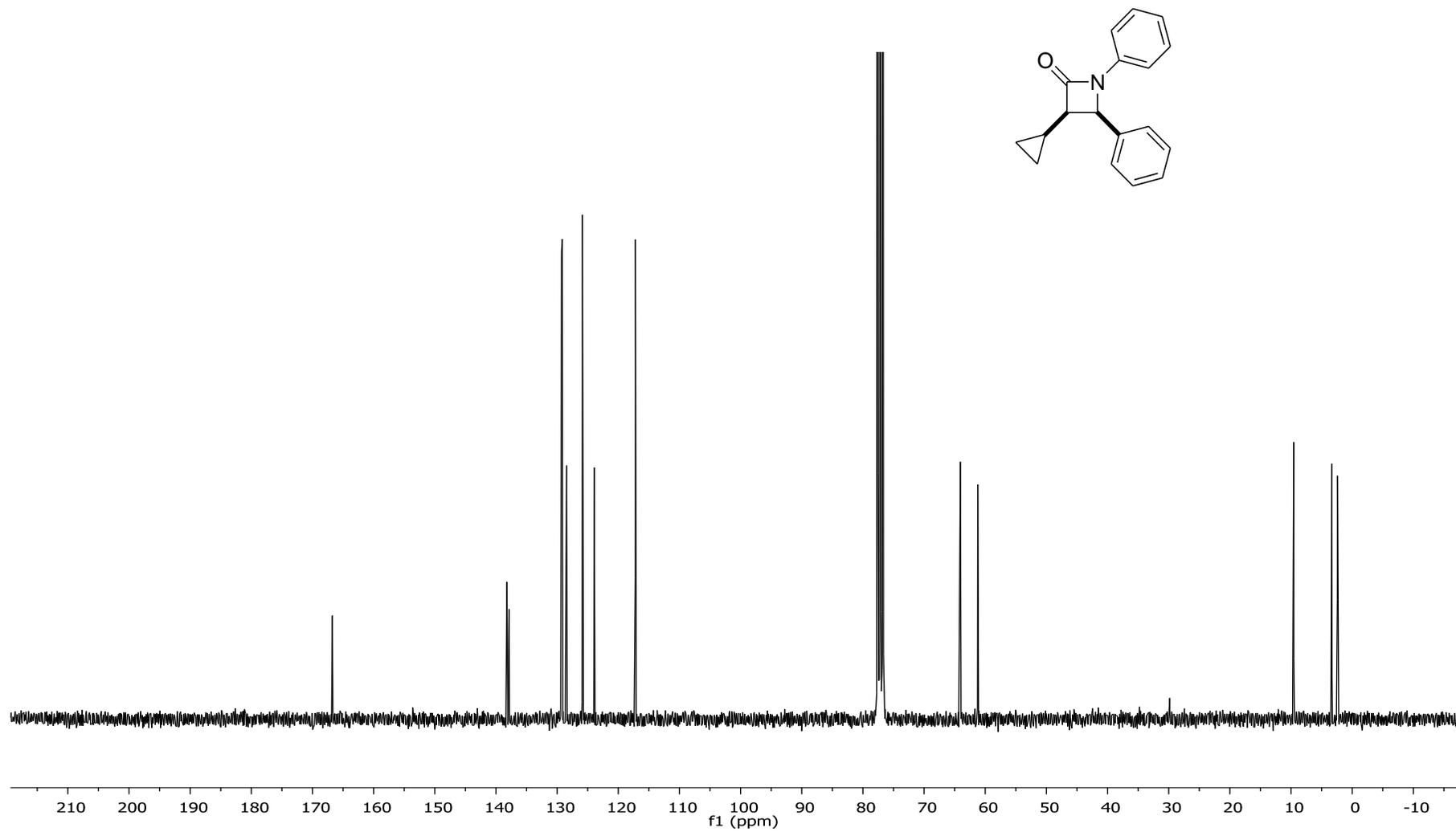
DEPT spectrum of *cis*-3-cyclopropyl-*N*,4-diphenylazetidin-2-one (*c*-**1b**)
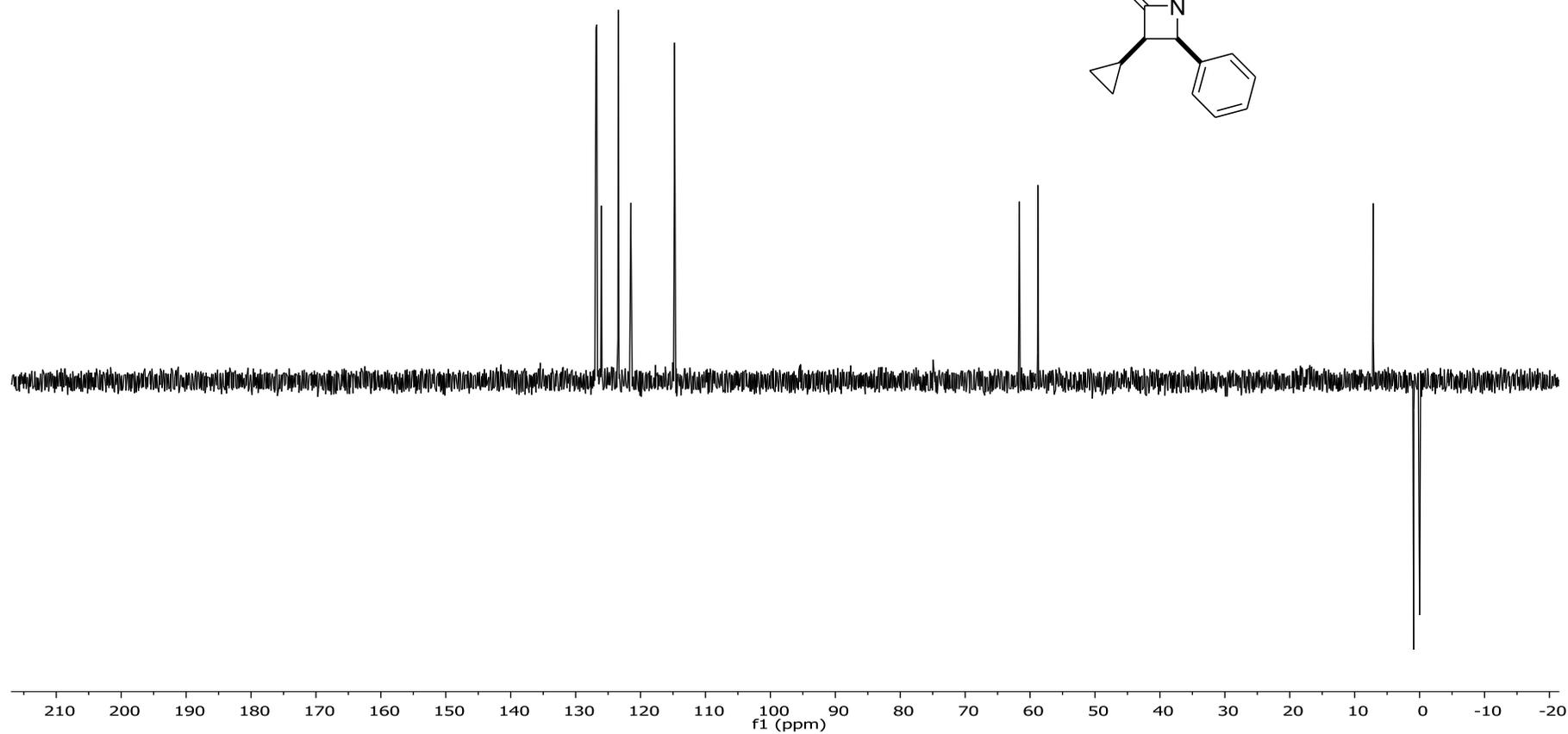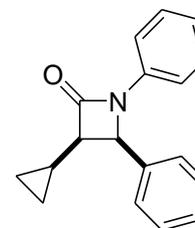
^{1}H-NMR spectrum of *trans*-N,3-diphenyl-4-methylazetidin-2-one (*t*-**1c**)
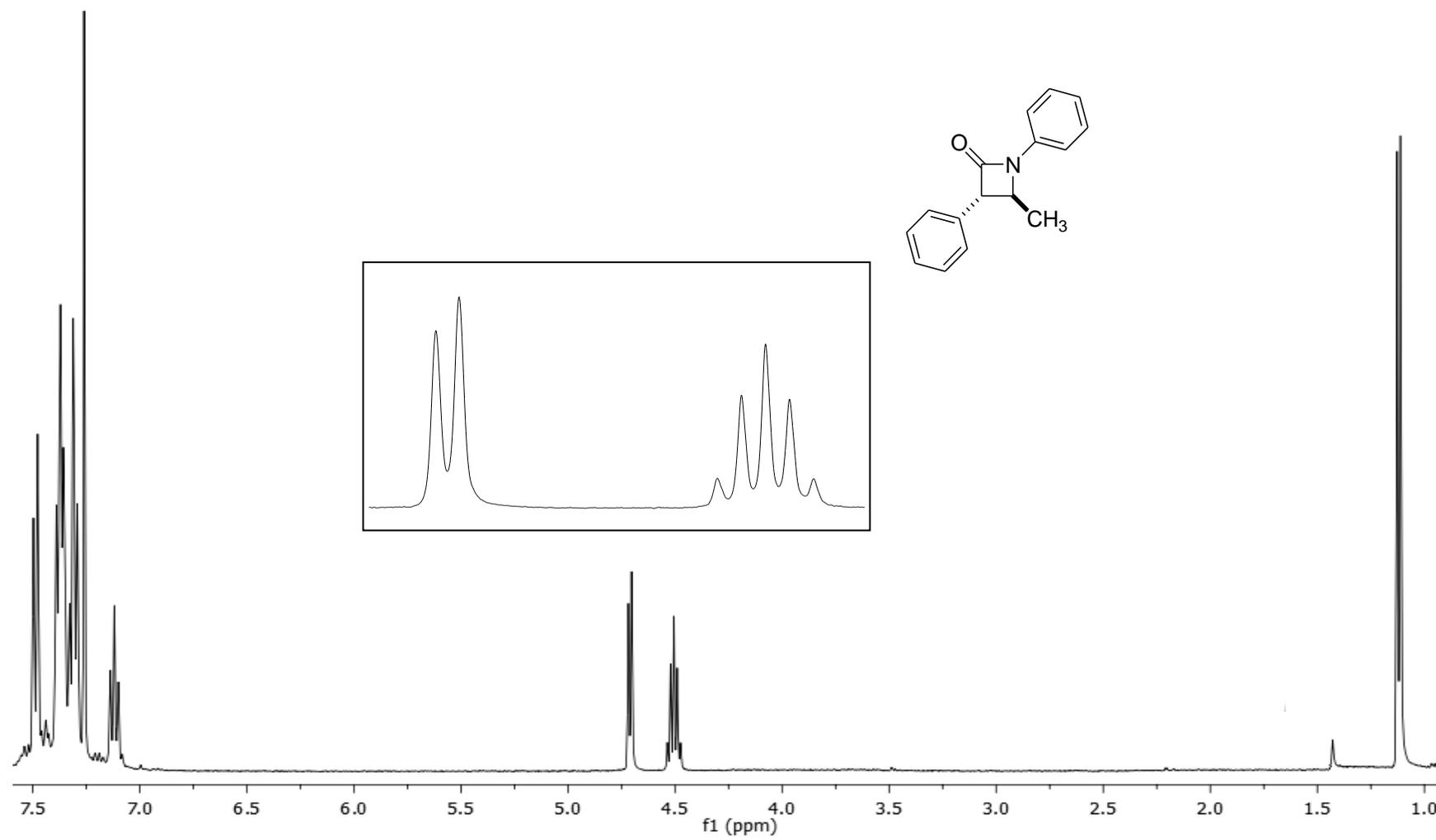
^{13}C-NMR spectrum of *trans-N*,3-diphenyl-4-methylazetidin-2-one (*t*-**1c**)
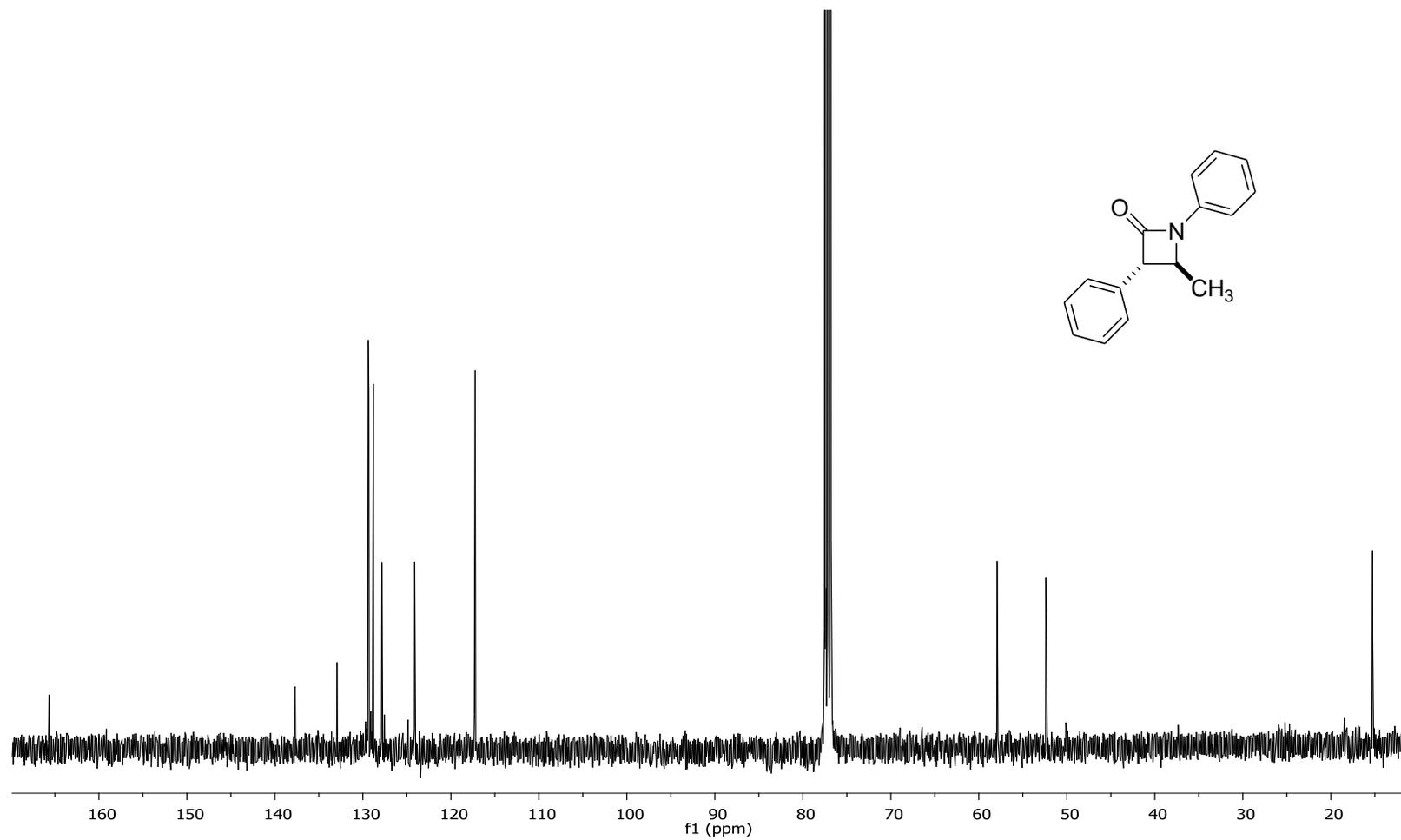
^{1}H-NMR spectrum of *cis-N*,3-diphenyl-4-methylazetidin-2-one (*c*-**1c**)
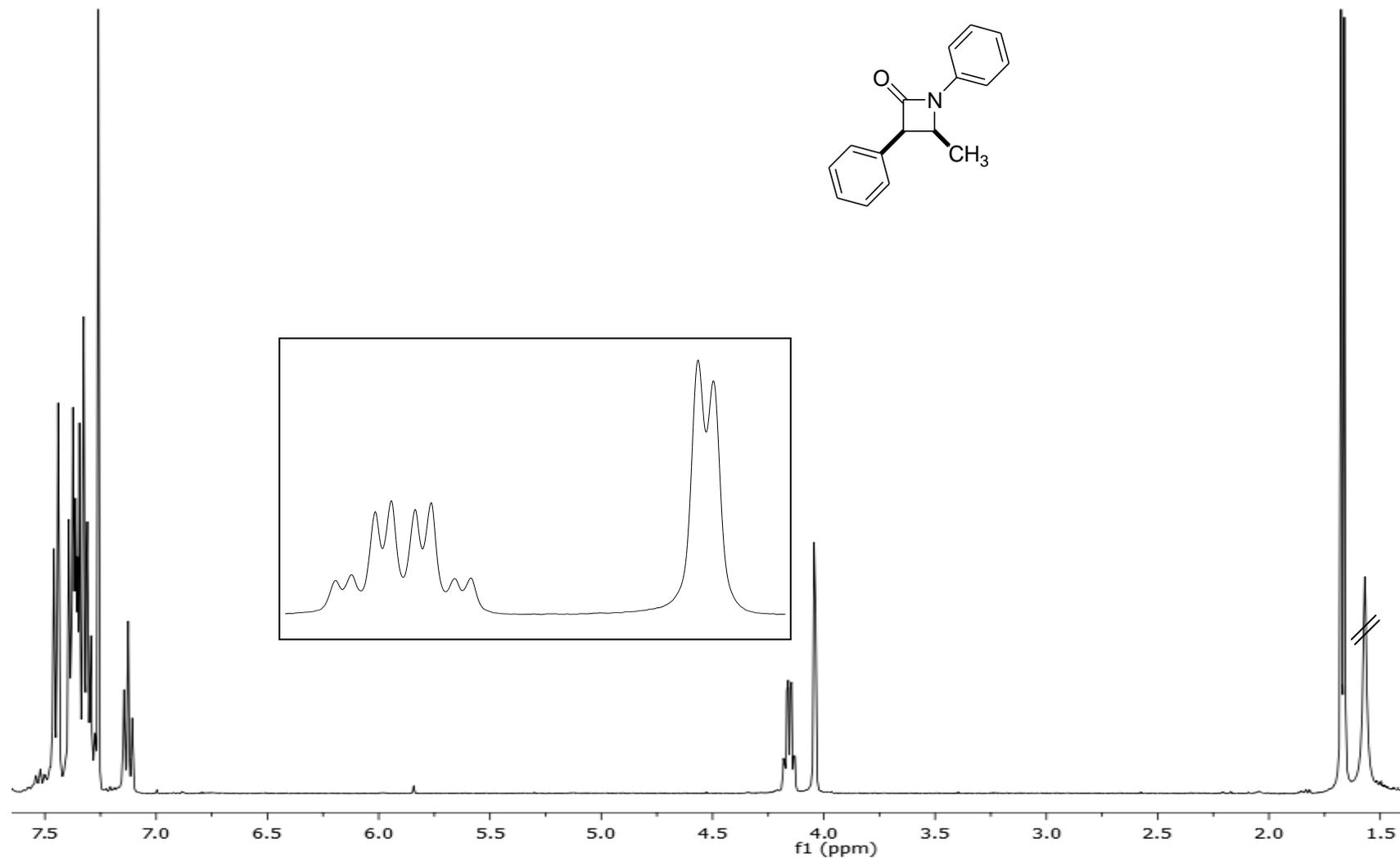
^{13}C-NMR spectrum of *cis-N*,3-diphenyl-4-methylazetidin-2-one (*c*-**1c**)
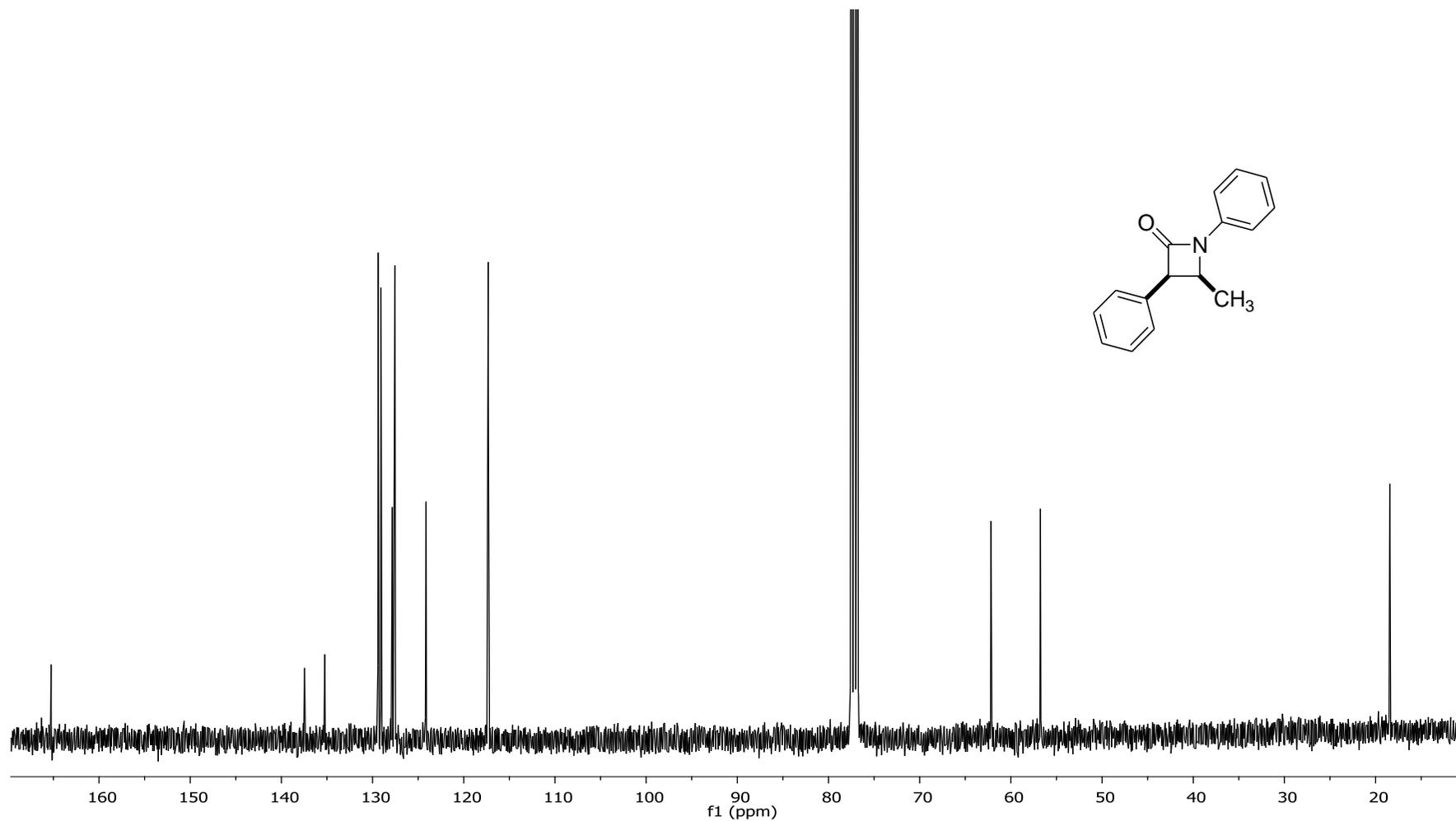
^{1}H-NMR spectrum of 2-cyclopropyl-N,3-diphenylpropanamide (**2b**)
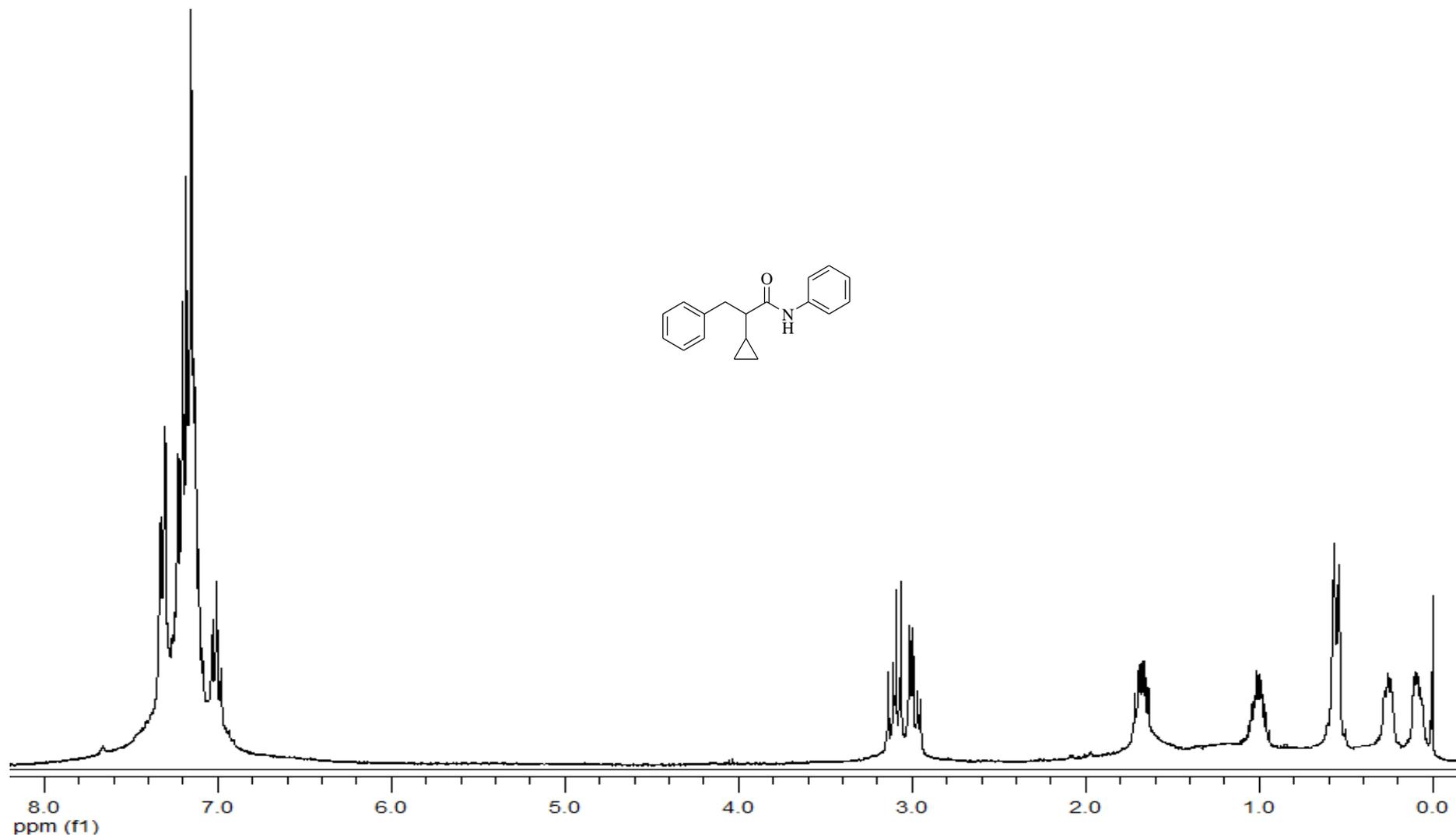
^{13}C-NMR spectrum of 2-cyclopropyl-*N*,3-diphenylpropanamide (**2b**)
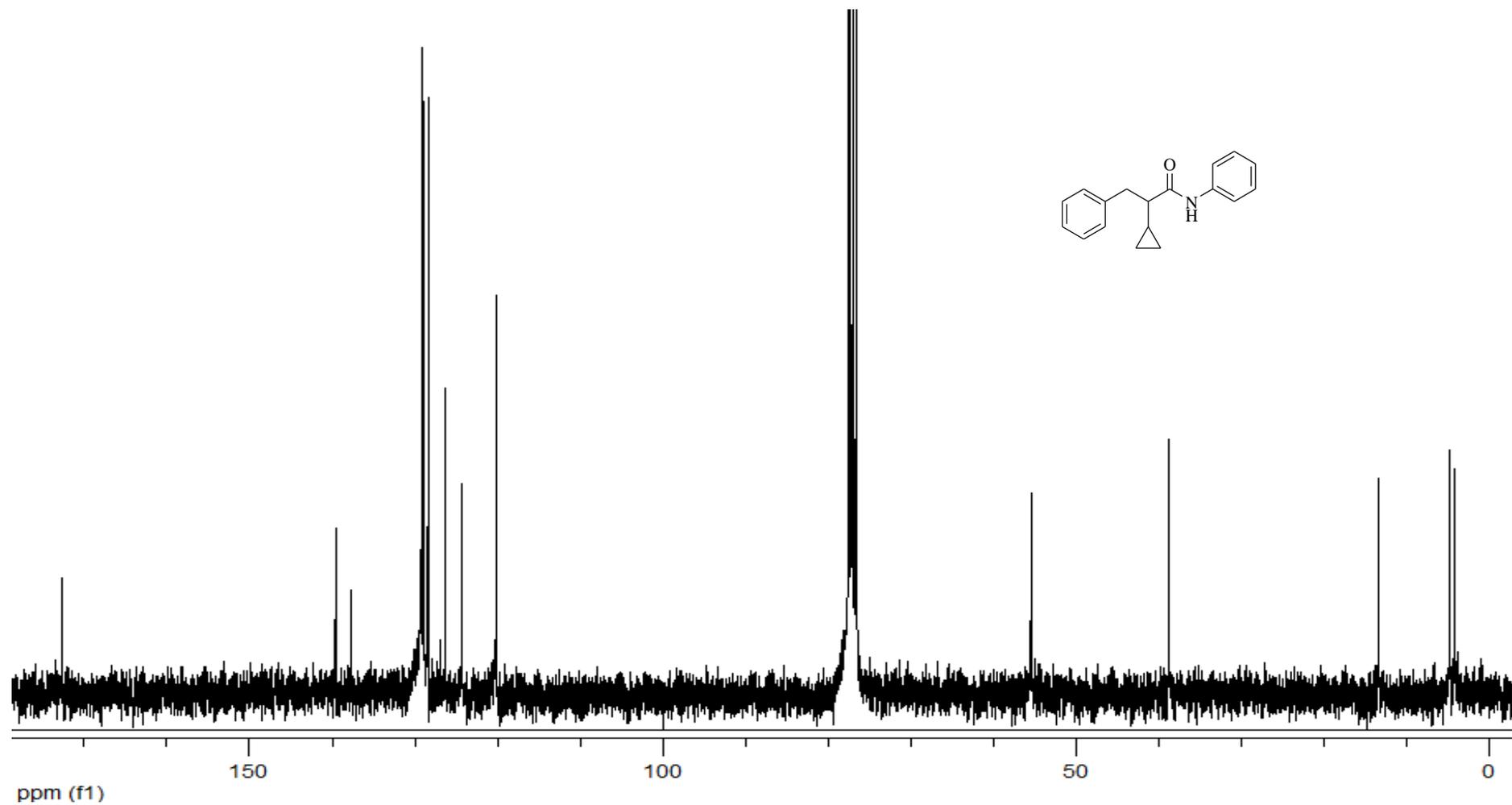
X-Ray structure of 2-cyclopropyl-*N*,3-diphenylpropanamide (**2b**): crystallographic data have been deposited with the Cambridge Crystallographic Data Centre (CCDC 860535 & 860536)
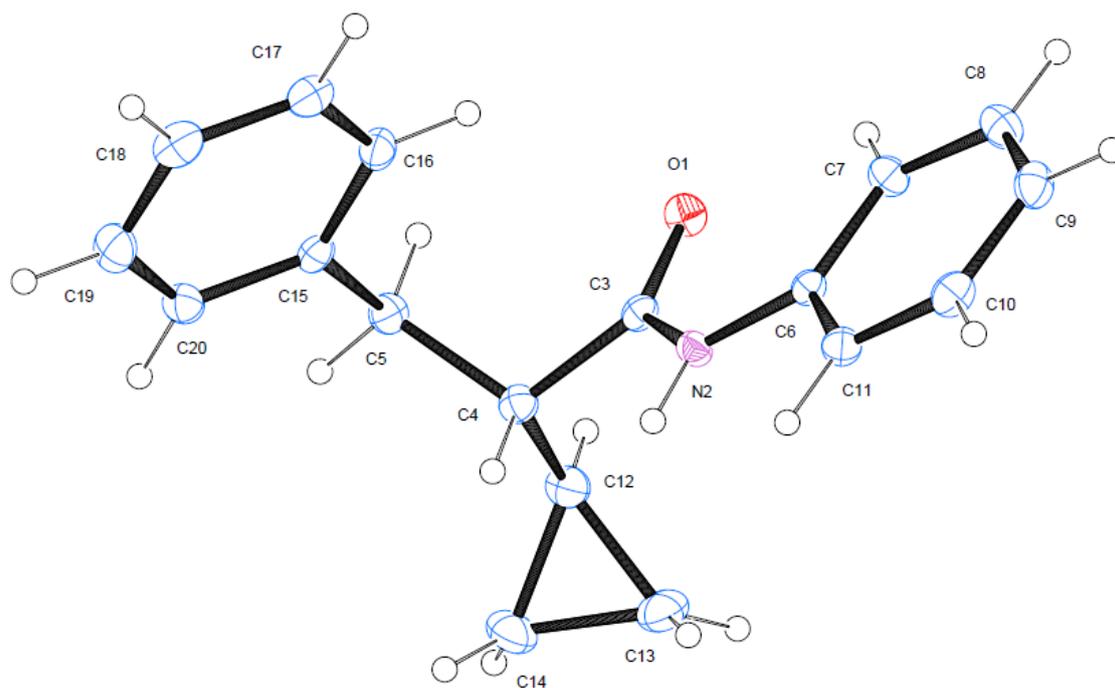
Crystal data and structure refinement for 2-cyclopropyl-*N*,3-diphenylpropanamide, **2b**

Empirical formula	$C_{18}H_{19}NO$
Formula weight	265.34
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 9.7754(7) Å $\alpha = 90°$
	b = 17.6008(15) Å $\beta = 113.841(4)°$
	c = 9.5625(7) Å $\gamma = 90°$
Volume	1504.9(2) $Å^3$
Z	4
Density (calculated)	1.171 Mg/m^3
Absorption coefficient	0.072 mm^{-1}
F(000)	568
Crystal size	0.46 x 0.16 x 0.03 mm^3
Theta range for data collection	2.28 to 26.37°
Index ranges	-12<=h<=11, 0<=k<=22, 0<=l<=11
Reflections collected	23367
Independent reflections	3070 [R(int) = 0.0634]
Completeness to theta = 26.37°	100.0 %
Max. and min. transmission	0.9887 and 0.9145
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3070 / 0 / 185
Goodness-of-fit on F^2	1.025
Final R indices [I>2sigma(I)]	R1 = 0.0476, wR2 = 0.0997
R indices (all data)	R1 = 0.0863, wR2 = 0.1153
Largest diff. peak and hole	0.394 and -0.227 $e.Å^{-3}$

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2x 10^3). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	1710(1)	2154(1)	3894(1)	25(1)
N(2)	2294(2)	2118(1)	1813(2)	21(1)
C(3)	1461(2)	2348(1)	2568(2)	21(1)
C(4)	193(2)	2889(1)	1688(2)	24(1)
C(5)	-1306(2)	2580(1)	1618(2)	25(1)
C(6)	3561(2)	1636(1)	2324(2)	20(1)
C(7)	4194(2)	1319(1)	3779(2)	25(1)
C(8)	5464(2)	872(1)	4178(2)	30(1)
C(9)	6096(2)	727(1)	3148(2)	30(1)
C(10)	5449(2)	1034(1)	1694(2)	29(1)
C(11)	4198(2)	1490(1)	1282(2)	25(1)
C(12)	550(2)	3658(1)	2450(2)	30(1)
C(13)	1693(2)	4147(1)	2213(2)	39(1)
C(14)	63(2)	4355(1)	1482(2)	40(1)
C(15)	-1881(2)	1904(1)	576(2)	23(1)
C(16)	-1186(2)	1198(1)	940(2)	26(1)
C(17)	-1718(2)	583(1)	-36(2)	30(1)
C(18)	-2971(2)	654(1)	-1384(2)	33(1)
C(19)	-3679(2)	1351(1)	-1759(2)	34(1)
C(20)	-3134(2)	1974(1)	-801(2)	29(1)

Bond lengths [Å] and angles [°]

O(1)-C(3)	1.2385(19)
N(2)-C(3)	1.350(2)
N(2)-C(6)	1.415(2)
N(2)-H(2)	0.875(19)
C(3)-C(4)	1.520(2)
C(4)-C(12)	1.509(3)
C(4)-C(5)	1.539(2)
C(4)-H(4)	1.0000

C(5)-C(15)	1.508(2)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(6)-C(7)	1.391(2)
C(6)-C(11)	1.396(2)
C(7)-C(8)	1.387(3)
C(7)-H(7)	0.9500
C(8)-C(9)	1.381(2)
C(8)-H(8)	0.9500
C(9)-C(10)	1.383(3)
C(9)-H(9)	0.9500
C(10)-C(11)	1.381(3)
C(10)-H(10)	0.9500
C(11)-H(11)	0.9500
C(12)-C(14)	1.495(3)
C(12)-C(13)	1.499(3)
C(12)-H(12)	1.0000
C(13)-C(14)	1.504(3)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-C(16)	1.391(3)
C(15)-C(20)	1.395(2)
C(16)-C(17)	1.384(3)
C(16)-H(16)	0.9500
C(17)-C(18)	1.379(3)
C(17)-H(17)	0.9500
C(18)-C(19)	1.381(3)
C(18)-H(18)	0.9500
C(19)-C(20)	1.390(3)
C(19)-H(19)	0.9500
C(20)-H(20)	0.9500
C(3)-N(2)-C(6)	128.87(15)
C(3)-N(2)-H(2)	114.0(12)
C(6)-N(2)-H(2)	117.1(12)
O(1)-C(3)-N(2)	123.61(16)

O(1)-C(3)-C(4)	121.25(14)
N(2)-C(3)-C(4)	115.13(14)
C(12)-C(4)-C(3)	108.44(14)
C(12)-C(4)-C(5)	111.57(14)
C(3)-C(4)-C(5)	110.63(14)
C(12)-C(4)-H(4)	108.7
C(3)-C(4)-H(4)	108.7
C(5)-C(4)-H(4)	108.7
C(15)-C(5)-C(4)	113.67(13)
C(15)-C(5)-H(5A)	108.8
C(4)-C(5)-H(5A)	108.8
C(15)-C(5)-H(5B)	108.8
C(4)-C(5)-H(5B)	108.8
H(5A)-C(5)-H(5B)	107.7
C(7)-C(6)-C(11)	119.53(16)
C(7)-C(6)-N(2)	124.04(15)
C(11)-C(6)-N(2)	116.42(15)
C(8)-C(7)-C(6)	119.38(16)
C(8)-C(7)-H(7)	120.3
C(6)-C(7)-H(7)	120.3
C(9)-C(8)-C(7)	121.11(17)
C(9)-C(8)-H(8)	119.4
C(7)-C(8)-H(8)	119.4
C(8)-C(9)-C(10)	119.35(17)
C(8)-C(9)-H(9)	120.3
C(10)-C(9)-H(9)	120.3
C(11)-C(10)-C(9)	120.41(16)
C(11)-C(10)-H(10)	119.8
C(9)-C(10)-H(10)	119.8
C(10)-C(11)-C(6)	120.20(16)
C(10)-C(11)-H(11)	119.9
C(6)-C(11)-H(11)	119.9
C(14)-C(12)-C(13)	60.28(13)
C(14)-C(12)-C(4)	118.91(16)
C(13)-C(12)-C(4)	118.85(16)
C(14)-C(12)-H(12)	115.8
C(13)-C(12)-H(12)	115.8
C(4)-C(12)-H(12)	115.8

C(12)-C(13)-C(14)	59.73(13)
C(12)-C(13)-H(13A)	117.8
C(14)-C(13)-H(13A)	117.8
C(12)-C(13)-H(13B)	117.8
C(14)-C(13)-H(13B)	117.8
H(13A)-C(13)-H(13B)	114.9
C(12)-C(14)-C(13)	59.99(13)
C(12)-C(14)-H(14A)	117.8
C(13)-C(14)-H(14A)	117.8
C(12)-C(14)-H(14B)	117.8
C(13)-C(14)-H(14B)	117.8
H(14A)-C(14)-H(14B)	114.9
C(16)-C(15)-C(20)	117.95(16)
C(16)-C(15)-C(5)	121.76(16)
C(20)-C(15)-C(5)	120.29(16)
C(17)-C(16)-C(15)	121.10(17)
C(17)-C(16)-H(16)	119.5
C(15)-C(16)-H(16)	119.5
C(18)-C(17)-C(16)	120.59(19)
C(18)-C(17)-H(17)	119.7
C(16)-C(17)-H(17)	119.7
C(17)-C(18)-C(19)	119.08(18)
C(17)-C(18)-H(18)	120.5
C(19)-C(18)-H(18)	120.5
C(18)-C(19)-C(20)	120.67(18)
C(18)-C(19)-H(19)	119.7
C(20)-C(19)-H(19)	119.7
C(19)-C(20)-C(15)	120.60(18)
C(19)-C(20)-H(20)	119.7
C(15)-C(20)-H(20)	119.7

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Anisotropic displacement parameters (Å^2 x 10^3). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\, h^2 a^{*2} U^{11} + ... + 2\, h\, k\, a^*\, b^*\, U^{12}\,]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	28(1)	30(1)	19(1)	-2(1)	12(1)	1(1)

N(2)	21(1)	25(1)	18(1)	4(1)	8(1)	2(1)
C(3)	21(1)	20(1)	21(1)	-4(1)	9(1)	-5(1)
C(4)	25(1)	24(1)	24(1)	-1(1)	10(1)	-1(1)
C(5)	24(1)	25(1)	28(1)	0(1)	12(1)	2(1)
C(6)	20(1)	19(1)	21(1)	-2(1)	7(1)	-3(1)
C(7)	28(1)	27(1)	21(1)	0(1)	10(1)	2(1)
C(8)	32(1)	30(1)	23(1)	1(1)	6(1)	3(1)
C(9)	23(1)	27(1)	37(1)	-4(1)	10(1)	3(1)
C(10)	28(1)	31(1)	33(1)	-5(1)	18(1)	-2(1)
C(11)	25(1)	30(1)	21(1)	2(1)	10(1)	-1(1)
C(12)	33(1)	27(1)	27(1)	-1(1)	11(1)	-1(1)
C(13)	44(1)	29(1)	43(1)	0(1)	17(1)	-10(1)
C(14)	45(1)	24(1)	39(1)	6(1)	7(1)	3(1)
C(15)	20(1)	26(1)	25(1)	-1(1)	12(1)	-3(1)
C(16)	20(1)	29(1)	30(1)	-1(1)	10(1)	-1(1)
C(17)	32(1)	25(1)	38(1)	-2(1)	20(1)	-2(1)
C(18)	41(1)	33(1)	30(1)	-9(1)	18(1)	-10(1)
C(19)	33(1)	46(1)	20(1)	-3(1)	6(1)	-6(1)
C(20)	27(1)	32(1)	28(1)	5(1)	12(1)	1(1)

Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2x 10^3)

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	x	y	z	U(eq)

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H(2)	2000(20)	2306(11)	890(20)	30(5)
H(4)	129	2939	621	29
H(5A)	-1184	2435	2661	30
H(5B)	-2062	2991	1263	30
H(7)	3761	1408	4492	30
H(8)	5907	662	5177	36
H(9)	6965	420	3435	35
H(10)	5869	931	975	35
H(11)	3770	1705	287	30
H(12)	523	3690	3483	35
H(13A)	2163	3950	1542	47

H(13B)	2356	4459	3084	47
H(14A)	-274	4796	1904	47
H(14B)	-467	4287	363	47
H(16)	-333	1136	1873	32
H(17)	-1216	109	226	36
H(18)	-3342	231	-2045	40
H(19)	-4547	1404	-2682	41
H(20)	-3620	2451	-1086	34

Torsion angles [°]

C(6)-N(2)-C(3)-O(1)	-0.2(3)
C(6)-N(2)-C(3)-C(4)	178.26(16)
O(1)-C(3)-C(4)-C(12)	66.5(2)
N(2)-C(3)-C(4)-C(12)	-112.00(16)
O(1)-C(3)-C(4)-C(5)	-56.1(2)
N(2)-C(3)-C(4)-C(5)	125.35(16)
C(12)-C(4)-C(5)-C(15)	167.37(15)
C(3)-C(4)-C(5)-C(15)	-71.82(18)
C(3)-N(2)-C(6)-C(7)	-1.3(3)
C(3)-N(2)-C(6)-C(11)	179.61(17)
C(11)-C(6)-C(7)-C(8)	1.0(3)
N(2)-C(6)-C(7)-C(8)	-178.12(16)
C(6)-C(7)-C(8)-C(9)	-1.0(3)
C(7)-C(8)-C(9)-C(10)	0.1(3)
C(8)-C(9)-C(10)-C(11)	0.9(3)
C(9)-C(10)-C(11)-C(6)	-1.0(3)
C(7)-C(6)-C(11)-C(10)	0.0(3)
N(2)-C(6)-C(11)-C(10)	179.17(16)
C(3)-C(4)-C(12)-C(14)	146.07(16)
C(5)-C(4)-C(12)-C(14)	-91.85(19)
C(3)-C(4)-C(12)-C(13)	76.09(19)
C(5)-C(4)-C(12)-C(13)	-161.84(16)
C(4)-C(12)-C(13)-C(14)	108.73(19)
C(4)-C(12)-C(14)-C(13)	-108.63(19)
C(4)-C(5)-C(15)-C(16)	70.0(2)
C(4)-C(5)-C(15)-C(20)	-109.61(18)

C(20)-C(15)-C(16)-C(17)	0.3(2)
C(5)-C(15)-C(16)-C(17)	-179.36(15)
C(15)-C(16)-C(17)-C(18)	-1.2(3)
C(16)-C(17)-C(18)-C(19)	0.8(3)
C(17)-C(18)-C(19)-C(20)	0.5(3)
C(18)-C(19)-C(20)-C(15)	-1.4(3)
C(16)-C(15)-C(20)-C(19)	1.0(2)
C(5)-C(15)-C(20)-C(19)	-179.33(15)

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Hydrogen bonds [Å and °].

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D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(2)...O(1)#1	0.875(19)	2.05(2)	2.9105(19)	169.3(17)

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Symmetry transformations used to generate equivalent atoms: #1 x,-y+1/2,z-1/2

Geometries of the stationary points

c-**1a**

E (RB+HF - LYP) = -940,482232907 a.u.

C	0.27901600	1.44105300	1.00652900
C	0.29201000	1.32900200	-0.39025500
C	0.77068900	2.40567300	-1.14973700
C	1.23941800	3.56632300	-0.52963800
C	1.22548200	3.66756900	0.86394100
C	0.74069400	2.60267400	1.62880000
C	-0.16938400	0.07874500	-1.09859200
N	-1.18410600	-0.74592200	-0.40979800
C	-2.54298100	-0.49665300	-0.14884200
C	-3.34290400	-1.48624800	0.45030200
C	-4.69202100	-1.22503000	0.68912900
C	-5.25833600	0.00634800	0.34348800
C	-4.45687100	0.98539500	-0.24873600
C	-3.10449000	0.74227100	-0.49539800
C	0.76448200	-1.21475400	-1.08734900
C	-0.41074000	-1.89268900	-0.36135400
O	-0.63441200	-3.00392000	0.07492700
C	2.12608500	-1.17922200	-0.44290200
C	2.32753400	-1.56616400	0.88917700
C	3.60273900	-1.51576700	1.45931900
C	4.69464600	-1.07791300	0.70676800
C	4.50599100	-0.69603900	-0.62503000
C	3.23255600	-0.75195200	-1.19345700
H	-0.48340800	0.32883200	-2.12008200
H	0.84728400	-1.61170600	-2.10676300
H	-2.90427300	-2.44184200	0.71342500
H	-5.30498200	-1.99540800	1.15016500
H	-6.31021300	0.20011900	0.53484200
H	-4.88113400	1.94861000	-0.52050000
H	-2.48755200	1.51369800	-0.94532400
H	1.49156300	-1.93250700	1.47800900
H	3.74142300	-1.82653700	2.49180900
H	5.68623700	-1.04178500	1.15067200
H	5.35021300	-0.36113600	-1.22254500
H	3.09505200	-0.46107700	-2.23321400
H	0.77417700	2.33721700	-2.23633200
H	1.60788600	4.39111800	-1.13436100
H	1.58383900	4.57124500	1.35012100
H	0.71996600	2.67585200	2.71314600
H	-0.10373600	0.62239600	1.60911800

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c-**1a**^{.-}

E (UB+HF - LYP) = -940,475487116 a.u.

C	0.98849600	2.26457200	-1.07179200
C	0.29762900	1.27640500	-0.34916800
C	0.09449500	1.45314400	1.02277700
C	0.56611900	2.60609000	1.67098400
C	1.26982800	3.57983600	0.94635300
C	1.48204500	3.40891800	-0.42153400
C	-0.17475900	0.03884000	-1.07094100
N	-1.22376000	-0.74616300	-0.39603000
C	-2.56603300	-0.47115300	-0.18351300
C	-3.41009800	-1.43075000	0.44278900
C	-4.75981500	-1.14778900	0.62878000
C	-5.32055400	0.07320200	0.22068400
C	-4.47624800	1.02938300	-0.37890400
C	-3.12496500	0.76947800	-0.57783000
C	0.73510200	-1.25796100	-1.00835100
C	-0.40891200	-1.86590600	-0.20627200
O	-0.64462700	-2.96815800	0.29408500
C	2.12663600	-1.19280100	-0.44102000
C	3.14613600	-0.57555500	-1.19412800
C	4.44653100	-0.46719900	-0.67752600
C	4.75362200	-1.01090200	0.57004500
C	3.75374200	-1.66430900	1.30894200
C	2.44558100	-1.73762600	0.80726600
H	-0.45601900	0.29211100	-2.10585000
H	0.78979200	-1.69836600	-2.03496200
H	-2.98513400	-2.37760200	0.75650400
H	-5.39002300	-1.89890600	1.10368200
H	-6.37729600	0.28001400	0.37123600
H	-4.87930100	1.99063700	-0.69363400
H	-2.48880900	1.52422500	-1.03193600
H	1.66898900	-2.23688700	1.37969600
H	3.98743400	-2.10690300	2.27513000
H	5.76414100	-0.93029300	0.96770100
H	5.21679500	0.04133600	-1.25570100
H	2.91474900	-0.17189100	-2.17816800
H	1.14486200	2.13589400	-2.14162700
H	2.02979300	4.15952500	-0.98852400
H	1.64803100	4.46767900	1.45044500
H	0.39567700	2.73399100	2.73754900
H	-0.44779600	0.69634500	1.58212700

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_c_-1a-TS(N-C2)
E (UB+HF - LYP) = -940,451007888 a.u.
1 imaginary frequency -44,83 cm**-1

C	-0.29609200	1.52192900	1.11686700
C	0.07012400	1.07630600	-0.16092700
C	0.74706100	1.96758000	-1.00573000
C	1.06552100	3.26304500	-0.58821600
C	0.70340800	3.69286700	0.69223700
C	0.01895100	2.81571100	1.54088500
C	-0.25766200	-0.34648200	-0.62625300
N	-1.34311000	-1.00204100	0.04923100
C	-2.63399500	-0.65356800	-0.13158100
C	-3.65034700	-1.38280000	0.57007900
C	-4.99858600	-1.09667800	0.41375700
C	-5.43758400	-0.07305500	-0.44838100
C	-4.46550100	0.65714900	-1.14241200
C	-3.10317100	0.39184200	-0.99336300
C	0.84977600	-1.41353400	-0.31296200
C	0.26959500	-1.95569800	1.02986600
O	0.25197800	-3.10727100	1.38964000
C	2.31125500	-1.04854300	-0.25313500
C	2.85273200	-0.29103500	0.80120000
C	4.21309500	0.02241800	0.83722600
C	5.06918500	-0.41087100	-0.18064600
C	4.54856100	-1.17026800	-1.23280700
C	3.18707400	-1.48502600	-1.26151500
H	-0.38767400	-0.29374200	-1.72557000
H	0.72309300	-2.21239300	-1.05892800
H	-3.32493100	-2.18305500	1.23102200
H	-5.73063100	-1.68325300	0.97008000
H	-6.49665300	0.14581800	-0.56695400
H	-4.77160700	1.46214100	-1.81201900
H	-2.38398700	0.99834200	-1.53719200
H	2.19745600	0.05025100	1.59626700
H	4.60563700	0.61119800	1.66407700
H	6.12825300	-0.16209600	-0.15244800
H	5.20163100	-1.52197000	-2.02950000
H	2.79101000	-2.08398900	-2.07973900
H	1.03106000	1.63899000	-2.00484700
H	1.59457200	3.93554600	-1.26149000
H	0.94452400	4.70182800	1.02191700
H	-0.27836200	3.14381200	2.53546100
H	-0.83784500	0.83730000	1.76298600

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c-**1a-TS(C2-C3)**
E (UB+HF - LYP) = -940,444226993 a.u.
1 imaginary frequency -112,36 cm**-1

C	-0.06696800	-0.09830200	-1.05085300
C	1.22142300	-0.89332500	-1.22131400
H	-0.47243100	0.05734500	-2.06531100
H	1.35694800	-1.27559200	-2.23045900
C	2.42682400	-0.81388100	-0.45804700
C	0.06958900	1.29608300	-0.44209600
N	-0.97239900	-0.99974500	-0.30312600
C	-0.36257000	-2.30217800	-0.37902500
C	-2.33688000	-0.75498900	-0.09691100
O	-0.77322700	-3.26380000	0.24772400
C	-3.08285000	-1.54798600	0.80917900
C	-4.44835900	-1.32913000	0.98264100
C	-5.11728700	-0.31469800	0.28575100
C	-4.38527700	0.47813200	-0.60454500
C	-3.02052800	0.26361200	-0.80080200
H	-2.57505300	-2.33651300	1.34998100
H	-4.99633100	-1.95846900	1.68229300
H	-6.18047000	-0.14235700	0.43817700
H	-4.87821500	1.27840400	-1.15438800
H	-2.47907600	0.90146500	-1.49110200
C	0.60028200	2.32224000	-1.23905800
C	0.76034400	3.61702900	-0.74319700
C	0.38333000	3.91653200	0.57147200
C	-0.15057200	2.90561100	1.37318400
C	-0.30644500	1.60912600	0.87036900
H	0.90555600	2.09222200	-2.25849200
H	1.18122100	4.39185500	-1.38126600
H	0.50657500	4.92408500	0.96355100
H	-0.44953600	3.12229200	2.39698900
H	-0.72900200	0.83279300	1.50087800
C	2.51978100	-0.38903400	0.90484400
C	3.72954600	-0.38412400	1.59134900
C	4.92048600	-0.81634200	0.98621100
C	4.85539800	-1.26706500	-0.34468700
C	3.65443000	-1.26490300	-1.04147000
H	1.62170800	-0.07954500	1.42734400
H	3.74315700	-0.04760400	2.62808700
H	5.86093000	-0.81400300	1.53289700
H	5.75889400	-1.61880300	-0.84324300
H	3.63555800	-1.61340500	-2.07381600

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c-**1a-TS(C3-C4)**
E (UB+HF - LYP) = -940,470784418 a.u.
1 imaginary frequency -255,86 cm**-1

C	-0.20852200	0.22514700	-1.07117700
C	0.93163600	-1.15848200	-1.03881200
H	-0.47713700	0.38799600	-2.12211600
H	0.96419800	-1.41033600	-2.10959500
C	2.27415700	-1.16099300	-0.45006200
C	0.07182200	1.48350500	-0.38467900
N	-1.10523000	-0.75390300	-0.42730100
C	-0.23305700	-1.83119400	-0.34577900
C	-2.47326800	-0.65145100	-0.16355500
O	-0.42200400	-2.95543400	0.10953600
C	-3.18737100	-1.73352800	0.39935000
C	-4.55428600	-1.61227500	0.64362000
C	-5.24275700	-0.42825100	0.34797100
C	-4.53138600	0.64401000	-0.20404600
C	-3.16546800	0.54049200	-0.46426400
H	-2.65541500	-2.64825500	0.63219200
H	-5.08815100	-2.45747300	1.07466300
H	-6.30916400	-0.34325400	0.54418000
H	-5.04275200	1.57669100	-0.43458100
H	-2.62058800	1.38159400	-0.87947700
C	2.53866400	-1.54964900	0.88894400
C	3.82156400	-1.49793900	1.41891200
C	4.90810300	-1.03341000	0.64437200
C	4.66474500	-0.64066100	-0.68002700
C	3.38235600	-0.70246300	-1.21973700
H	1.72118500	-1.92070300	1.50226000
H	3.98738400	-1.82107900	2.44588700
H	5.90907000	-0.97841600	1.06664300
H	5.48684900	-0.27993400	-1.29800900
H	3.21494100	-0.38966900	-2.24984700
C	0.32807900	2.66455900	-1.13094200
C	0.67590400	3.85818700	-0.51278700
C	0.79068600	3.93008200	0.89534300
C	0.54664100	2.76842900	1.64714700
C	0.19749300	1.56918200	1.03412500
H	0.24365200	2.62794300	-2.21778700
H	0.85782900	4.74420800	-1.11989500
H	1.06365900	4.86243700	1.38411200
H	0.63318200	2.80259500	2.73279900
H	0.00948800	0.68665100	1.63989100

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c-**1a-TS(N-C4)**
E (UB+HF - LYP) = -940,46705545 a.u.
1 imaginary frequency -501,33 cm**-1

C	0.02058800	0.24914600	-1.23627900
C	0.90916300	-1.05697500	-1.20654500
H	-0.28629000	0.49809500	-2.25515500
H	1.07316300	-1.37712000	-2.24866300
C	2.24248800	-1.05039700	-0.50282100
C	0.27480200	1.44788200	-0.46127400
N	-1.15808000	-0.83310600	-0.66332900
C	-0.26131700	-1.85432800	-0.61831700
C	-2.46999900	-0.72727800	-0.22884900
O	-0.37583200	-3.02847200	-0.26002400
C	-3.02070400	-1.60846900	0.73328800
C	-4.33291700	-1.44018900	1.16712000
C	-5.12983400	-0.39078500	0.67964500
C	-4.58384700	0.48590400	-0.26756600
C	-3.27837700	0.32254400	-0.72611600
H	-2.41159000	-2.42535500	1.10510900
H	-4.74242500	-2.13810800	1.89630900
H	-6.15111200	-0.26110600	1.03054800
H	-5.18223800	1.30944900	-0.65388500
H	-2.86083400	1.01335800	-1.45279100
C	2.53956300	-1.92623300	0.55028500
C	3.79397500	-1.89991100	1.17083900
C	4.76978900	-0.98644400	0.75223200
C	4.48709100	-0.11765800	-0.30602900
C	3.24171500	-0.15854500	-0.93883000
H	1.78479300	-2.63647200	0.87475400
H	4.00399000	-2.58792000	1.98758200
H	5.74094400	-0.95567200	1.24263400
H	5.23711500	0.59740600	-0.63905800
H	3.02425800	0.52673200	-1.75430900
C	0.04151300	2.73618500	-1.03985200
C	0.22618300	3.90749500	-0.32464100
C	0.63908100	3.86955800	1.03274800
C	0.82566700	2.60780300	1.63556500
C	0.63814800	1.42813700	0.92990600
H	-0.27402700	2.79009300	-2.08326800
H	0.05330700	4.86621900	-0.81340500
H	0.77851300	4.78658500	1.60035000
H	1.11612000	2.55322500	2.68489100
H	0.77288900	0.47547300	1.43479200

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c-**1a-IN(N-C2)**

E (UB+HF - LYP) = -940,451937542 a.u.

C	-0.35692700	1.53541600	1.31275700
C	-0.01255200	1.02352100	0.05289600
C	0.56960700	1.89471300	-0.87848700
C	0.81980100	3.23414800	-0.56377800
C	0.48835800	3.72764700	0.70143700
C	-0.10361000	2.87073400	1.63690200
C	-0.28002900	-0.44898900	-0.29566600
N	-1.41572200	-1.03790800	0.35239200
C	-2.65449500	-0.72580800	-0.07977200
C	-3.77756200	-1.34963400	0.56656400
C	-5.08555100	-1.11681700	0.17137200
C	-5.38731600	-0.24719000	-0.89650300
C	-4.31678700	0.38446700	-1.54057500
C	-2.99284800	0.16992300	-1.15248500
C	0.88716400	-1.40695200	0.12290600
C	0.72064000	-1.65787900	1.64044600
O	0.89733300	-2.68544500	2.22296800
C	2.31556700	-1.02624800	-0.20382700
C	3.01539200	-0.03559300	0.50756100
C	4.33464300	0.28620400	0.18034900
C	4.98649500	-0.37103700	-0.86769800
C	4.30500700	-1.36064200	-1.58230100
C	2.98750400	-1.68438100	-1.24723900
H	-0.32367800	-0.49818900	-1.40553300
H	0.65983700	-2.36545200	-0.36227100
H	-3.55806100	-2.03005300	1.38723700
H	-5.89551100	-1.62222000	0.69954700
H	-6.41564100	-0.06718700	-1.20323500
H	-4.51493600	1.07395500	-2.36306900
H	-2.20420600	0.70689300	-1.67232200
H	2.51996300	0.48792800	1.31934600
H	4.85314500	1.05795000	0.74557800
H	6.01326400	-0.11671600	-1.12262200
H	4.79877400	-1.88499300	-2.39818200
H	2.46609600	-2.46083900	-1.80345500
H	0.82875200	1.51692700	-1.86680500
H	1.27046200	3.89086000	-1.30629100
H	0.67716600	4.77014000	0.95166800
H	-0.37949300	3.24813700	2.62019500
H	-0.83953500	0.86816600	2.02057000

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c-1a-IN(C2-C3)
E (UB+HF - LYP) = -940,455246199 a.u.

C	3.91720500	0.61999800	0.53909900
C	2.64698500	0.15122500	0.07086900
C	2.70016800	-0.92332300	-0.87487000
C	3.90909200	-1.44877300	-1.32099500
C	5.13859600	-0.95927600	-0.85337500
C	5.11608600	0.08325300	0.09186000
C	1.44096800	0.72217700	0.56080900
C	0.09645500	0.48157600	-0.06830500
N	-0.54234400	-0.64771000	0.66371200
C	-1.56849200	-1.43213800	0.11050400
C	-1.91313600	-2.69651100	0.64684800
C	-2.92265400	-3.46084500	0.06418900
C	-3.61822000	-3.01325000	-1.06554700
C	-3.28438900	-1.76665400	-1.60063800
C	-2.28357500	-0.98221100	-1.02409400
C	-0.73431200	1.76079900	-0.07710200
C	-0.67266600	2.62920900	-1.17766200
C	-1.37433600	3.83683400	-1.18535700
C	-2.15535300	4.20187800	-0.08241600
C	-2.22444200	3.34398900	1.01942800
C	-1.52360000	2.13415800	1.02076300
C	0.08967800	-0.78277200	1.92320100
O	-0.13037200	-1.70971700	2.69002600
H	0.21558000	0.15797500	-1.11266600
H	1.52711300	1.58655900	1.21168600
H	-1.37975900	-3.05615600	1.51646500
H	-3.16280100	-4.42909400	0.50057500
H	-4.40043500	-3.62073400	-1.51544200
H	-3.81073400	-1.38843400	-2.47553300
H	-2.06968500	-0.00820400	-1.44868000
H	-0.05851800	2.35498000	-2.03413100
H	-1.31181400	4.49275400	-2.05177400
H	-2.70546600	5.14073200	-0.08469300
H	-2.83031400	3.61503600	1.88213000
H	-1.58360600	1.46738400	1.87630600
H	1.77339400	-1.35851900	-1.24138400
H	3.89366600	-2.26756100	-2.04047300
H	6.07904600	-1.38024000	-1.20186600
H	6.05377900	0.48097500	0.48055800
H	3.92959200	1.42820000	1.26946300

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c-**1a-IN(C3-C4)**
E (UB+HF - LYP) = -940,502339192 a.u.

C	-0.70018400	3.51446800	-1.01512100
C	-0.60701500	2.33825100	-0.21375800
C	0.18500800	2.42287700	0.97026300
C	0.83407200	3.60420800	1.30742400
C	0.73276300	4.75043800	0.50185900
C	-0.04684000	4.68942100	-0.66423600
C	-1.33507800	1.18155500	-0.61212000
N	-1.27331100	-0.07192300	-0.04622200
C	-2.40832100	-0.88962900	-0.04048700
C	-2.28811100	-2.29599000	0.04699300
C	-3.41933500	-3.10486700	0.01014000
C	-4.70330300	-2.55469500	-0.11634400
C	-4.83101000	-1.16507100	-0.18868300
C	-3.70561700	-0.33981100	-0.14255000
C	0.03283400	-0.65554200	0.45117100
O	0.03736200	-1.05998600	1.63463500
C	1.02589000	-0.66983300	-0.52367500
C	2.37691000	-1.14594600	-0.34925200
C	3.28320800	-1.10109000	-1.44444300
C	4.59707900	-1.54877400	-1.33653700
C	5.07832200	-2.06672000	-0.12539500
C	4.20350300	-2.12054100	0.96863000
C	2.88585800	-1.67525200	0.86976200
H	-2.05240100	1.29452600	-1.42462200
H	0.76795100	-0.27715000	-1.50320400
H	-1.30375200	-2.73754800	0.14993000
H	-3.29616800	-4.18422700	0.07783600
H	-5.58142000	-3.19580900	-0.14605900
H	-5.81747900	-0.71039700	-0.26418400
H	-3.82798000	0.73882300	-0.15033500
H	2.21808400	-1.72551700	1.72274500
H	4.55535700	-2.51856700	1.92039600
H	6.10497100	-2.41717000	-0.03786500
H	5.25437000	-1.49262000	-2.20410200
H	2.93084100	-0.69995900	-2.39421900
H	-1.29710700	3.48040300	-1.92559300
H	-0.14082800	5.56636000	-1.30307800
H	1.24989200	5.66738000	0.77513900
H	1.43252700	3.63487400	2.21619300
H	0.27362300	1.55519100	1.61564500

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c-**1a-IN(N-C4)**
E (UB+HF - LYP) = -940,506891414 a.u.

C	2.91358900	0.85962500	-1.18201200
C	2.61836000	0.10913500	-0.01109300
C	3.73322200	-0.39701600	0.71583900
C	5.04014000	-0.15720200	0.28260100
C	5.30568600	0.58554400	-0.87359700
C	4.21981000	1.09325600	-1.60236300
N	1.27478500	-0.04977100	0.28660700
C	0.85535900	-0.71524900	1.36139500
O	1.48619200	-1.26673600	2.29655400
C	-0.72294200	-0.79683100	1.45751300
C	-1.30383900	0.57257100	1.66165000
C	-1.73399900	1.53767400	0.71309700
C	-2.32841500	2.75052700	1.17929700
C	-2.79620000	3.72193600	0.30355000
C	-2.68978100	3.53569800	-1.08383300
C	-2.09293000	2.36029600	-1.56819600
C	-1.62089100	1.38269900	-0.70128300
C	-1.39338300	-1.65687500	0.38188800
C	-2.79070800	-1.81118200	0.39994900
C	-3.44420100	-2.64793600	-0.50696000
C	-2.70818900	-3.35966800	-1.46035800
C	-1.31836900	-3.21865200	-1.48849700
C	-0.66863800	-2.37708600	-0.57866900
H	-1.34056900	0.89474900	2.70243200
H	-0.87692800	-1.33582400	2.40102700
H	3.54359900	-0.96984300	1.61467600
H	5.86886700	-0.56097000	0.86505700
H	6.32886200	0.76551900	-1.19904400
H	4.39555800	1.67739300	-2.50569600
H	2.07137600	1.25632900	-1.74423900
H	-2.41310600	2.90715300	2.25363300
H	-3.24340000	4.63290600	0.69823900
H	-3.05248500	4.29571100	-1.77244700
H	-1.98346200	2.21415300	-2.64132800
H	-1.11911400	0.50627600	-1.09139600
H	0.40848300	-2.25704900	-0.62416900
H	-0.73036300	-3.76260900	-2.22549300
H	-3.21185100	-4.01151100	-2.17171000
H	-4.52830600	-2.74162100	-0.47108700
H	-3.37230000	-1.25606400	1.13333800

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t-**1a**

E (RB+HF - LYP) = -940,485595361 a.u.

C	-1.21408100	2.15030700	1.01728300
C	-0.42719600	1.77458600	-0.08136200
C	-0.10641500	2.73967300	-1.04599900
C	-0.55366400	4.05712400	-0.91366900
C	-1.33549500	4.42312800	0.18490200
C	-1.66586000	3.46474000	1.14847900
C	0.12149600	0.37510500	-0.21877600
N	-0.69240100	-0.72880500	0.34048200
C	-1.95316900	-1.22592500	-0.03132700
C	-2.50876100	-2.32698600	0.64480100
C	-3.75717300	-2.81173200	0.25484500
C	-4.46334000	-2.21709800	-0.79607900
C	-3.90556400	-1.12310700	-1.46213400
C	-2.65654600	-0.62504100	-1.08715500
C	1.26323700	-0.05803700	0.78820600
C	0.29262900	-1.18716500	1.19825000
O	0.33497000	-2.13139000	1.95890300
C	2.61000800	-0.43110800	0.22743300
C	2.76503100	-1.53809100	-0.62252000
C	4.01388800	-1.85539000	-1.15847500
C	5.13144700	-1.07253800	-0.85079600
C	4.99035900	0.02737600	-0.00177700
C	3.73820700	0.34323000	0.53264300
H	0.40741300	0.17783800	-1.25872900
H	1.37336900	0.67624400	1.59289400
H	-1.95862500	-2.78986000	1.45604000
H	-4.17968000	-3.66435600	0.78047500
H	-5.43588500	-2.60153000	-1.09099100
H	-4.44246100	-0.64893900	-2.27981000
H	-2.23554600	0.23061500	-1.60573200
H	1.90830100	-2.16658100	-0.85618300
H	4.11627500	-2.71992800	-1.80945100
H	6.10475200	-1.32309400	-1.26474000
H	5.85345900	0.63898600	0.24881300
H	3.63535000	1.19950300	1.19582700
H	0.49786500	2.45845700	-1.90648900
H	-0.29572000	4.79332800	-1.67075300
H	-1.69005600	5.44546400	0.28728300
H	-2.28089100	3.73965800	2.00161900
H	-1.48509700	1.40862700	1.76469600

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t-**1a**[.-]

E (UB+HF - LYP) = -940,4795831 a.u.

C	3.54161800	0.45725500	0.08058900
C	2.57632500	-0.56896800	0.26633100
C	2.91755300	-1.87390600	-0.14373600
C	4.16227500	-2.15367900	-0.70485100
C	5.11125200	-1.12466200	-0.89040700
C	4.78380900	0.17609000	-0.49131200
C	1.23165300	-0.20859200	0.78877700
C	0.21599200	-1.29613100	1.10881400
O	0.21056200	-2.30485500	1.80937300
C	0.08291500	0.36664700	-0.22990500
N	-0.77181500	-0.73454600	0.32019800
C	-2.04898100	-1.16134700	-0.04179300
C	-2.54093100	-2.41114400	0.40129200
C	-3.80611600	-2.83966600	0.00673600
C	-4.60931100	-2.05378700	-0.83402200
C	-4.12035900	-0.81416600	-1.26564900
C	-2.86267800	-0.35923100	-0.87142800
C	-0.37668300	1.76271300	-0.06567600
C	-0.84064600	2.25852100	1.19412200
C	-1.13461800	3.61228400	1.35596800
C	-0.98078100	4.52549900	0.30326900
C	-0.51325800	4.04598100	-0.94955600
C	-0.21509400	2.69823000	-1.11447400
H	0.35495700	0.15742100	-1.27113000
H	1.30598400	0.53444400	1.60383300
H	-1.92032800	-3.01978000	1.04912500
H	-4.16910400	-3.80361700	0.35926800
H	-5.59659000	-2.39552200	-1.13606000
H	-4.73001700	-0.18262800	-1.90932100
H	-2.50725500	0.61607300	-1.18634100
H	2.20085200	-2.67847000	0.00128500
H	4.40344700	-3.17522400	-0.99392000
H	6.08004200	-1.33928200	-1.33674700
H	5.50568100	0.98142900	-0.62396700
H	3.30397300	1.47244900	0.39296500
H	0.15259600	2.34573200	-2.07892100
H	-0.39147300	4.73187600	-1.78642600
H	-1.21268000	5.57886700	0.44299500
H	-1.49678200	3.96306400	2.32237100
H	-1.00871600	1.56617100	2.01608700

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t-**1a-TS(N-C2)**

E (UB+HF - LYP) = -940,454545412 a.u.

1 imaginary frequency -62,73 cm**-1

C	1.80689800	1.82994700	0.92743500
C	0.91909000	1.63175100	-0.13954000
C	0.87897900	2.59411500	-1.15890800
C	1.69217900	3.73107000	-1.11490300
C	2.56871700	3.92146400	-0.04222700
C	2.62227600	2.96352800	0.97677700
C	-0.01846400	0.41781200	-0.17559300
N	0.43239800	-0.77953300	0.48985800
C	1.49627900	-1.49602000	0.06242200
C	1.87837400	-2.66324600	0.80132200
C	2.93835800	-3.46630100	0.40604700
C	3.68922500	-3.17383500	-0.74868200
C	3.33735200	-2.03804400	-1.48748700
C	2.28085500	-1.21116500	-1.10179000
C	-1.31072500	0.68688600	0.65660500
C	-0.85921000	-0.04514100	1.97228500
O	-1.51623300	-0.75216400	2.69459900
C	-2.58507700	0.15109700	0.05400500
C	-2.67657600	-1.17778900	-0.40190100
C	-3.86719000	-1.66711100	-0.93956200
C	-5.00058800	-0.84857500	-1.02685800
C	-4.92750900	0.46856700	-0.56499500
C	-3.73172200	0.95760800	-0.02937200
H	-0.28656600	0.25293200	-1.23741900
H	-1.44988600	1.74999500	0.89130000
H	1.30051700	-2.90352400	1.69102000
H	3.18856500	-4.34333200	1.00388100
H	4.51796100	-3.80861900	-1.05493900
H	3.90248800	-1.78158000	-2.38450200
H	2.05360200	-0.33141600	-1.69754800
H	-1.79996400	-1.81465000	-0.31817900
H	-3.91422700	-2.69756700	-1.28718400
H	-5.92859500	-1.23547100	-1.44347900
H	-5.79968700	1.11784100	-0.62229600
H	-3.68378700	1.98523000	0.32827200
H	0.20353400	2.44623500	-2.00126100
H	1.64612400	4.46302900	-1.91981100
H	3.20850100	4.80121900	-0.00471900
H	3.30795600	3.09723300	1.81164900
H	1.84743800	1.07678200	1.70894100

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t-**1a-TS(C2-C3)**
E (UB+HF - LYP) = -940,452625423 a.u.
1 imaginary frequency -135,21 cm**-1

C	1.12757500	1.93577400	-1.12833000
C	0.34596700	1.54983100	-0.02784300
C	-0.00212500	2.52841500	0.91573500
C	0.40727700	3.85530800	0.76451700
C	1.18017200	4.23071900	-0.34039800
C	1.53692000	3.26247100	-1.28451700
C	-0.17974400	0.12804900	0.11948000
N	0.74385800	-0.89732800	-0.40746800
C	2.04380200	-1.11905400	0.05171500
C	2.93733400	-1.96035900	-0.65669000
C	4.22024600	-2.19786700	-0.16768500
C	4.67071000	-1.60466400	1.01923700
C	3.79501700	-0.76904800	1.72074600
C	2.50173700	-0.53175700	1.25505700
C	-1.43199300	-0.08468800	-0.70879600
C	-2.72332900	-0.35183800	-0.16037100
C	-2.93664600	-0.95708300	1.11836400
C	-4.21440400	-1.23735500	1.59307800
C	-5.35757700	-0.94947600	0.83078700
C	-5.17522700	-0.37682500	-0.44254800
C	-3.90470600	-0.08761200	-0.92152700
C	-0.07941400	-1.77677200	-1.18175600
O	0.36576700	-2.59374000	-1.97381100
H	-0.38820700	-0.04628600	1.18451700
H	-1.42766200	0.45480300	-1.65557400
H	2.59683400	-2.42410800	-1.57407100
H	4.88265900	-2.85390200	-0.73058300
H	5.67870900	-1.78667300	1.38525500
H	4.11866100	-0.29202000	2.64455900
H	1.84710500	0.12401000	1.81910700
H	-2.07913200	-1.22651300	1.73054400
H	-4.32322000	-1.70037000	2.57400700
H	-6.35329000	-1.17168900	1.20800100
H	-6.04217300	-0.15011100	-1.06318300
H	-3.79258100	0.35920800	-1.90884100
H	-0.61106600	2.24469800	1.77246100
H	0.12390300	4.59602500	1.51000200
H	1.50411600	5.26251900	-0.46038300
H	2.14422300	3.53947200	-2.14436800
H	1.41842700	1.18513600	-1.85820100

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t-**1a-TS(C3-C4)**
E (UB+HF - LYP) = -940,479070267 a.u.
1 imaginary frequency -181,62 cm**-1

C	-1.31982500	2.12935800	0.98239300
C	-0.53662800	1.75721900	-0.15456700
C	-0.16767100	2.80690500	-1.04869600
C	-0.56402900	4.11946000	-0.83470400
C	-1.34830200	4.46774200	0.28761600
C	-1.71301900	3.44730600	1.18611000
C	-0.00294800	0.42292500	-0.33512900
N	-0.70609500	-0.72124600	0.26176800
C	-1.97328600	-1.22838500	-0.05327500
C	-2.44797000	-2.41870100	0.53787600
C	-3.70887100	-2.90972100	0.19839700
C	-4.52092700	-2.24244500	-0.72576700
C	-4.04937900	-1.06140700	-1.30777100
C	-2.79319000	-0.55190500	-0.97815400
C	0.31342600	-1.26062600	1.03305600
O	0.32918500	-2.30856600	1.66820400
C	1.34361800	-0.17703400	0.80661300
C	2.67810800	-0.48735000	0.32565500
C	2.96883900	-1.65588400	-0.44014700
C	4.22917300	-1.86820100	-0.98705900
C	5.26683400	-0.93276600	-0.81240900
C	4.99741700	0.23100100	-0.06520500
C	3.74063100	0.45025800	0.48458500
H	0.35896900	0.20911100	-1.34535000
H	1.32063600	0.59225600	1.58491900
H	-1.81612600	-2.94182900	1.24512700
H	-4.05701900	-3.83046100	0.66302400
H	-5.50314200	-2.63252100	-0.98314600
H	-4.66653400	-0.52113900	-2.02294400
H	-2.44317000	0.37574700	-1.41771800
H	2.19408600	-2.40751500	-0.57642100
H	4.41432100	-2.77957700	-1.55510900
H	6.25020600	-1.10316200	-1.24468700
H	5.78301100	0.97051700	0.08798200
H	3.55304400	1.35993800	1.05384900
H	0.44138400	2.56364400	-1.91914200
H	-0.26658000	4.88866300	-1.54694300
H	-1.65980700	5.49622600	0.45374000
H	-2.31937400	3.68936600	2.05883200
H	-1.62673400	1.36148400	1.68946600

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S37

t-**1a-TS(N-C4)**
E (UB+HF - LYP) = -940,475955448 a.u.
1 imaginary frequency -386,31 cm**-1

C	-0.45418500	2.48192900	1.22633800
C	-0.26148800	1.84190100	-0.04706900
C	-0.55339800	2.62385800	-1.20462900
C	-0.95457600	3.94637700	-1.11659000
C	-1.10378200	4.57556000	0.15034100
C	-0.85420600	3.81276000	1.30429700
C	0.17160600	0.46221400	-0.16986700
N	-0.81882200	-0.76342800	0.44911500
C	-2.05915600	-1.26760300	0.08489400
C	-2.28123500	-2.65256500	-0.10962600
C	-3.52306600	-3.10943400	-0.54353400
C	-4.56998300	-2.21133100	-0.81347300
C	-4.35042100	-0.83946200	-0.62342000
C	-3.12045800	-0.36531000	-0.17090500
C	1.21349300	-0.17602500	0.80759700
C	0.22676300	-1.30693900	1.12812900
O	0.33053500	-2.35213100	1.77356600
C	2.56495900	-0.51001100	0.22887700
C	3.04810100	-1.82315000	0.14473000
C	4.30053800	-2.08947100	-0.42279500
C	5.08878300	-1.04459500	-0.91999500
C	4.61798600	0.26956100	-0.83645100
C	3.37164300	0.53698500	-0.26149600
H	0.35868000	0.17376400	-1.20704600
H	1.34033000	0.47849000	1.68289400
H	-1.47879800	-3.34946600	0.11058500
H	-3.68021400	-4.17974300	-0.67100300
H	-5.53579100	-2.57493800	-1.15740900
H	-5.15196300	-0.12925200	-0.82054700
H	-2.95870500	0.69640900	-0.01036800
H	2.44252700	-2.63399200	0.53850800
H	4.65830400	-3.11597100	-0.47609800
H	6.06083000	-1.25210100	-1.36347700
H	5.22308400	1.09071500	-1.21664400
H	3.00966600	1.56039100	-0.19337300
H	-0.44152600	2.16161000	-2.18592900
H	-1.15536100	4.50752200	-2.02859000
H	-1.42111600	5.61304400	0.22406700
H	-0.98571500	4.26705300	2.28676100
H	-0.30424900	1.91601200	2.14320100

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t-**1a-IN(N-C2)**
E (UB+HF - LYP) = -940,4558007 a.u.

C	-2.12647400	-1.63727000	0.82789000
C	-1.16770100	-1.52870900	-0.18742000
C	-1.20483000	-2.45730500	-1.23853500
C	-2.16127300	-3.47647600	-1.27317800
C	-3.10772000	-3.58006000	-0.24829700
C	-3.08605100	-2.65341100	0.79961100
C	-0.08665800	-0.42961800	-0.14784200
N	-0.37900300	0.71807700	0.66151700
C	-1.26479000	1.62887300	0.20265300
C	-1.52275300	2.79051800	1.00905500
C	-2.39188500	3.79405900	0.60915100
C	-3.07421700	3.72615200	-0.62205600
C	-2.85162200	2.60289800	-1.42738700
C	-1.98680700	1.57797000	-1.03883400
C	1.23709200	-1.02189400	0.43580500
C	1.06077700	-0.97700000	1.97312800
O	1.85931000	-0.69273700	2.81316700
C	2.50402700	-0.34702500	-0.04704400
C	2.67366100	1.04584800	0.04229700
C	3.84894400	1.64625000	-0.41260500
C	4.88405500	0.87287400	-0.95151700
C	4.73111600	-0.51387000	-1.03278600
C	3.55064800	-1.11373900	-0.58270300
H	0.12785400	-0.17772600	-1.20868400
H	1.30419000	-2.09341400	0.19901400
H	-0.99857600	2.85703000	1.96082400
H	-2.54570100	4.65311900	1.26372000
H	-3.75594400	4.51549300	-0.93192900
H	-3.37288900	2.51364500	-2.38189600
H	-1.87032000	0.71838500	-1.69297800
H	1.86046800	1.63289700	0.46002800
H	3.95850700	2.72681700	-0.34347900
H	5.79981000	1.34601000	-1.30092100
H	5.52682500	-1.12974400	-1.44831900
H	3.43808900	-2.19491600	-0.65235100
H	-0.47772800	-2.37378400	-2.04667100
H	-2.17315900	-4.18299600	-2.10184200
H	-3.85874900	-4.36764200	-0.27165000
H	-3.82453000	-2.71867400	1.59685000
H	-2.10483900	-0.90351600	1.62799400

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t-**1a-IN(C2-C3)**

E (UB+HF - LYP) = -940,455254169 a.u.

C	3.92521000	0.57120400	0.55568500
C	2.65274400	0.11670100	0.07798000
C	2.70264500	-0.94343600	-0.88465000
C	3.90962800	-1.46909600	-1.33562400
C	5.14098500	-0.99408100	-0.85776700
C	5.12194800	0.03419800	0.10323000
C	1.45032900	0.68968500	0.57232600
C	0.10427700	0.46860700	-0.05933000
N	-0.55728600	-0.65008300	0.66933500
C	0.06997200	-0.80662400	1.92738100
O	-0.17424400	-1.73038300	2.69084100
C	-0.70593800	1.76166300	-0.06894600
C	-1.49497900	2.14734100	1.02412800
C	-2.17785000	3.36798800	1.01839300
C	-2.09156700	4.22326700	-0.08382500
C	-1.31107200	3.84522900	-1.18330600
C	-0.62741100	2.62780200	-1.17101000
C	-1.59617500	-1.41446500	0.10881700
C	-1.97434900	-2.66849100	0.64663300
C	-2.99475300	-3.41290600	0.05686100
C	-3.66907100	-2.95464100	-1.08130600
C	-3.30231500	-1.71804700	-1.61789600
C	-2.28970900	-0.95379800	-1.03474500
H	0.22129600	0.14410800	-1.10341200
H	1.54128300	1.54230100	1.23782300
H	-1.45780200	-3.03613300	1.52297700
H	-3.26070500	-4.37363100	0.49493100
H	-4.46053400	-3.54621800	-1.53623700
H	-3.81175600	-1.33163000	-2.49919100
H	-2.05007100	0.01294200	-1.46176800
H	1.77451300	-1.36787900	-1.26045000
H	3.89107400	-2.27658500	-2.06778300
H	6.07984500	-1.41508100	-1.21047500
H	6.06096200	0.42070600	0.50010500
H	3.94044400	1.36804600	1.29839400
H	-0.01269300	2.34351700	-2.02373300
H	-1.23505800	4.49931300	-2.05007000
H	-2.62762900	5.17020500	-0.08969600
H	-2.78357800	3.64846500	1.87819900
H	-1.56993400	1.48258600	1.88013200

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t-**1a-IN(C3-C4)**

E (UB+HF - LYP) = -940,506038993 a.u.

C	3.47384000	-0.53017900	0.57417000
C	2.51648000	-1.37431700	-0.06646100
C	3.00536100	-2.61064000	-0.59034100
C	4.34329900	-2.96650400	-0.49916100
C	5.27117900	-2.11220900	0.12329200
C	4.81159700	-0.90040700	0.66149100
C	1.12195200	-1.10150500	-0.17514600
N	0.43103400	0.03696600	0.14354800
C	0.87949400	1.35431900	-0.01584100
C	0.32744300	2.38809400	0.77310600
C	0.72732700	3.70894700	0.58422200
C	1.68597600	4.04328900	-0.38159100
C	2.23288600	3.02264600	-1.16709300
C	1.83801100	1.69641100	-0.99467700
C	-1.00122200	-0.17109500	0.63732200
O	-1.13032000	-0.25175400	1.87667700
C	-1.91960600	-0.23867500	-0.40262300
C	-3.34162200	-0.45717300	-0.26619700
C	-4.00073100	-0.64202500	0.98061200
C	-5.37828300	-0.84906600	1.04519100
C	-6.16818400	-0.88239800	-0.11240200
C	-5.53826300	-0.70227900	-1.35201100
C	-4.16281000	-0.49587500	-1.42585600
H	0.47119800	-1.93530400	-0.42714500
H	-1.53761000	-0.10541500	-1.41167800
H	-0.40381600	2.13244500	1.53255000
H	0.28677000	4.48690400	1.20496300
H	1.99695400	5.07622900	-0.52047300
H	2.96949200	3.25939500	-1.93298000
H	2.25538400	0.91771500	-1.62435300
H	-3.40169500	-0.61773300	1.88450000
H	-5.84555200	-0.98694800	2.02020600
H	-7.24275200	-1.04362600	-0.05133500
H	-6.12611000	-0.72258700	-2.26955700
H	-3.69415400	-0.35703000	-2.39978100
H	2.29944300	-3.28516600	-1.07204700
H	4.67303200	-3.91847900	-0.91236800
H	6.32055700	-2.38860700	0.19354500
H	5.51042000	-0.23470700	1.16575000
H	3.14901500	0.40205900	1.02191400

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t-**1a-IN(N-C4)**

E (UB+HF - LYP) = -940,51487288 a.u.

C	-3.08058500	-1.71440300	-1.47738600
C	-2.46592100	-1.09253600	-0.34533700
C	-2.86678400	-1.57142800	0.94085000
C	-3.81908400	-2.57522700	1.07068900
C	-4.41843200	-3.15643100	-0.05814700
C	-4.03184200	-2.71433500	-1.33524300
C	-1.51538400	-0.06053400	-0.53783100
C	-0.81435400	0.70207300	0.53930200
C	-0.64143400	2.17048400	0.17189100
C	0.17896600	2.57330100	-0.89611100
C	0.31419800	3.92416000	-1.22329600
C	-0.36391800	4.90566600	-0.49074500
C	-1.17685000	4.51849400	0.57766600
C	-1.31182200	3.16423600	0.90138600
C	0.56984300	0.01516000	0.90606600
O	0.78038100	-0.16660100	2.12670700
N	1.29814900	-0.27299700	-0.17429000
C	2.55812900	-0.84301400	-0.08632500
C	3.20120900	-1.13004900	-1.32102400
C	4.47075200	-1.69793600	-1.38143100
C	5.16947100	-2.00850000	-0.20562900
C	4.55669900	-1.73476300	1.02272100
C	3.28216000	-1.16684300	1.09560600
H	-1.22281500	0.15890200	-1.56154900
H	-1.39270500	0.66467300	1.46628300
H	2.82037100	-0.96393000	2.05349500
H	5.08109500	-1.96867900	1.94960300
H	6.16294900	-2.45153100	-0.24772400
H	4.92148000	-1.90125700	-2.35283200
H	2.65790700	-0.89104100	-2.23280500
H	0.73222000	1.80955800	-1.43530100
H	0.96117900	4.21341600	-2.04965200
H	-0.25398100	5.95803500	-0.74576600
H	-1.70503000	5.26897000	1.16338700
H	-1.94465400	2.87160000	1.73719700
H	-2.78525700	-1.38427700	-2.47150500
H	-4.47794600	-3.16162600	-2.22204600
H	-5.16111800	-3.94304700	0.05332400
H	-4.09430900	-2.92075800	2.06570600
H	-2.39958100	-1.16068900	1.83053800

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c-**1b**

E (RB+HF - LYP) = -826,12574919 a.u.

C	0.81961600	1.41020100	1.06358200
C	1.00945300	1.07529500	-0.28428600
C	1.76272000	1.93781000	-1.09330100
C	2.32987500	3.10052400	-0.56632100
C	2.14125100	3.42227300	0.78068600
C	1.38141800	2.57491900	1.59223600
C	0.44953400	-0.19413000	-0.88359800
N	-0.73648800	-0.77681000	-0.21997100
C	-2.06429700	-0.32244600	-0.15023700
C	-3.05292300	-1.11190500	0.46472000
C	-4.36806900	-0.64965600	0.51244200
C	-4.71644800	0.58729600	-0.04005800
C	-3.72893000	1.36715200	-0.64695600
C	-2.40737700	0.92106200	-0.70453300
C	1.18961200	-1.56558100	-0.58919900
C	-0.13598900	-1.99364800	0.06824000
O	-0.55328100	-2.99574300	0.61186000
C	2.44110200	-1.59094200	0.24751300
H	0.27779600	-0.04885700	-1.95806600
H	1.34835500	-2.12762800	-1.51851400
H	-2.78253400	-2.07208900	0.88886000
H	-5.12712700	-1.26655700	0.98691500
H	-5.74368900	0.93877600	0.00347300
H	-3.98278400	2.33216300	-1.07833200
H	-1.64537800	1.53972400	-1.16806800
H	1.90658800	1.69765100	-2.14534300
H	2.91176800	3.75674100	-1.20869500
H	2.57550500	4.32973400	1.19225100
H	1.21935300	2.82272100	2.63823800
H	0.21814200	0.76480800	1.69836300
C	3.29390200	-2.83927500	0.26758500
C	3.80065800	-1.59412200	-0.41890600
H	2.37458700	-1.04743200	1.18719600
H	3.83540600	-1.58873500	-1.50629700
H	4.59988300	-1.02818900	0.05220600
H	3.74297200	-3.13041800	1.21321300
H	2.98216900	-3.67775600	-0.35014000

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c-**1b**·⁻

E (UB+HF - LYP) = -826,11301126 a.u.

C	-2.43485600	0.93428100	-0.72366900
C	-2.08001700	-0.31460700	-0.15249700
C	-3.10627500	-1.11105000	0.43290500
C	-4.42681200	-0.67682500	0.39394400
C	-4.78647400	0.54223300	-0.20730200
C	-3.76292300	1.34356300	-0.75434400
N	-0.76036500	-0.74167100	-0.13902800
C	-0.11483000	-1.90507600	0.28437700
O	-0.52249800	-2.88557300	0.91164800
C	0.43378400	-0.20024100	-0.82061900
C	1.15390700	-1.56448500	-0.49389900
C	2.49626500	-1.57100400	0.19527500
C	3.77004800	-1.70672100	-0.61023300
C	3.29699800	-2.85109400	0.25700200
C	1.01786700	1.06327700	-0.25273900
C	0.60250600	1.61449100	0.96613700
C	1.18292400	2.78440000	1.46762300
C	2.22520000	3.41914000	0.75480300
C	2.63448500	2.88702800	-0.46936700
C	2.03607100	1.73024300	-0.98285700
H	0.26262100	-0.08246500	-1.90783700
H	1.21997200	-2.19612700	-1.41005500
H	-2.83826100	-2.05520900	0.89396000
H	-5.19660800	-1.30615200	0.83978900
H	-5.82339600	0.86849700	-0.23211300
H	-4.00717400	2.30180900	-1.21033500
H	-1.66093800	1.57308000	-1.13972700
H	2.36289100	1.32520100	-1.93913400
H	3.42735700	3.37542700	-1.03551900
H	2.69434700	4.31880000	1.14864700
H	0.83696600	3.19417500	2.41424700
H	-0.19318700	1.12671200	1.52337600
H	2.55853900	-0.92822800	1.07001500
H	3.67366600	-1.81258800	-1.68982200
H	4.63786800	-1.13360700	-0.29171400
H	3.84166500	-3.07068600	1.17291700
H	2.87901100	-3.72767900	-0.23391000

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c-**1b-TS(N-C2)**
E (UB+HF - LYP) = -826,09123891 a.u.
1 imaginary frequency -71,82 cm**-1

C	0.49831200	1.38171300	1.24816400
C	0.70323300	1.06449100	-0.10313100
C	1.25414100	2.04675100	-0.93776400
C	1.60610600	3.30713700	-0.44304300
C	1.40599900	3.60776900	0.90748300
C	0.84801400	2.63797900	1.74914000
C	0.35037900	-0.32445500	-0.64615300
N	-0.76159800	-0.98942500	-0.01381300
C	-2.04340500	-0.59298500	-0.15005500
C	-3.07124500	-1.33500600	0.52053600
C	-4.41193600	-0.99963000	0.40199200
C	-4.83097300	0.08828400	-0.38856100
C	-3.84619300	0.83141300	-1.05069700
C	-2.49089800	0.51694400	-0.93933100
C	1.41919700	-1.41610300	-0.33366600
C	0.74087700	-2.02937200	0.91726900
O	0.67320800	-3.20655800	1.20393600
C	2.86234100	-1.01902100	-0.11069100
H	0.23222200	-0.21870900	-1.74235100
H	1.37815200	-2.16954500	-1.13938700
H	-2.76134100	-2.18344200	1.12626800
H	-5.15422100	-1.59758900	0.93208500
H	-5.88441300	0.34521800	-0.47768600
H	-4.13663500	1.68476400	-1.66528500
H	-1.75972800	1.13264400	-1.45585600
H	1.40527500	1.82097700	-1.99307800
H	2.02925300	4.05438800	-1.11278000
H	1.67203700	4.58846800	1.29781700
H	0.67802900	2.86485400	2.80028200
H	0.05474900	0.62601200	1.89024000
C	3.95354800	-2.05834600	-0.22174800
C	3.83501400	-0.97286800	-1.26999000
H	3.01102500	-0.26257900	0.65707300
H	3.46311200	-1.25278500	-2.25392500
H	4.58253900	-0.18206000	-1.28568400
H	4.78357200	-2.01101200	0.48023400
H	3.65683600	-3.06934400	-0.49129200

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c-**1b-TS(C3-C4)**
E (UB+HF - LYP) = -826,09548299 a.u.
1 imaginary frequency -371,38 cm**-1

C	1.81160400	1.98860700	-1.22568300
C	0.98292200	1.13357200	-0.42095300
C	0.87227200	1.49066000	0.96656100
C	1.53219600	2.59550600	1.48597600
C	2.35039600	3.41585000	0.67879800
C	2.46860400	3.08520200	-0.69180100
C	0.39840200	-0.04186100	-0.99343200
N	-0.70087400	-0.73682800	-0.32318700
C	-0.23368200	-2.05139100	-0.25783600
C	1.18125700	-1.87630200	-0.68547100
C	2.27000500	-1.72842400	0.32461300
C	3.05539700	-2.92561900	0.84654000
C	3.71213700	-1.92548400	-0.08229500
C	-2.00276000	-0.25246400	-0.13389200
C	-2.31197600	1.08964800	-0.44719300
C	-3.61077800	1.57170300	-0.28192600
C	-4.62857900	0.74982500	0.21298200
C	-4.31832300	-0.57637800	0.54193900
C	-3.02933000	-1.08115000	0.37304400
O	-0.88812200	-3.07144800	-0.02490100
H	0.28871000	-0.02503200	-2.08074500
H	1.45508000	-2.56412500	-1.50014400
H	-2.80011100	-2.11257400	0.60886400
H	-5.09295800	-1.23522000	0.93137300
H	-5.63724200	1.13462000	0.34778400
H	-3.82170800	2.60966500	-0.53354000
H	-1.52590400	1.74408700	-0.80621700
H	1.92332500	1.75850600	-2.28576400
H	3.08497000	3.70434000	-1.34453100
H	2.86518900	4.27880700	1.09448700
H	1.40798900	2.83402500	2.54275900
H	0.23996900	0.88952900	1.61677600
H	2.10810700	-0.93726700	1.05435200
H	3.90424700	-2.23472600	-1.10856600
H	4.46020500	-1.24708400	0.32247700
H	3.35472000	-2.93278000	1.89452100
H	2.79792800	-3.90438200	0.44782100

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c-**1b-TS(N-C4)**

E (UB+HF - LYP) = -826,10879020 a.u.

1 imaginary frequency -320,04 cm**-1

C	2.35759300	1.02514600	-0.38005000
C	2.08941200	-0.32803500	-0.04559800
C	3.17780700	-1.17621000	0.27888300
C	4.47951800	-0.68532900	0.27016600
C	4.74216100	0.66356300	-0.04091700
C	3.66656800	1.50363400	-0.36503400
N	0.77149900	-0.75661800	0.02845100
C	0.20004300	-1.98145800	-0.14088100
O	0.63649800	-3.03449300	-0.60656800
C	-0.58698900	-0.19064200	0.85825500
C	-1.14043500	-1.61399800	0.51895300
C	-2.39368300	-1.76374200	-0.31041000
C	-3.74332000	-1.84392000	0.36286200
C	-3.14844300	-3.07320100	-0.29015100
C	-1.15553000	1.07157100	0.39665000
C	-1.46333600	1.34331200	-0.98080600
C	-1.98563700	2.57277600	-1.36989500
C	-2.22202200	3.60158400	-0.44088300
C	-1.86964500	3.37030300	0.91682200
C	-1.34888800	2.14820900	1.31114200
H	-0.30404500	-0.12606900	1.91448700
H	-1.27023800	-2.19671000	1.44499400
H	2.98113900	-2.22023100	0.50479800
H	5.30383900	-1.35861800	0.50318600
H	5.76145300	1.04375900	-0.03810500
H	3.85161800	2.54659200	-0.61906800
H	1.52930600	1.67522800	-0.64661900
H	-1.08624400	1.99234700	2.35831400
H	-2.00918000	4.15751600	1.65706100
H	-2.63896300	4.55528900	-0.75609400
H	-2.20688900	2.74076200	-2.42451300
H	-1.25112300	0.59161200	-1.73662600
H	-2.38242900	-1.24458500	-1.26475800
H	-3.76599900	-1.79923300	1.44995300
H	-4.58543200	-1.35101500	-0.11751800
H	-3.58295100	-3.43024700	-1.22142700
H	-2.76737700	-3.86551600	0.35067900

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c-**1b-IN(N-C2)**

E (UB+HF - LYP) = -826,09340132 a.u.

C	-2.47805000	0.20462800	-1.01261900
C	-2.06316100	-0.73051200	-0.00033000
C	-3.14020600	-1.39705300	0.68332000
C	-4.47183000	-1.16965300	0.37426500
C	-4.84839900	-0.26097900	-0.63649900
C	-3.82542700	0.41423500	-1.31320900
N	-0.79887100	-1.04226500	0.34587500
C	0.28605600	-0.41505200	-0.35633200
C	1.50256200	-1.34391600	-0.07947600
C	2.87337300	-0.84310100	-0.50621500
C	3.34399200	-1.06384900	-1.92664100
C	3.98725300	-1.82447500	-0.78722000
C	0.57008000	1.04564100	0.03790200
C	0.34840400	1.48888800	1.35037100
C	0.61844300	2.80966000	1.71713000
C	1.10691300	3.72229800	0.77485400
C	1.31769800	3.29857100	-0.54056500
C	1.04960100	1.97290600	-0.89887500
C	1.53069500	-1.66062200	1.42435300
O	1.82538100	-2.69857200	1.93980400
H	0.15401400	-0.41223600	-1.46043900
H	1.29148800	-2.29764300	-0.58680700
H	-2.86406500	-2.10713500	1.46079500
H	-5.24248100	-1.70962600	0.92685100
H	-5.89537300	-0.08462300	-0.87490200
H	-4.08066900	1.13541600	-2.09190500
H	-1.72974100	0.77886400	-1.55199100
H	1.20616100	1.65176400	-1.92834100
H	1.68156400	4.00054000	-1.28964600
H	1.30790600	4.75368800	1.05941400
H	0.43743300	3.13212000	2.74120600
H	-0.05642600	0.77935100	2.06574600
H	3.17442400	0.09812500	-0.05175900
H	2.68451800	-1.61011300	-2.59769300
H	3.91222700	-0.27096700	-2.40887300
H	4.99865700	-1.55517300	-0.49008700
H	3.76141300	-2.88360900	-0.68641700

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c-**1b-IN(C3-C4)**

E (UB+HF - LYP) = -826,12711379 a.u.

C	2.61218200	-1.79208500	-0.25236500
C	2.08467400	-0.50296800	-0.00865200
C	2.99846500	0.55486100	0.21491000
C	4.36940700	0.32701100	0.16538000
C	4.88707100	-0.94895800	-0.10598300
C	3.99162000	-2.00255200	-0.30913400
N	0.70987200	-0.26728400	-0.00007800
C	0.20413800	1.03798600	0.59549500
O	0.41430100	1.20336100	1.82668200
C	-0.14742200	-1.13868300	-0.62866000
C	-1.48753000	-1.43946100	-0.25345000
C	-2.09178600	-1.02075000	0.97084300
C	-3.39416900	-1.39115300	1.28164800
C	-4.15990200	-2.18516700	0.41040700
C	-3.58138500	-2.61048700	-0.79627800
C	-2.27963400	-2.24802500	-1.12157700
C	-0.39229100	1.85427000	-0.33877100
C	-0.97620100	3.16304900	0.03436500
C	-2.27364300	3.66628400	-0.58510500
C	-0.96318100	4.34710000	-0.92027900
H	0.26684900	-1.67599000	-1.48202000
H	-0.46851700	1.52271900	-1.37167800
H	2.61195900	1.54387800	0.43151800
H	5.04761500	1.16059800	0.34037900
H	5.96125700	-1.11652300	-0.14394900
H	4.36552700	-3.00810000	-0.49675100
H	1.93518600	-2.63358500	-0.36148300
H	-1.84751700	-2.58028500	-2.06485000
H	-4.15443400	-3.22750000	-1.48733300
H	-5.17988100	-2.46446600	0.66540100
H	-3.82509200	-1.05647300	2.22409200
H	-1.51868500	-0.41251100	1.66396700
H	-0.83836600	3.40914800	1.08544900
H	-2.73470600	3.03936500	-1.34633500
H	-2.98754500	4.19551100	0.04598300
H	-0.77891900	5.34486200	-0.52155300
H	-0.54071700	4.18183300	-1.91050200

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c-1b-IN(N-C4)

E (UB+HF - LYP) = -826,15458048 a.u.

C	3.27192700	-1.15481000	-1.41635200
C	2.54808900	-0.45878000	-0.39779400
C	2.89280100	-0.76536100	0.95586300
C	3.89853000	-1.67775800	1.25129600
C	4.60826000	-2.33139600	0.23078200
C	4.27674000	-2.06100600	-1.10822300
C	1.54914200	0.48134400	-0.75032300
C	0.75044700	1.31658700	0.19447700
C	0.37416000	2.65703500	-0.42474700
C	0.11124700	3.84968900	0.45735500
C	1.35191900	3.81104800	-0.41602000
C	-0.53756200	0.52962600	0.65474600
O	-0.58999700	0.20523500	1.86622600
N	-1.38423000	0.31790200	-0.35607500
C	-2.59533000	-0.32919400	-0.18798300
C	-3.38882300	-0.48643600	-1.35797500
C	-4.63087700	-1.11447800	-1.33336300
C	-5.15189600	-1.61951200	-0.13257800
C	-4.39014600	-1.47549300	1.03322900
C	-3.14154200	-0.84852700	1.02079900
H	1.28961700	0.55728400	-1.80497800
H	1.31856500	1.50409200	1.11325600
H	-2.56253400	-0.74696600	1.92992600
H	-4.77483000	-1.86082900	1.97809100
H	-6.12321500	-2.11067200	-0.10850400
H	-5.20073800	-1.21220800	-2.25763000
H	-2.98420000	-0.09464600	-2.28875600
H	3.01965500	-0.95782700	-2.45681600
H	4.80788900	-2.56888600	-1.91179500
H	5.39278300	-3.04497100	0.47239400
H	4.12858800	-1.89569900	2.29287800
H	2.33072100	-0.30327700	1.76152900
H	-0.26639200	2.55869600	-1.29834500
H	2.31323400	3.65702200	0.07141900
H	1.39645300	4.46811900	-1.28336100
H	-0.69479600	4.52774700	0.18380100
H	0.23625300	3.72037000	1.53049400

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t-**1b**
E (RB+HF - LYP) = -826,12775306 a.u.

C	0.57811300	1.80374300	1.17650800
C	0.93385100	1.31054400	-0.08737800
C	1.60535900	2.15803400	-0.97925900
C	1.92913000	3.46779100	-0.61434400
C	1.57485800	3.94924900	0.64843300
C	0.89562800	3.11364700	1.54093400
C	0.65409500	-0.11975400	-0.48471900
N	-0.55542000	-0.75447100	0.08871400
C	-1.91995500	-0.48420600	-0.10670800
C	-2.89616400	-1.27997800	0.51984000
C	-4.24649900	-1.00242600	0.30803400
C	-4.64257300	0.05646700	-0.51574900
C	-3.66756500	0.84364700	-1.13334300
C	-2.31105900	0.58048200	-0.93397000
C	1.49227900	-1.25015100	0.22527900
C	0.12939100	-1.79736800	0.69360200
O	-0.25128100	-2.76339600	1.32285500
C	2.33068500	-2.15429900	-0.64096800
H	0.68108300	-0.22084300	-1.57720300
H	2.08094700	-0.85517300	1.06169700
H	-2.58788900	-2.10328800	1.15392200
H	-4.99530100	-1.62335300	0.79343300
H	-5.69723200	0.26525200	-0.67314400
H	-3.95893000	1.67170600	-1.77460500
H	-1.56114000	1.20401200	-1.41051400
H	1.87779600	1.78959300	-1.96667700
H	2.45099800	4.11121400	-1.31823900
H	1.81963400	4.96919600	0.93337100
H	0.60798300	3.48390300	2.52171500
H	0.03889000	1.16506600	1.87181900
C	3.40664900	-3.01289800	-0.01872800
C	3.79245200	-1.83706600	-0.88364800
H	1.79170900	-2.60036800	-1.47645200
H	4.20062000	-2.03299300	-1.87184400
H	4.21012600	-0.95911000	-0.39623200
H	3.56022600	-2.93319800	1.05457600
H	3.54660300	-4.01590400	-0.41235900

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t-**1b·⁻**

E (UB+HF - LYP) = -826,11241438 a.u.

C	-2.29559600	0.59614700	-1.03888300
C	-1.91909200	-0.39480300	-0.09809100
C	-2.94743000	-1.10525100	0.59359800
C	-4.28278200	-0.82986600	0.31397000
C	-4.65918100	0.13713900	-0.63241000
C	-3.63603100	0.85108200	-1.30154200
N	-0.58297700	-0.67965800	0.14194800
C	0.10354500	-1.64482700	0.88066600
O	-0.28266500	-2.51992600	1.66355500
C	0.63943900	-0.12592800	-0.47063600
C	1.45055300	-1.25491200	0.26413700
C	2.10655200	-2.31588000	-0.60104000
C	3.54579200	-2.15973400	-1.04146500
C	3.17303900	-3.20976500	-0.01833000
C	0.99557000	1.29069600	-0.10450500
C	0.40255900	1.95199400	0.97018300
C	0.80053700	3.25427600	1.32838500
C	1.82693300	3.89613900	0.59821900
C	2.43282100	3.23899000	-0.46827400
C	2.02709000	1.93845800	-0.83239700
H	0.64248400	-0.25205900	-1.56675800
H	2.19420300	-0.84773200	0.96732800
H	-2.66814400	-1.85834200	1.32206600
H	-5.05202400	-1.38592200	0.84990600
H	-5.70738100	0.34235900	-0.83604700
H	-3.89347100	1.61826600	-2.03020200
H	-1.52597200	1.17050400	-1.54810500
H	2.48962700	1.43515900	-1.67973000
H	3.22657200	3.73101300	-1.02953500
H	2.14147400	4.90320400	0.86831300
H	0.31542300	3.76072700	2.15956100
H	-0.38836300	1.45573700	1.52647000
H	1.43420800	-2.78528300	-1.31950500
H	3.81945700	-2.48489800	-2.04324200
H	4.08047500	-1.27582300	-0.69580200
H	3.45764700	-3.03712500	1.01816000
H	3.19003300	-4.25650200	-0.31445700

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t-**1b-TS(N-C2)**
E (UB+HF - LYP) = -826,09149440 a.u.
1 imaginary frequency -85,34 cm**-1

C	-2.30458200	0.00284000	-1.02682200
C	-1.70193000	-0.86856700	-0.06191300
C	-2.59306700	-1.76635900	0.61252100
C	-3.95266100	-1.78974900	0.33784000
C	-4.52344400	-0.93264000	-0.62308400
C	-3.67375700	-0.04441200	-1.29367500
N	-0.38539300	-0.91644100	0.23146700
C	0.60370000	-0.05946800	-0.37906200
C	1.85647800	-0.72953600	0.25481700
C	2.49353500	-1.77191200	-0.64449100
C	3.59527100	-1.39073900	-1.61300200
C	3.90160800	-2.24531300	-0.39889700
C	0.52265400	1.43616400	-0.05662500
C	0.06528200	1.88098000	1.19290600
C	0.03780000	3.24302500	1.50112800
C	0.46396800	4.19211600	0.56430100
C	0.91412100	3.76213900	-0.68744700
C	0.93892100	2.39641100	-0.98991600
C	1.13793700	-1.33524000	1.49605600
O	1.32184200	-2.43089600	1.98871800
H	0.63707900	-0.15244900	-1.48220700
H	-2.16192900	-2.43928200	1.35007700
H	-4.58834000	-2.49199700	0.87840000
H	-5.59035700	-0.95768200	-0.83468800
H	-4.08575300	0.63657300	-2.03974000
H	-1.68438800	0.71912500	-1.55859900
H	1.28166900	2.06803100	-1.97102700
H	1.23861800	4.48870000	-1.43097200
H	0.43658800	5.25352200	0.80405900
H	-0.32400200	3.56706200	2.47546400
H	-0.27074200	1.13767300	1.91047100
H	3.61174300	-1.85931200	-2.59563300
H	3.94006400	-0.35783200	-1.61034000
H	4.45178500	-1.78855800	0.42156700
H	4.12557500	-3.29971200	-0.54641100
H	2.62411900	-0.01131800	0.58006800
H	1.79028900	-2.52873800	-0.98831400

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t-**1b-TS(C3-C4)**
E (UB+HF - LYP) = -826,10011038 a.u.
1 imaginary frequency -337,49 cm**-1

C	-2.42492300	0.73841000	-0.63642100
C	-1.95142600	-0.47457900	-0.08505400
C	-2.89740100	-1.41394300	0.38977900
C	-4.26120300	-1.14092100	0.30288100
C	-4.73035800	0.05625000	-0.25730700
C	-3.79484400	0.98580700	-0.72475700
N	-0.58168400	-0.72932800	-0.00781200
C	0.09810800	-1.90729400	0.34498400
O	-0.38044900	-3.02724700	0.56672500
C	0.50542300	0.02866800	-0.63036000
C	0.80148800	1.37671100	-0.22638300
C	0.53555300	1.87031000	1.09465100
C	0.96275500	3.13057200	1.49348700
C	1.68887800	3.97257500	0.62620600
C	1.98340200	3.49224400	-0.67272500
C	1.55829600	2.23876600	-1.08482300
C	1.48642400	-1.43425400	0.19984100
C	2.51435100	-2.35792300	-0.36054700
C	3.88559000	-1.82755100	-0.73894900
C	3.74950200	-2.76465700	0.43689700
H	0.58533900	-0.16068300	-1.70444500
H	1.85969900	-0.81862600	1.02470000
H	-2.54164600	-2.35088000	0.80049000
H	-4.96912800	-1.88093600	0.67342200
H	-5.79700700	0.26095200	-0.31984900
H	-4.13126800	1.92766900	-1.15525900
H	-1.71077000	1.47994900	-0.97668600
H	1.79532100	1.89535600	-2.09245200
H	2.54530900	4.11851300	-1.36604100
H	2.01707600	4.95858500	0.94660400
H	0.72284600	3.47479800	2.49992500
H	-0.03635200	1.25152400	1.78321400
H	2.11502300	-3.13540200	-1.01076100
H	4.35288200	-2.20181200	-1.64875100
H	4.08266500	-0.77641700	-0.53708000
H	3.85200000	-2.34886800	1.43725400
H	4.11570200	-3.78558900	0.33819800

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t-**1b-TS(N-C4)**

E (UB+HF - LYP) = -826,11327938 a.u.

1 imaginary frequency -171,38 cm**-1

C	-2.39899500	1.00397000	0.14549300
C	-2.00860200	-0.36097800	0.10789900
C	-2.99117000	-1.34513400	-0.16176200
C	-4.31282600	-0.97482400	-0.38883000
C	-4.69631600	0.38223300	-0.37714800
C	-3.72323900	1.35658400	-0.10771900
N	-0.66661000	-0.68832700	0.26222700
C	-0.03062500	-1.80813800	0.71695500
O	-0.44496100	-2.82225600	1.27816700
C	0.68489900	-0.13580000	-0.46215200
C	1.35674800	-1.36324400	0.22633600
C	2.11328600	-2.33074600	-0.65065000
C	3.59589900	-2.14773600	-0.89235400
C	3.10181300	-3.29737400	-0.04182800
C	1.12392400	1.23206100	-0.17922500
C	1.44797800	1.67033500	1.15187200
C	1.88329600	2.97275100	1.38475900
C	2.01222300	3.90478900	0.34144100
C	1.66269000	3.49363200	-0.97758100
C	1.22866000	2.19869500	-1.21652200
H	0.55130200	-0.29730000	-1.53785800
H	1.99526700	-1.04157700	1.06183500
H	-2.70112600	-2.39181000	-0.15982900
H	-5.05767100	-1.74795500	-0.57405700
H	-5.72956400	0.66724200	-0.56289300
H	-4.00388100	2.40879600	-0.08209100
H	-1.65521500	1.76099600	0.37473400
H	0.96545700	1.90165100	-2.23273200
H	1.73547200	4.19801700	-1.80535500
H	2.35363400	4.91858900	0.53765600
H	2.12243900	3.27423400	2.40522700
H	1.33256000	0.98546900	1.98942200
H	1.53896700	-2.71551700	-1.49393400
H	3.98824000	-2.36788000	-1.88309200
H	4.08420300	-1.31166700	-0.39701800
H	3.25485000	-3.24648500	1.03386100
H	3.15317100	-4.30492000	-0.44870600

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t-**1b-IN(N-C2)**

E (UB+HF - LYP) = -826,15456981 a.u.

C	-2.39614800	0.48924800	-0.98205400
C	-2.07632600	-0.41510700	0.08382500
C	-3.20281400	-0.98625700	0.76404300
C	-4.50958400	-0.69250500	0.40504500
C	-4.79776100	0.19552200	-0.65041100
C	-3.71886500	0.77534200	-1.32739300
N	-0.83536100	-0.76607500	0.49596200
C	0.31163800	-0.30833700	-0.25506400
C	1.36566400	-1.37671900	0.13257500
C	2.49310600	-1.62593300	-0.84811500
C	3.80355900	-0.87561800	-0.73788800
C	3.74545400	-2.35006700	-0.40745400
C	0.78447500	1.11495500	0.04751900
C	0.58268200	1.67682600	1.31729400
C	1.04301200	2.96128300	1.61623700
C	1.71314900	3.71696700	0.64687900
C	1.91116200	3.17315600	-0.62602400
C	1.44897100	1.88569500	-0.91766100
C	0.45970900	-2.61652900	0.29599500
O	0.55064400	-3.46821700	1.14381100
H	0.16383700	-0.37785500	-1.35299100
H	1.78460300	-1.13790800	1.12388800
H	-2.99113700	-1.67834900	1.57641700
H	-5.32771600	-1.16163500	0.95312500
H	-5.82474200	0.42603100	-0.92648100
H	-3.90791900	1.47470900	-2.14335700
H	-1.59570500	0.98335700	-1.52583800
H	1.60023100	1.47160400	-1.91361500
H	2.41967200	3.75355900	-1.39452700
H	2.06556700	4.72080200	0.87702200
H	0.86971700	3.37965100	2.60644400
H	0.03855700	1.08837700	2.05167000
H	2.15667600	-1.84622200	-1.86125900
H	4.30125800	-0.56936400	-1.65615100
H	3.91092000	-0.16806800	0.08037700
H	3.80974400	-2.64607800	0.63707400
H	4.20230400	-3.05587800	-1.09810700

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t-**1b-IN(C3-C4)**

E (UB+HF - LYP) = -826,12739972 a.u.

C	1.79587200	1.64509800	-0.80388100
C	0.51749700	1.54871000	-0.21900500
C	0.08611200	2.59939500	0.61921100
C	0.91464500	3.69011400	0.86941100
C	2.19265900	3.77301100	0.29883400
C	2.62077100	2.73928200	-0.54023000
N	-0.31753400	0.44403500	-0.45350800
C	-1.79646900	0.65398100	-0.49646900
O	-2.21973400	1.71953000	-1.01359300
C	0.14642500	-0.79022600	-0.87293800
C	1.22611500	-1.53721500	-0.32723800
C	1.96084300	-1.17005300	0.84266200
C	2.98930200	-1.97069700	1.32703800
C	3.34792600	-3.16793800	0.68692800
C	2.63360700	-3.55379300	-0.46211100
C	1.60504100	-2.76439300	-0.95612700
C	-2.50892700	-0.40400400	0.05428800
C	-3.98680300	-0.42778200	0.03752600
C	-4.76182800	-1.73638800	-0.03680000
C	-4.79856100	-0.91415900	1.23252900
H	-0.46975600	-1.26838500	-1.62893900
H	-1.97806200	-1.20951500	0.55498400
H	-0.90651200	2.55225700	1.05200300
H	0.55674700	4.48782300	1.51821300
H	2.83640200	4.62645300	0.50114200
H	3.60517700	2.78421600	-1.00338800
H	2.13244100	0.85526900	-1.46763800
H	1.06152300	-3.07999100	-1.84544300
H	2.88646600	-4.48282000	-0.97163300
H	4.15654000	-3.78459200	1.07254600
H	3.52191900	-1.65900100	2.22461200
H	1.69913300	-0.25765000	1.36775000
H	-4.42261000	0.40641300	-0.50853200
H	-5.65917400	-1.78152900	-0.65392200
H	-4.18137300	-2.65775700	-0.03166800
H	-4.24217400	-1.28027600	2.09388300
H	-5.72143100	-0.39307000	1.48756200

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t-**1b-IN(N-C4)**

E (UB+HF - LYP) = -826,15456981 a.u.

C	3.39045700	-0.45068400	-1.36403400
C	2.58677500	-0.32134900	-0.19766500
C	3.11727700	-0.88043400	1.00042400
C	4.36160600	-1.51586100	1.00675900
C	5.13355000	-1.63172300	-0.15546500
C	4.62754700	-1.08862500	-1.34598300
N	1.38292100	0.34129300	-0.35681800
C	0.51622400	0.50322200	0.64560400
O	0.53800000	0.10478600	1.83640100
C	-0.75470500	1.32929400	0.20787700
C	-0.35656600	2.67610200	-0.38110300
C	-1.31333800	3.84719700	-0.34376800
C	-0.07061300	3.84314900	0.52753700
C	-1.57967000	0.53438500	-0.75043900
C	-2.55638600	-0.43250300	-0.40676500
C	-2.82414800	-0.82536700	0.94192800
C	-3.80962900	-1.76106600	1.23301900
C	-4.57264300	-2.35318500	0.21332000
C	-4.31581700	-1.99769600	-1.12200900
C	-3.33163300	-1.06762100	-1.42662500
H	-1.37109500	0.67468500	-1.80999300
H	-1.31557800	1.50418500	1.13425000
H	2.52916100	-0.80317600	1.90608700
H	4.73425600	-1.93129700	1.94365600
H	6.10096100	-2.13075500	-0.13658100
H	5.20534800	-1.16412500	-2.26739800
H	2.99803600	-0.02864300	-2.28679000
H	-3.13789800	-0.80353400	-2.46484500
H	-4.88885700	-2.45739300	-1.92582800
H	-5.34083800	-3.08537700	0.45187500
H	-3.98083900	-2.04686000	2.26949400
H	-2.21522000	-0.41419600	1.74138900
H	0.28169800	2.58679600	-1.25725100
H	-1.34714400	4.52473000	-1.19571800
H	-2.27644300	3.70005900	0.14227800
H	-0.19716600	3.69173800	1.59766400
H	0.74745900	4.51242300	0.26856700

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c-**1c**

E (RB+HF - LYP) = -748,74228024 a.u.

C	-0.00140000	1.17432500	-0.51926900
C	1.04384500	0.11402900	-1.05294800
H	-0.32465300	1.86710200	-1.30725800
H	1.17826300	0.22994200	-2.13519300
C	2.38842900	-0.02958400	-0.38596900
N	-0.95359600	0.04744200	-0.36606100
C	-0.06010000	-0.92503000	-0.77797500
C	-2.32674900	0.02013000	-0.07575500
O	-0.16222500	-2.13076400	-0.88598100
C	-2.99128300	-1.20865000	0.09098900
C	-4.35826000	-1.21902100	0.36685400
C	-5.07797700	-0.02532700	0.48462200
C	-4.41344900	1.19189100	0.31679600
C	-3.04605800	1.22097100	0.03671600
H	-2.43434700	-2.13347400	-0.00538100
H	-4.86380800	-2.17324800	0.49204000
H	-6.14210000	-0.04414900	0.70322000
H	-4.95864700	2.12864100	0.40097600
H	-2.54386700	2.17368400	-0.09999400
C	2.57798500	-0.85408800	0.73298300
C	3.82972000	-0.94437500	1.34770700
C	4.91301100	-0.21441000	0.85198300
C	4.73878800	0.60242600	-0.26898400
C	3.48752900	0.68849400	-0.88298800
H	1.75048000	-1.44594100	1.11454500
H	3.95844100	-1.59310200	2.21045700
H	5.88714400	-0.28874100	1.32850200
H	5.57739000	1.16595300	-0.67039600
H	3.36258000	1.31786700	-1.76234200
C	0.33635500	1.92961100	0.75837900
H	1.16046200	2.62731400	0.57042500
H	-0.52202800	2.50769300	1.11653400
H	0.64535000	1.24611800	1.55529300

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c-**1c**˙⁻

E (UB+HF - LYP) = -748,72821926 a.u.

C	-0.01208100	-1.10204400	0.56484100
C	1.02844900	-0.01040400	1.02250000
H	-0.32927700	-1.75067800	1.39605300
H	1.15463400	-0.08258600	2.13417200
C	2.39413200	0.05666600	0.39030900
N	-0.97415800	-0.00233300	0.33876300
C	-0.03663300	0.99898400	0.62067900
C	-2.33130100	-0.01618600	0.07675200
O	-0.15301900	2.22990700	0.66917700
C	-3.05111400	1.20295400	-0.09203300
C	-4.41337700	1.17716000	-0.35944100
C	-5.12374500	-0.03526600	-0.47500800
C	-4.40920900	-1.23853100	-0.32306900
C	-3.04503600	-1.23983800	-0.05191600
H	-2.51386200	2.14058100	-0.00168100
H	-4.93975300	2.12358400	-0.47944600
H	-6.19142600	-0.04134100	-0.68016400
H	-4.92798300	-2.19276700	-0.40870100
H	-2.52537300	-2.18482300	0.07829400
C	2.77278400	1.11559700	-0.44264100
C	4.05473700	1.16176900	-1.01217300
C	4.96593400	0.11431300	-0.78121000
C	4.60133800	-0.94173500	0.05405600
C	3.33498600	-0.96262800	0.65932400
H	2.06305600	1.91708600	-0.62779500
H	4.33650100	2.00428600	-1.64083400
H	5.95147400	0.13139400	-1.24447700
H	5.30408200	-1.75233600	0.24627700
H	3.06565200	-1.77458300	1.33366100
C	0.32668900	-1.93436900	-0.66724700
H	1.13995500	-2.63300800	-0.43663500
H	-0.53869700	-2.51631200	-1.00582300
H	0.65496100	-1.29007000	-1.48999600

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c-**1c-TS(N-C2)**
E (UB+HF - LYP) = -748,70764138 a.u.
1 imaginary frequency -44,77 cm**-1

C	-2.85552400	-1.21607400	-0.89620000
C	-2.25475400	-0.09764700	-0.29215800
C	-3.10087600	0.85554200	0.30258300
C	-4.48807300	0.69206000	0.29953100
C	-5.06853600	-0.43364900	-0.29466200
C	-4.24219400	-1.38860900	-0.89598200
C	-0.75171100	0.04421000	-0.27709700
C	-0.21488300	1.49875800	-0.40585200
O	0.09933000	2.05395800	-1.43367700
C	0.07023900	-0.38015000	0.98169100
C	-0.63089600	-0.13459800	2.32301300
N	1.21343100	0.50411300	0.84464800
C	2.40176000	0.06229900	0.36822100
C	3.40375300	1.04327300	0.06073100
C	4.66428900	0.69530800	-0.40020900
C	5.03117500	-0.65101300	-0.59122300
C	4.07275100	-1.63075800	-0.30722900
C	2.79599000	-1.30000800	0.15060200
H	0.30135400	-1.45478800	0.91660600
H	-0.34054900	-0.51925800	-1.13021600
H	3.13191700	2.08691100	0.19974600
H	5.38271000	1.48592000	-0.62035600
H	6.02224400	-0.91964200	-0.95097100
H	4.32136800	-2.68422000	-0.44655500
H	2.09702200	-2.10608500	0.35856600
H	-2.65734800	1.73681500	0.75779200
H	-5.11940500	1.44889800	0.76189600
H	-6.14918700	-0.56190000	-0.29427000
H	-4.67754600	-2.26592800	-1.37139100
H	-2.22053600	-1.95953200	-1.37517500
H	-1.54829200	-0.73030900	2.42709400
H	0.05534800	-0.39747400	3.13761200
H	-0.88282900	0.92647800	2.43194700

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c-**1c-TS(C2-C3)**
E (UB+HF - LYP) = -748,70707603 a.u.
1 imaginary frequency -110,19 cm**-1

C	0.00722700	-0.79749900	-0.61148900
C	-1.28822300	-0.12850500	-1.01794700
H	0.39430500	-1.29764100	-1.51507800
H	-1.31591600	0.11831900	-2.07786500
C	-2.55907800	-0.11613600	-0.38582100
N	0.96280800	0.28984400	-0.25041700
C	0.32410400	1.55001800	-0.39984800
C	2.33918300	0.07229500	-0.05884500
O	0.88987700	2.60766200	-0.15569900
C	3.13145500	0.99849000	0.66092100
C	4.50083800	0.78940500	0.82114200
C	5.13179700	-0.34174300	0.29019300
C	4.35765600	-1.26491000	-0.41928700
C	2.98798300	-1.06271600	-0.59739000
H	2.65761300	1.87936100	1.07271500
H	5.08178400	1.52233900	1.37886400
H	6.19894800	-0.50110700	0.42899800
H	4.82073200	-2.15477300	-0.84331700
H	2.41890800	-1.79313700	-1.16248300
C	-2.82177600	-0.33224700	1.00935600
C	-4.10948400	-0.28912700	1.53458400
C	-5.22717700	-0.01115700	0.73179300
C	-5.00071300	0.24357200	-0.63482800
C	-3.72309400	0.19417800	-1.17102700
H	-1.99449500	-0.50158600	1.68887000
H	-4.24408000	-0.45996700	2.60324800
H	-6.22934600	0.02368800	1.15322500
H	-5.84111500	0.48054600	-1.28807400
H	-3.58315500	0.39249200	-2.23336200
C	-0.05404200	-1.86706400	0.49402500
H	-0.89203300	-2.54932800	0.31335700
H	0.87098000	-2.45484600	0.52450500
H	-0.18173400	-1.41568500	1.48171000

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c-**1c-TS(C3-C4)**
E (UB+HF - LYP) = -748,70889263 a.u.
1 imaginary frequency -383,01 cm**-1

C	-0.22930100	1.40437400	-0.41238100
C	1.13888300	0.05088000	-0.96341900
H	-0.56522900	2.06921700	-1.21797200
H	1.11524400	0.32167700	-2.02474100
C	2.46204000	-0.11493600	-0.42882600
N	-0.99990400	0.17197500	-0.32920800
C	-0.02440300	-0.80470800	-0.55085900
C	-2.36841600	0.02564800	-0.09718100
O	-0.14199900	-2.02258500	-0.42850200
C	-2.99004400	-1.24647200	-0.06738500
C	-4.36756100	-1.34726700	0.12398200
C	-5.16612100	-0.21110600	0.30367900
C	-4.55092100	1.04759100	0.28776900
C	-3.17634500	1.16886100	0.08905900
H	-2.37631600	-2.12978000	-0.19239700
H	-4.82318400	-2.33633400	0.13682100
H	-6.23965800	-0.30340500	0.45281800
H	-5.14643200	1.94798300	0.42986600
H	-2.71342800	2.15044100	0.06505300
C	2.73809500	-0.77089300	0.81833800
C	4.01607900	-0.81472200	1.35209200
C	5.11201600	-0.19947300	0.69950200
C	4.86446500	0.45499400	-0.52587300
C	3.59028400	0.50126700	-1.07319900
H	1.92403500	-1.27097100	1.33897500
H	4.17774400	-1.34175800	2.29304800
H	6.11083300	-0.22961500	1.12906000
H	5.68841200	0.93260800	-1.05807200
H	3.43052300	1.01812800	-2.02021100
C	0.10340200	2.08215400	0.89252000
H	0.70279700	2.98173200	0.69764000
H	-0.77387400	2.39044200	1.49144000
H	0.71094100	1.41933900	1.52423500

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S63

c-**1c-TS(N-C4)**

E (UB+HF - LYP) = -748,70959719 a.u.

1 imaginary frequency -592,15 cm**-1

C	-0.18353200	0.55941700	1.35521700
C	-1.03561700	-0.59115600	0.80823100
H	0.23190500	0.37548500	2.35045200
H	-1.14754600	-1.36170500	1.58371900
C	-2.40155800	-0.29727300	0.24095700
N	0.99911800	-0.06062600	0.10819800
C	0.09437200	-1.03930800	-0.16827200
C	2.36087800	-0.02185400	-0.08583400
O	0.16140800	-2.02863800	-0.89785900
C	3.22055100	-1.10182900	0.29767000
C	4.60012000	-0.97887600	0.21377300
C	5.20719900	0.21308700	-0.24037900
C	4.36954500	1.28038800	-0.63083600
C	2.98672900	1.17175100	-0.56091900
H	2.77001600	-2.03269700	0.63397000
H	5.22547400	-1.82495000	0.50104900
H	6.28978600	0.30325000	-0.29417900
H	4.81169100	2.20588800	-1.00095900
H	2.35199400	1.99992200	-0.87160900
C	-2.57238500	0.21865900	-1.06028900
C	-3.84226400	0.52495300	-1.55361800
C	-4.98221600	0.32097200	-0.76751300
C	-4.83035700	-0.20984200	0.52346700
C	-3.55836400	-0.50989900	1.01281700
H	-1.69875100	0.36031000	-1.69184500
H	-3.94291900	0.91977300	-2.56353400
H	-5.97050900	0.56416800	-1.15256700
H	-5.70518100	-0.39305200	1.14561700
H	-3.45052600	-0.91625200	2.01824800
C	-0.49272600	2.00709300	1.07625300
H	-1.34612600	2.38283200	1.66192400
H	0.37900200	2.62823000	1.32391200
H	-0.72564500	2.16458800	0.01694900

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c-**1c-IN(N-C2)**

E (UB+HF - LYP) = -748,70592428 a.u.

C	0.19270300	-0.21023600	0.15942300
C	-0.99295200	0.62710400	-0.40983000
H	0.24462500	-1.12569300	-0.47060400
H	-0.78054500	0.77091200	-1.47809200
C	-2.38945100	0.05624600	-0.26476000
N	1.32966900	0.65388500	0.00690700
C	-0.90746200	2.03252000	0.22611100
C	2.56150900	0.11870100	-0.03149500
O	-1.07804600	3.08200900	-0.31708300
C	3.68985900	1.00716300	-0.15595700
C	4.99506500	0.54979900	-0.22952700
C	5.29851000	-0.82788500	-0.18914500
C	4.22670000	-1.72078200	-0.06669200
C	2.90418400	-1.28166100	0.01814500
H	3.47193000	2.07288000	-0.19440400
H	5.80435900	1.27597400	-0.32321200
H	6.32584800	-1.18200800	-0.24544400
H	4.42338300	-2.79414900	-0.02871600
H	2.11800400	-2.02575900	0.11910600
C	-3.14121000	0.17824500	0.91726900
C	-4.42067600	-0.37334200	1.01861900
C	-4.98144600	-1.06523800	-0.05947100
C	-4.24849900	-1.19216600	-1.24317800
C	-2.97203800	-0.63212500	-1.34213300
H	-2.71794100	0.71323800	1.76243400
H	-4.98136200	-0.26164500	1.94467000
H	-5.97721300	-1.49627400	0.02073500
H	-4.67114100	-1.72397000	-2.09343100
H	-2.41083400	-0.73103500	-2.26901900
C	-0.03365700	-0.66643900	1.61711900
H	-0.21340800	0.20518600	2.25839400
H	-0.87654600	-1.36508500	1.71706400
H	0.87068800	-1.16526500	1.98182900

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c-**1c-IN(C2-C3)**

E (UB+HF - LYP) = -748,70022269 a.u.

C	-3.78218300	-0.40562500	-0.94374200
C	-2.48501500	-0.32325000	-0.33706100
C	-2.46753500	0.26093900	0.97270100
C	-3.63302500	0.66705000	1.61446400
C	-4.89132300	0.54349300	1.00362000
C	-4.93801100	0.01065100	-0.29823000
C	-1.33781100	-0.74364900	-1.06703600
C	0.00899900	-1.17825300	-0.52997000
N	0.85856000	0.04431800	-0.46591800
C	2.21186600	0.04008900	-0.08414200
C	2.81781800	1.21534100	0.41734300
C	4.16933300	1.22551300	0.75964800
C	4.95882500	0.07588800	0.63089800
C	4.36910000	-1.09020100	0.13065100
C	3.02101200	-1.10842400	-0.23076900
C	0.25051600	1.05630800	-1.26309300
O	0.72265500	2.17634400	-1.38306300
H	0.43965100	-1.86195700	-1.28185900
H	-1.53827500	-1.07229500	-2.08476500
H	2.21515300	2.10869600	0.52154400
H	4.60956200	2.14477300	1.14295000
H	6.00920800	0.08917700	0.91381600
H	4.96294600	-1.99573500	0.01456900
H	2.59109000	-2.02076500	-0.63251000
H	-1.51386900	0.43710000	1.46096400
H	-3.55823500	1.10963200	2.60819100
H	-5.79724300	0.86694000	1.51159400
H	-5.89589800	-0.08311800	-0.81084000
H	-3.85144800	-0.81910100	-1.94967000
C	-0.00699900	-1.94333800	0.80640700
H	0.99850000	-2.25984800	1.10747700
H	-0.42413100	-1.34176500	1.61697200
H	-0.63158300	-2.83789400	0.69735600

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c-**1c-IN(C3-C4)**

E (UB+HF - LYP) = -748,74170611 a.u.

C	-3.68435000	0.55754900	-0.11156900
C	-2.36794800	0.04186800	-0.02214500
C	-2.20585200	-1.36442800	-0.09432000
C	-3.30491200	-2.19795400	-0.26451300
C	-4.60586600	-1.67895500	-0.37192600
C	-4.77648200	-0.29440900	-0.28840100
N	-1.26153000	0.87863500	0.09469200
C	-1.35440500	2.23337800	-0.14742000
C	-0.31802100	3.20608600	0.31493700
C	0.05031400	0.28398500	0.54768100
O	0.06320500	-0.21462200	1.69471900
C	1.05323700	0.37875400	-0.41653600
C	2.42094500	-0.05122400	-0.26806200
C	3.33265300	0.10856600	-1.34964400
C	4.66504200	-0.28563900	-1.26088000
C	5.16404400	-0.86246100	-0.08364700
C	4.28479400	-1.03080600	0.99596600
C	2.94871900	-0.64090400	0.91635100
H	-2.11522400	2.55152600	-0.85620900
H	0.78137000	0.82499800	-1.37006400
H	-1.21089300	-1.78591300	-0.00811200
H	-3.14460600	-3.27367400	-0.31564900
H	-5.45952900	-2.33922000	-0.50799500
H	-5.77562400	0.13573200	-0.34762100
H	-3.84896900	1.62434700	-0.00308500
H	2.27848500	-0.78043700	1.75755100
H	4.64866500	-1.47783100	1.92131900
H	6.20492500	-1.17223100	-0.01148200
H	5.32318100	-0.14226400	-2.11802800
H	2.96738400	0.55423600	-2.27477300
H	-0.76109600	4.21111200	0.37232600
H	0.06132600	2.94141300	1.30990900
H	0.56420800	3.27431300	-0.34392000

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c-**1c-IN(N-C4)**

E (UB+HF - LYP) = -748,74702219 a.u.

C	1.31944400	2.32274800	0.61336700
C	1.29669900	1.31101700	-0.49942900
H	0.93905500	3.30829900	0.34140100
H	1.64959800	1.81252300	-1.40858000
C	2.22003300	0.12030100	-0.26372000
N	-0.90661100	0.49774200	0.17893900
C	-0.18020500	0.87960200	-0.87768200
C	-2.20842900	0.04290400	0.05705500
O	-0.47946700	0.96300600	-2.09308000
C	-2.95630400	-0.14404100	-1.14146400
C	-4.26639100	-0.62815200	-1.10266200
C	-4.89850000	-0.94525500	0.10569700
C	-4.17977100	-0.76653700	1.29713700
C	-2.87304400	-0.28724000	1.27098600
H	-2.48293500	0.10092700	-2.08360000
H	-4.80527600	-0.75916400	-2.04172200
H	-5.92063600	-1.31986400	0.12087400
H	-4.64435600	-1.00426800	2.25433900
H	-2.31697800	-0.14983700	2.19615600
C	1.84365500	-0.98843800	0.51328900
C	2.72523300	-2.05408000	0.71714700
C	4.00403200	-2.04030600	0.14986300
C	4.39099900	-0.94536600	-0.62869400
C	3.50594200	0.11845200	-0.82926900
H	0.84301800	-1.00105500	0.93626100
H	2.40735900	-2.90391800	1.31895000
H	4.68675000	-2.87348600	0.30714800
H	5.37937300	-0.92046900	-1.08509900
H	3.81419600	0.96586400	-1.43945500
C	1.35225300	1.98504500	2.06898200
H	1.52630700	2.88205000	2.67923400
H	0.39552000	1.53631500	2.38606500
H	2.13714800	1.25390200	2.30648700

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t-**1c**
E (RB+HF - LYP) = -748,74073207 a.u.

C	-0.05124500	1.30618400	-0.09801500
C	-1.13459000	0.63763100	0.82034200
H	-0.28166500	1.19455200	-1.16480200
H	-1.37884800	1.27286900	1.67926200
C	-2.39714200	0.11094700	0.18746100
N	0.89647400	0.26248700	0.36885300
C	-0.02220700	-0.37455300	1.18372700
C	2.22776300	-0.01742000	0.02295000
O	0.05905000	-1.35458300	1.89466200
C	2.95988600	-0.97963600	0.74202100
C	4.27879500	-1.25168800	0.37963000
C	4.88569500	-0.57896100	-0.68613800
C	4.15272800	0.37284000	-1.39923800
C	2.82968700	0.65395800	-1.05348200
H	2.48772700	-1.50481300	1.56434200
H	4.83664900	-1.99780200	0.93988500
H	5.91501100	-0.79565300	-0.95825800
H	4.60761400	0.90030900	-2.23391400
H	2.26643600	1.38575000	-1.62461000
C	-2.35178900	-0.85084800	-0.83491900
C	-3.52567200	-1.31876400	-1.42643900
C	-4.76840900	-0.83550700	-1.00344300
C	-4.82657000	0.11615500	0.01677000
C	-3.64840400	0.58313700	0.60679600
H	-1.39338100	-1.24794800	-1.16286700
H	-3.47091500	-2.06715000	-2.21297700
H	-5.68265600	-1.20311800	-1.46215600
H	-5.78705300	0.49444200	0.35763500
H	-3.70144500	1.32058400	1.40507500
C	0.32451900	2.74411200	0.23664600
H	-0.51219400	3.40887400	-0.00962500
H	0.54936900	2.85057400	1.30430000
H	1.19935900	3.08225800	-0.32858300

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t-**1c**⁻·

E (UB+HF - LYP) = -748,72939746 a.u.

C	0.02763600	1.23516900	-0.23763800
C	1.13327500	0.37538800	-0.93421900
H	0.25939300	1.46010300	0.81354500
H	1.38069900	0.79066500	-1.93021400
C	2.41683000	0.09239200	-0.19311200
N	-0.89833400	0.09487100	-0.38170300
C	0.06298100	-0.73174200	-0.99226200
C	-2.22136200	-0.04195100	-0.00970800
O	-0.04400800	-1.82229300	-1.56891200
C	-2.99815500	-1.14900000	-0.46587700
C	-4.32042600	-1.28402500	-0.06725600
C	-4.93783300	-0.34757100	0.79118300
C	-4.16088100	0.72827200	1.26576800
C	-2.83199700	0.88201100	0.88707500
H	-2.53114800	-1.87626400	-1.12166500
H	-4.89175100	-2.13687800	-0.43296000
H	-5.97701300	-0.46140100	1.08974000
H	-4.60094900	1.45641700	1.94680600
H	-2.25309900	1.71311300	1.28263100
C	2.38948400	-0.32861400	1.14989800
C	3.58932600	-0.58765300	1.83804900
C	4.81671900	-0.47201800	1.18043800
C	4.85354100	-0.08699200	-0.16625900
C	3.65213200	0.21721400	-0.83555900
H	1.43298800	-0.47260200	1.64783200
H	3.55816700	-0.89081700	2.88349000
H	5.74266400	-0.68983200	1.71204300
H	5.80312700	-0.02626800	-0.69588700
H	3.67440700	0.53845400	-1.87679400
C	-0.38795400	2.50417000	-0.97592400
H	0.42904400	3.23700800	-0.94005300
H	-0.60432900	2.28206900	-2.02785700
H	-1.28169000	2.96019100	-0.53503200

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t-**1c-TS(N-C2)**

E (UB+HF - LYP) = -748,70360227 a.u.

1 imaginary frequency -77,04 cm**-1

C	-3.62007600	0.53750600	-0.31965800
C	-2.26561600	0.22263400	-0.11864300
C	-1.90855300	-1.13862600	-0.05738700
C	-2.86910900	-2.13758500	-0.21638200
C	-4.21416000	-1.80852000	-0.42897300
C	-4.58580600	-0.46172600	-0.47620100
C	-1.24217900	1.31050900	0.07535800
C	-0.58627900	1.33127200	1.51000900
O	-0.97868400	0.79956300	2.52049200
C	0.07680900	1.14984900	-0.72171500
C	0.60596300	2.51904100	-1.19908900
N	0.87871400	0.51711300	0.30275400
C	2.10926100	0.01468300	0.08277900
C	2.86020500	-0.49318700	1.19574100
C	4.11923500	-1.05254900	1.03776700
C	4.72464900	-1.15869200	-0.23004900
C	4.01064800	-0.67878100	-1.33484900
C	2.74667100	-0.10296800	-1.19834100
H	-0.08006600	0.50465900	-1.60814700
H	-1.72492600	2.28330600	-0.09384100
H	2.40248100	-0.42303600	2.17982100
H	4.64750500	-1.41892600	1.91880400
H	5.71296400	-1.59824100	-0.34633000
H	4.44797100	-0.75107400	-2.33192100
H	2.22883900	0.24761300	-2.08730100
H	-0.86840800	-1.39334900	0.12736200
H	-2.56776600	-3.18252800	-0.16713000
H	-4.96092000	-2.59116700	-0.54888200
H	-5.62723300	-0.18675000	-0.63644000
H	-3.91985200	1.58410700	-0.35691300
H	-0.05281300	2.95314700	-1.96669800
H	0.65732900	3.20855500	-0.34739700
H	1.61340200	2.43023700	-1.62039500

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t-**1c-TS(C2-C3)**
E (UB+HF - LYP) = -748,69987971 a.u.
1 imaginary frequency 123,48 cm**-1

C	0.06312600	-0.48254100	0.86416000
C	1.30216200	0.38265400	0.89333700
H	0.22578800	-1.37430200	0.24084800
H	1.37604500	1.01722200	1.77809700
C	2.54218500	0.04665200	0.27706800
N	-0.95070100	0.40443000	0.24530200
C	-0.22565300	1.52063900	-0.26650500
C	-2.27780200	0.05986700	-0.01459200
O	-0.75044000	2.56620400	-0.62207900
C	-3.26677500	1.05539900	-0.21527700
C	-4.58001900	0.69722800	-0.51317700
C	-4.96730300	-0.64651800	-0.60730500
C	-3.99572900	-1.63597500	-0.41359600
C	-2.67319400	-1.29503300	-0.13154900
H	-2.97540200	2.09626800	-0.14919000
H	-5.31692800	1.48440500	-0.66657400
H	-5.99821700	-0.91506100	-0.82710700
H	-4.26682000	-2.68823200	-0.48838900
H	-1.93648000	-2.08244800	-0.00404600
C	2.66374600	-0.84322500	-0.83947100
C	3.89377300	-1.11832400	-1.42844000
C	5.07921400	-0.52478600	-0.96430800
C	4.98546500	0.37647000	0.11468500
C	3.76430400	0.65285500	0.71298700
H	1.76889800	-1.30193900	-1.25368800
H	3.93056600	-1.80212500	-2.27701800
H	6.03690100	-0.74331700	-1.43155300
H	5.88486600	0.86401000	0.49173700
H	3.72293700	1.35142700	1.54844800
C	-0.37128900	-0.93503800	2.26815100
H	0.40240900	-1.58170500	2.69972400
H	-0.49304300	-0.06138800	2.92068600
H	-1.32036300	-1.48541000	2.26053100

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t-1c-TS(C3-C4)
E (UB+HF - LYP) = -748,70794451 a.u.
1 imaginary frequency -337,53 cm**-1

C	3.65024200	0.79125900	-0.66320500
C	2.51908900	-0.00283200	-0.28212600
C	2.77907200	-1.05161500	0.65941600
C	4.05433000	-1.28825100	1.15080600
C	5.15587000	-0.49618800	0.75596100
C	4.92233300	0.54716900	-0.16317100
C	1.19761100	0.34729100	-0.73055900
C	0.03842700	-0.60022200	-0.68129000
O	-0.06368500	-1.79036200	-0.97711100
N	-0.96307300	0.23683700	-0.17793600
C	-2.31895700	-0.03027700	0.02256300
C	-2.97366300	-1.08917500	-0.64955000
C	-4.33182800	-1.31862100	-0.44299500
C	-5.08264000	-0.51426800	0.42904500
C	-4.43616400	0.53015500	1.09901600
C	-3.07703400	0.77640600	0.90174900
C	-0.21929300	1.41660500	0.22436100
C	-0.62132200	2.72845500	-0.39090000
H	0.03237600	1.43968200	1.28835800
H	1.18585000	1.00778600	-1.60614600
H	-2.39567700	-1.72974600	-1.30465000
H	-4.81185300	-2.14316600	-0.96785700
H	-6.14368600	-0.69948600	0.58102800
H	-4.99397900	1.16434800	1.78648000
H	-2.58458600	1.58390700	1.43484900
H	1.95685000	-1.69135800	0.97203700
H	4.20629400	-2.10818000	1.85340600
H	6.15152900	-0.68245200	1.15245300
H	5.75244000	1.17381100	-0.49161800
H	3.49792800	1.60889600	-1.36853200
H	0.04923100	3.52278700	-0.03480300
H	-0.53062100	2.68701800	-1.48959600
H	-1.65754800	3.05584100	-0.17767900

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t-**1c-TS(N-C4)**
E (UB+HF - LYP) = -748,70706164 a.u.
1 imaginary frequency -557,58 cm**-1

C	-0.23338400	1.30685100	-0.66742500
C	-1.12470400	0.91165600	0.50228300
H	-0.33733900	0.67231300	-1.54878700
H	-1.37120800	1.78401000	1.12357500
C	-2.39262400	0.18894300	0.14863200
N	1.04954500	0.52161600	0.37450100
C	0.03515500	0.10605600	1.18045800
C	2.31593500	0.01774600	0.18274900
O	0.01267700	-0.67158400	2.13241300
C	2.55154100	-1.35911200	-0.13562500
C	3.82335900	-1.80682600	-0.46669700
C	4.92505600	-0.92563200	-0.51081000
C	4.70617200	0.43327400	-0.19377700
C	3.44165300	0.89628900	0.14519900
H	1.71763400	-2.05562600	-0.08885700
H	3.97099900	-2.86366600	-0.69143000
H	5.91634800	-1.28418900	-0.77874500
H	5.54282100	1.13237300	-0.20731100
H	3.28633900	1.94477400	0.39430500
C	-2.37281900	-1.12441700	-0.37759300
C	-3.55147600	-1.77010900	-0.74562100
C	-4.79545900	-1.13985200	-0.58849400
C	-4.83404100	0.15201800	-0.03731900
C	-3.65257100	0.79736900	0.32603800
H	-1.42155300	-1.64027200	-0.48363100
H	-3.50374500	-2.78102400	-1.14774900
H	-5.71410400	-1.64971900	-0.87057600
H	-5.78922100	0.65372000	0.11082600
H	-3.69764500	1.79822200	0.75395900
C	0.07102700	2.75040700	-0.95526000
H	-0.78725900	3.28744500	-1.39567900
H	0.35395500	3.27555400	-0.03148300
H	0.90882400	2.83947800	-1.65964500

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t-**1c-IN(N-C2)**
E (UB+HF - LYP) = -748,70976802 a.u.

C	-3.43310300	0.07044300	-0.78851600
C	-2.15803000	0.08299400	-0.20155700
C	-1.69434700	-1.09415400	0.41247800
C	-2.47980300	-2.24829600	0.41424200
C	-3.74744500	-2.25155500	-0.18010300
C	-4.22361600	-1.08317800	-0.78135400
C	-1.32178300	1.34505200	-0.22022900
C	-1.21181600	2.02374500	1.16801200
O	-1.82409100	1.79891700	2.16742100
C	0.13815200	1.17050000	-0.72838800
C	0.66396900	2.51807900	-1.27810600
N	0.89589100	0.66581300	0.38548500
C	2.08552300	0.07870600	0.15626900
C	2.84777700	-0.38003000	1.28911700
C	4.06693300	-1.02491800	1.15593700
C	4.63514500	-1.27220000	-0.11104500
C	3.92172700	-0.83805500	-1.23522000
C	2.69640600	-0.17882700	-1.12323300
H	0.08999500	0.46022100	-1.58190600
H	-1.83768800	2.09066900	-0.84472300
H	2.42126900	-0.19815200	2.27397900
H	4.59475600	-1.34775400	2.05472800
H	5.59345500	-1.77768200	-0.21095800
H	4.33209700	-1.01153300	-2.23187600
H	2.19280100	0.13589900	-2.03353700
H	-0.70789500	-1.07739200	0.86808600
H	-2.09961400	-3.15238400	0.88605500
H	-4.35708900	-3.15319200	-0.17171400
H	-5.20757000	-1.06820100	-1.24713700
H	-3.81036300	0.97580000	-1.26255600
H	0.58710800	3.29033800	-0.50308500
H	1.71878100	2.42605200	-1.55818000
H	0.09731500	2.84543300	-2.16475900

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t-**1c-IN(C2-C3)**
E (UB+HF - LYP) = -748,70927365 a.u.

C	2.52155300	-0.24819100	-1.21382700
C	2.04345200	0.06418000	0.08328100
C	2.81283300	-0.38963200	1.18486100
C	3.98731700	-1.11178100	0.98375400
C	4.44683700	-1.42094100	-0.30254700
C	3.69605800	-0.98104200	-1.39516700
N	0.85125800	0.78036200	0.25773100
C	0.29230300	1.29232400	1.45296600
O	0.76329300	1.08045000	2.56283900
C	-0.07192000	1.12857800	-0.86670500
C	0.40996200	2.38971800	-1.60463900
C	-1.44017600	1.31816000	-0.28423800
C	-2.40641200	0.28528500	-0.17957900
C	-3.77307700	0.58590500	0.13520000
C	-4.74548200	-0.39836600	0.23624500
C	-4.43204500	-1.75588200	0.03193700
C	-3.09938300	-2.08369300	-0.26484700
C	-2.11353000	-1.10679600	-0.36314700
H	-0.06475300	0.27862500	-1.56448800
H	-1.79620900	2.34164300	-0.19862100
H	2.46648900	-0.16505000	2.18456000
H	4.55041700	-1.44373000	1.85477300
H	5.36276700	-1.98959700	-0.44745600
H	4.02401100	-1.20501800	-2.40926200
H	1.97405800	0.07863700	-2.08981600
H	-1.08927400	-1.41299800	-0.56184900
H	-2.82165300	-3.12778700	-0.41173800
H	-5.19529300	-2.52666600	0.11354600
H	-5.76953300	-0.11051700	0.47621200
H	-4.04537100	1.62845200	0.29773900
H	-0.20822200	2.56845300	-2.49391800
H	0.31900800	3.25748600	-0.93969300
H	1.45866700	2.31498600	-1.91810500

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t-**1c-IN(C3-C4)**

E (UB+HF - LYP) = -748,74091994 a.u.

C	2.31276300	-1.18677400	0.75085700
C	2.30187000	-0.03403300	-0.06588700
C	3.52361500	0.39114900	-0.62849600
C	4.71180000	-0.29159500	-0.36279400
C	4.71729500	-1.42385600	0.45774200
C	3.50190200	-1.86472700	1.00249200
N	1.11354900	0.67609800	-0.29289100
C	1.13098800	2.03437700	-0.58273000
C	1.87886200	3.01998100	0.27088800
C	-0.16694600	-0.08678400	-0.39549200
O	-0.10700300	-1.21821800	-0.92575600
C	-1.27332300	0.59111300	0.13649200
C	-2.64110000	0.14486800	0.09808800
C	-3.07686800	-1.06208100	-0.52249600
C	-4.42217600	-1.42627700	-0.53106800
C	-5.40438700	-0.62722700	0.07281700
C	-4.99813200	0.56305600	0.69457100
C	-3.65733400	0.93707100	0.70645200
H	0.23950600	2.37989900	-1.09424900
H	-1.08758700	1.52914200	0.65210900
H	1.37892300	-1.54473800	1.16904800
H	3.48082700	-2.75062500	1.63500400
H	5.64314900	-1.95718200	0.66257600
H	5.63846400	0.05836300	-0.81574700
H	3.51917200	1.24512400	-1.29963200
H	-2.32728800	-1.69373600	-0.98613700
H	-4.71185000	-2.35747400	-1.01857200
H	-6.45196200	-0.92236000	0.06136900
H	-5.73651900	1.20596500	1.17424500
H	-3.36696700	1.86767400	1.19416600
H	1.84294900	4.01559800	-0.18949400
H	1.43358500	3.10898200	1.28181700
H	2.93380500	2.75885600	0.42116400

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t-**1c-IN(N-C4)**

E (UB+HF - LYP) = -748,74946510 a.u.

C	3.35665600	-0.07931400	1.34748800
C	2.40786500	-0.11772400	0.28896300
C	2.87202400	-0.62660100	-0.95749600
C	4.19271100	-1.05783800	-1.10986700
C	5.10855200	-1.00917700	-0.05237800
C	4.66965100	-0.51190900	1.18403800
N	1.13784400	0.34671900	0.59485900
C	0.15723400	0.37617600	-0.30891400
O	0.13240600	0.03119000	-1.51719900
C	-1.17342900	1.00190500	0.29154600
C	-1.46814100	2.30675900	-0.38585900
C	-0.60457300	3.50306100	-0.14016800
C	-2.34284600	0.03627900	0.21852700
C	-3.01526700	-0.35050900	1.38848700
C	-4.10499700	-1.22659000	1.34761400
C	-4.54671200	-1.73835400	0.12426900
C	-3.88167600	-1.36658200	-1.04991500
C	-2.79430300	-0.49054400	-1.00484800
H	-2.05046300	2.28052200	-1.30614200
H	-0.94577500	1.19450700	1.34622400
H	2.17466300	-0.67148700	-1.78425900
H	4.51103700	-1.44156000	-2.07986000
H	6.13432100	-1.34920000	-0.18507200
H	5.35951200	-0.46256700	2.02685200
H	3.01453700	0.30588200	2.30571200
H	-2.25315100	-0.23195700	-1.90954100
H	-4.20713100	-1.76890500	-2.00801000
H	-5.39349100	-2.42139100	0.08601300
H	-4.60536700	-1.51031300	2.27216700
H	-2.67425300	0.03931300	2.34595900
H	0.36473300	3.42410900	-0.66611200
H	-1.08668500	4.42832900	-0.48537000
H	-0.36313100	3.61393500	0.92609800

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