Electronic Supplementary Material (ESI)

A hybrid molecule of a GFP chromophore analogue and cholestene as a viscosity-dependent and cholesterol-responsive fluorescent sensor

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1. Synthetic methods of glycinate 8 and DAIN 13

Ethyl 2-((di(naphthalen-2-yl)methylene)amino)acetate (8)

A solution of 2-bromonaphthalene (10.0 g, 48.3 mmol) in THF (17 mL) was added to a stirred suspension of magnesium (1.17 g, 48.3 mmol) in THF (35 mL); the mixture was stirred under reflux for 30 min. A solution of 2-naphthonitrile (4.62 g, 30.2 mmol) in THF (18 mL) was then added to the solution of the Grignard reagent; the mixture was stirred overnight under reflux. Subsequent to the addition of MeOH (7.0 mL) at ice-water temperature, the mixture was stirred for 10 min and evaporated under reduced pressure. The residue was diluted with CH_2Cl_2 and was washed with a saturated solution of NH_4Cl, water, and brine; dried over $MgSO_4$; and concentrated under reduced pressure. The residue was recrystallized from ethyl acetate and hexane to obtain di(naphthalen-2-yl)methanimine (5.06 g, 60%). The obtained imine (4.00 g, 14.2 mmol) was treated with glycine ethyl ester hydrochloride (3.97 g, 28.4 mmol) in CH_2Cl_2 (120 mL) and stirred overnight.[1)] After filtration of the mixture, the filtrate was washed with water and then brine, dried over $MgSO_4$, and concentrated under reduced pressure. The residue was recrystallized from ether and hexane to yield **8** (4.16 g, 80%). ^{1}H-NMR ($CDCl_3$) δ: 8.17 (1H, dd, *J* = 8.7, 1.8 Hz), 7.99-7.94 (2H, m), 7.90-7.83 (3H, m), 7.81 (1H, s), 7.76 (1H, s), 7.70 (1H, d, *J* = 8.2 Hz), 7.62-7.56 (2H, m), 7.49 (1H, td, *J* = 7.5, 1.4 Hz), 7.42 (1H, td, *J* = 7.5, 1.4 Hz), 7.34 (1H, dd, *J* = 8.5, 1.6 Hz), 4.30 (2H, s), 4.22 (2H, q, *J* = 7.2 Hz), 1.27 (3H, t, *J* = 7.1 Hz). ^{13}C-NMR ($CDCl_3$) δ: 171.8, 170.7, 136.8, 134.5, 133.5, 133.2, 132.9, 132.7, 130.4, 128.9, 128.6, 128.3, 127.9, 127.9, 127.6, 127.2, 126.9, 126.8, 126.2, 125.3, 125.0, 60.9, 55.9, 14.2. HRMS (FAB) m/z: $[M + H]^+$ Calcd for $C_{25}H_{22}NO_2$ 368.1651; Found 368.1648. *Di(naphthalen-2-yl)methanimine*: ^{1}H-NMR ($CDCl_3$) δ: 9.95 (1H, br s), 8.04 (2H, br s), 7.94-7.84 (8H, m), 7.59-7.51 (4H, m). ^{13}C-NMR ($CDCl_3$) δ: 178.4, 136.8 (br), 134.2, 132.7 129.1 (br), 128.8, 128.2, 127.8, 127.3, 126.6, 125.3. HRMS (FAB) m/z: $[M + H]^+$ Calcd for $C_{21}H_{16}N$ 282.1283; Found 282.1284.

2-(Diphenylmethylene)-2,5,6,7-tetrahydro-3*H*-imidazo[1,2-*a*]azepin-3-one (DAIN **13**)

DAIN **13** was synthesised from 1,5,6,7-tetrahydro-2*H*-azepin-2-one,[2)] which was prepared by the Beckmann rearrangement of cyclohex-2-en-1-one oxime, using a routine method for DAIN synthesis. Methyl trifluoromethanesulfonate (509 µL, 4.50 mmol) was added to a stirred solution of 1,5,6,7-tetrahydro-2*H*-azepin-2-one (200 mg, 1.80 mmol) in CH_2Cl_2 (9.0 mL) at room temperature. The mixture was stirred at room temperature for 1 day. Triethylamine (877 µL, 6.31 mmol) was added at ice-water temperature, and the mixture was stirred for 30 min at room temperature. The solvent was removed under gently reduced pressure, and the residue was passed through a short pad of silica gel (ether/pentane = 2/1 containing 2% triethylamine) to obtain the corresponding crude material of methyl imidate (174 mg), which was subjected to the next reaction without purification. A mixture of the imidate (30 mg, 0.24 mmol), *N*-(diphenylmethylene)glycine ethyl ester (**7**) (320 mg, 1.20 mmol),

and acetic acid (27 μL, 0.48 mmol) in toluene (1.2 mL) was stirred at room temperature for 2.5 days. The mixture was diluted with ethyl acetate and was washed with 5% aqueous HCl. The acidic aqueous layer was re-extracted with ethyl acetate after neutralization with a saturated solution of $NaHCO_3$. The combined organic layers were washed with a saturated solution of $NaHCO_3$ and brine, dried over Na_2SO_4, and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (ethyl acetate/hexane = 1/4, then 1/2) to yield **13** (19 mg, 19% over 2 steps) as a yellow solid. ^{1}H-NMR ($CDCl_3$) δ: 7.60-7.58 (2H, m), 7.43-7.31 (8H, m), 6.42-6.34 (2H, m), 3.72-3.70 (2H, m), 2.62-2.59 (2H, m), 2.00-1.95 (2H, m). ^{13}C-NMR ($CDCl_3$) δ: 168.3, 159.1, 146.9, 141.9, 139.3, 138.2, 137.2, 132.6, 130.4, 129.5, 128.9, 127.9, 127.8, 120.6, 41.0, 32.6, 25.6. IR (KBr) ν_{max}: 1645, 1705 cm^{-1}. HRMS (FAB) m/z: $[M + H]^+$ Calcd for $C_{21}H_{19}N_2O$ 315.1498; Found 315.1495.

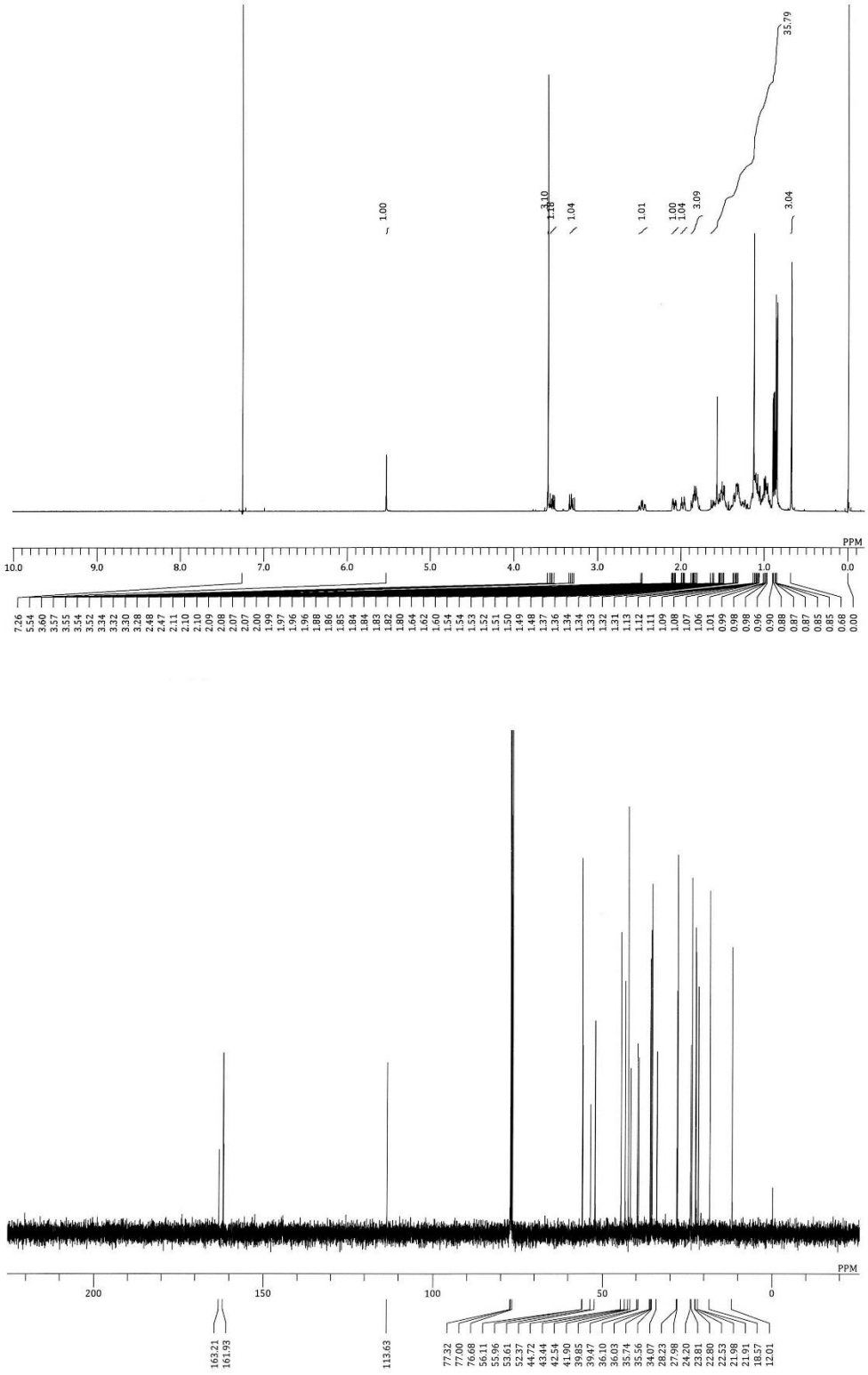
2. References

1) M. J. O'Donnell and R. L. Polt, *J. Org. Chem.* 1982, **47**, 2663–2666.

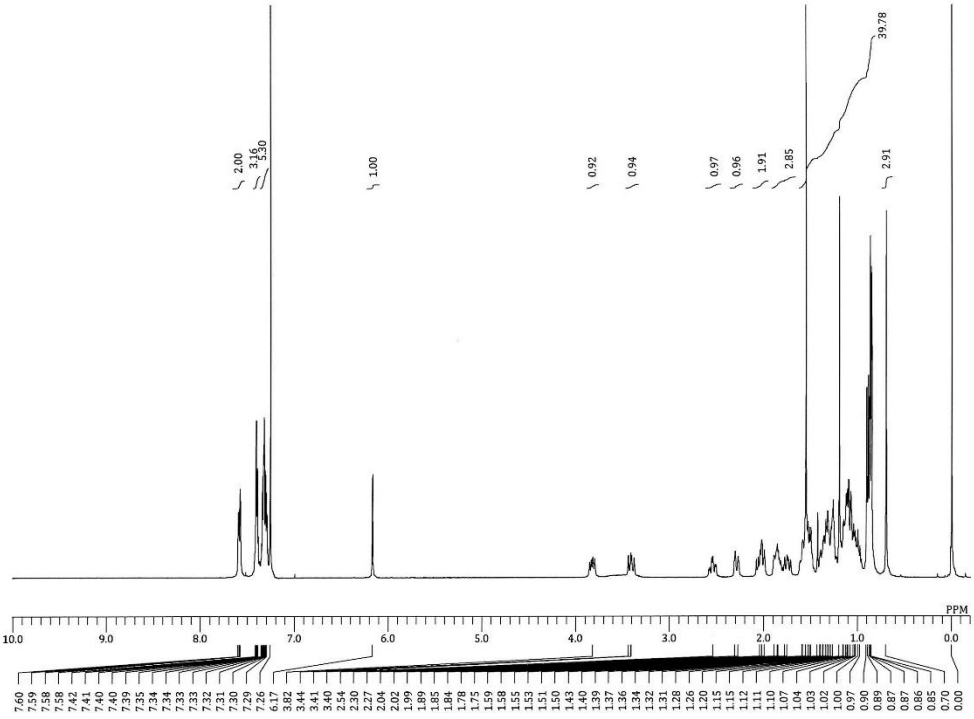
2) S. Álvarez, G. Domínguez, A. Gradillas and J. Pérez-Castells, *Eur. J. Org. Chem.* 2013, 3094–3102.

3. ^{1}H and ^{13}C NMR spectra of new compounds

Compound **6**



Compound **1**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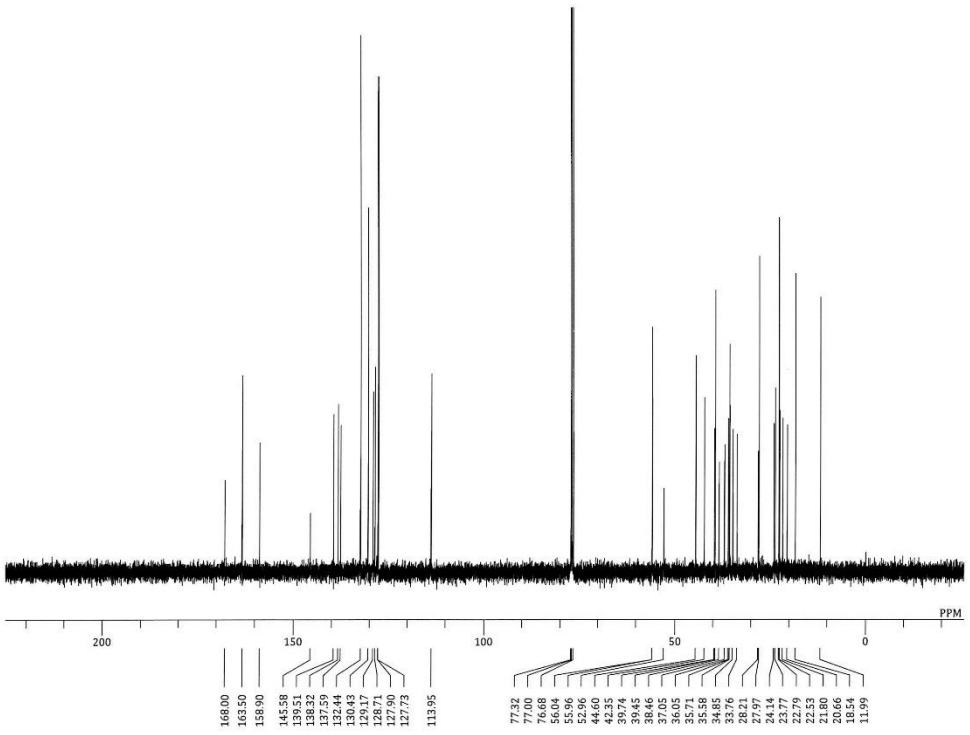
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11.99

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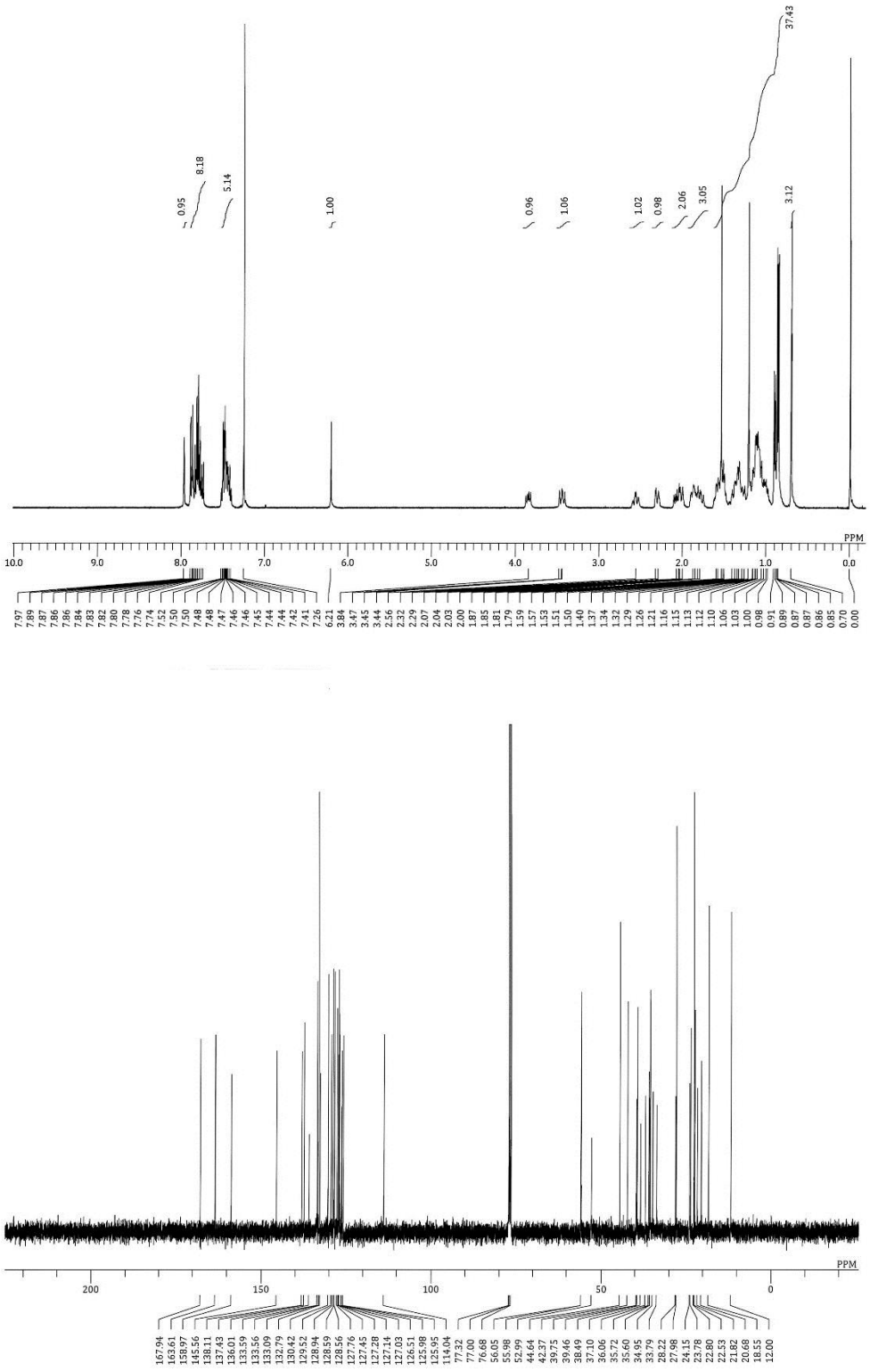
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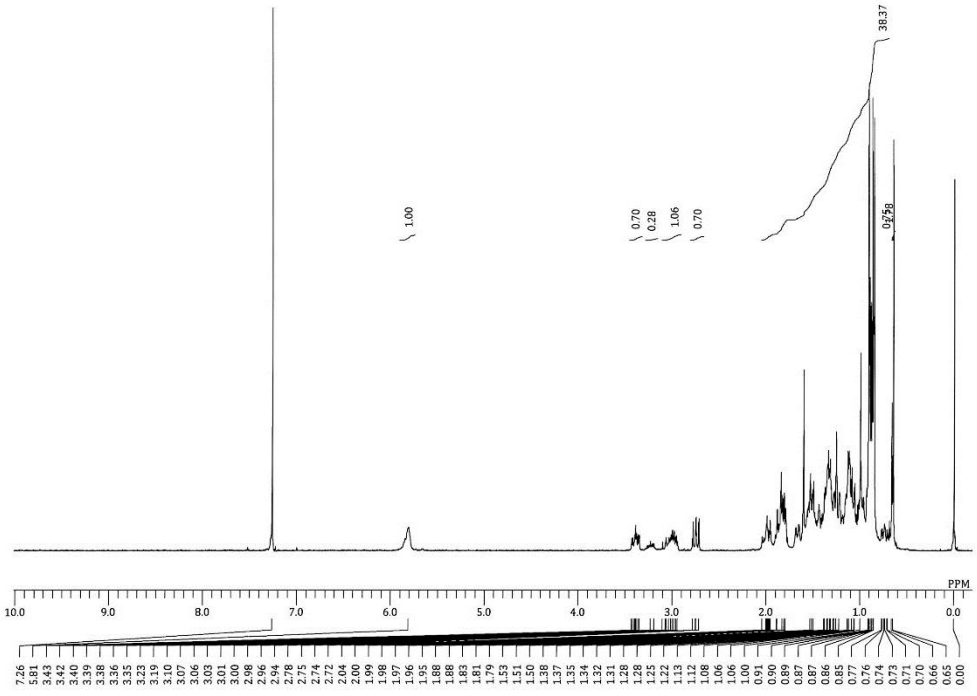
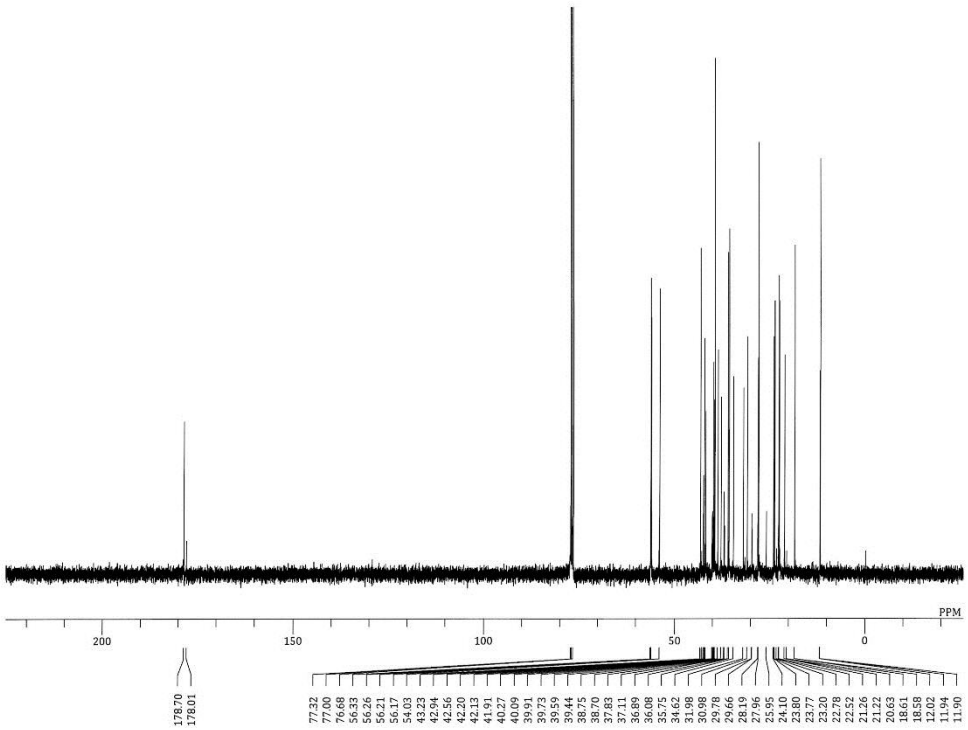
Compound **9** (from **5**)





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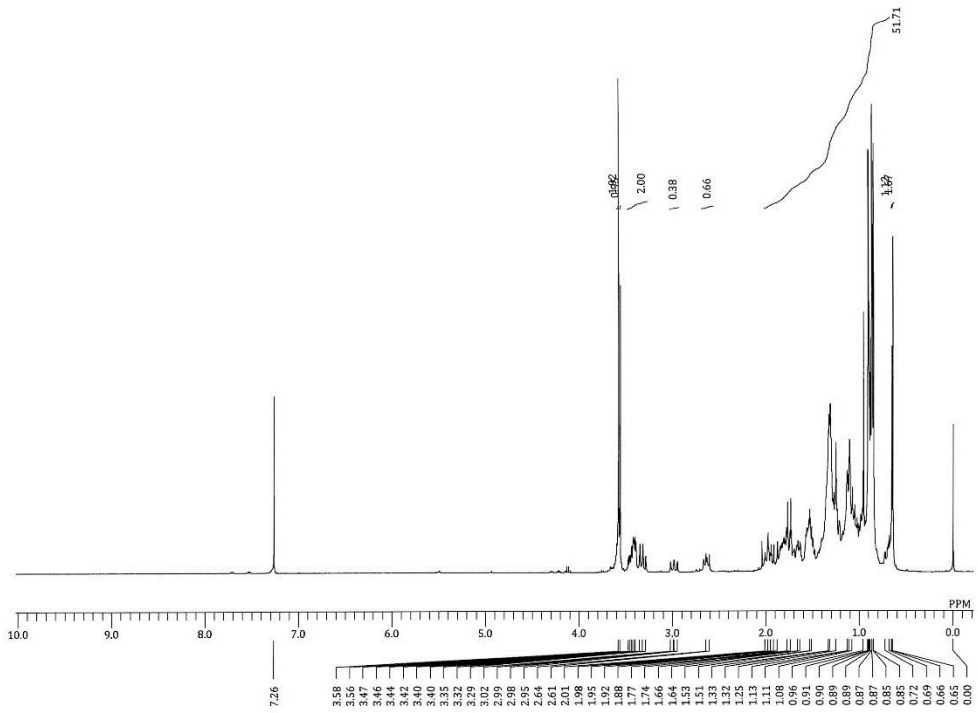

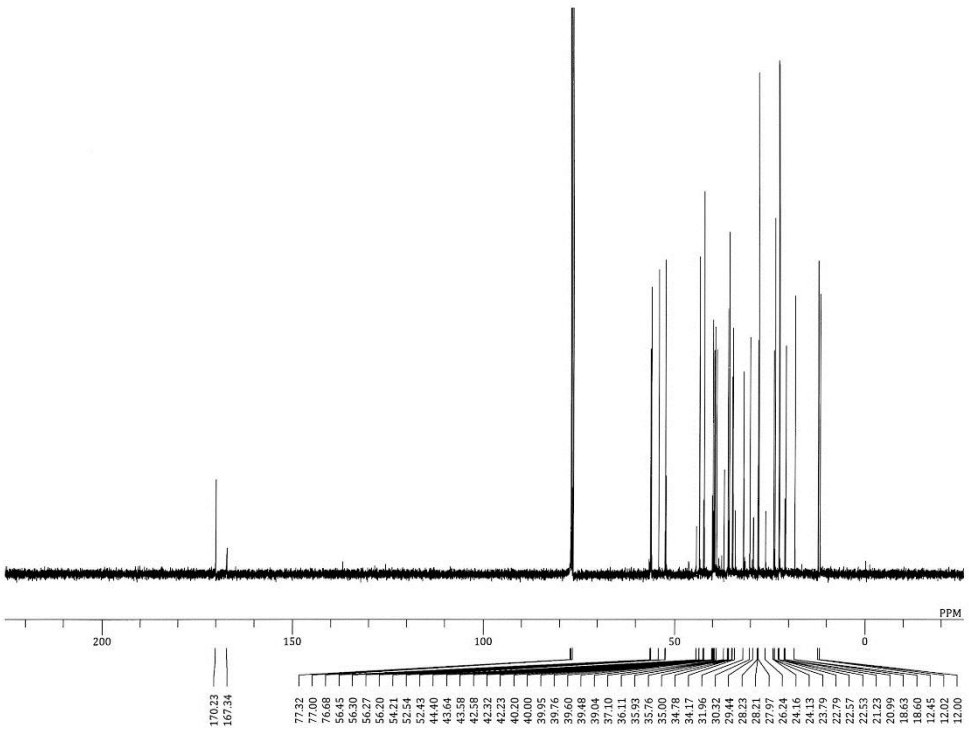

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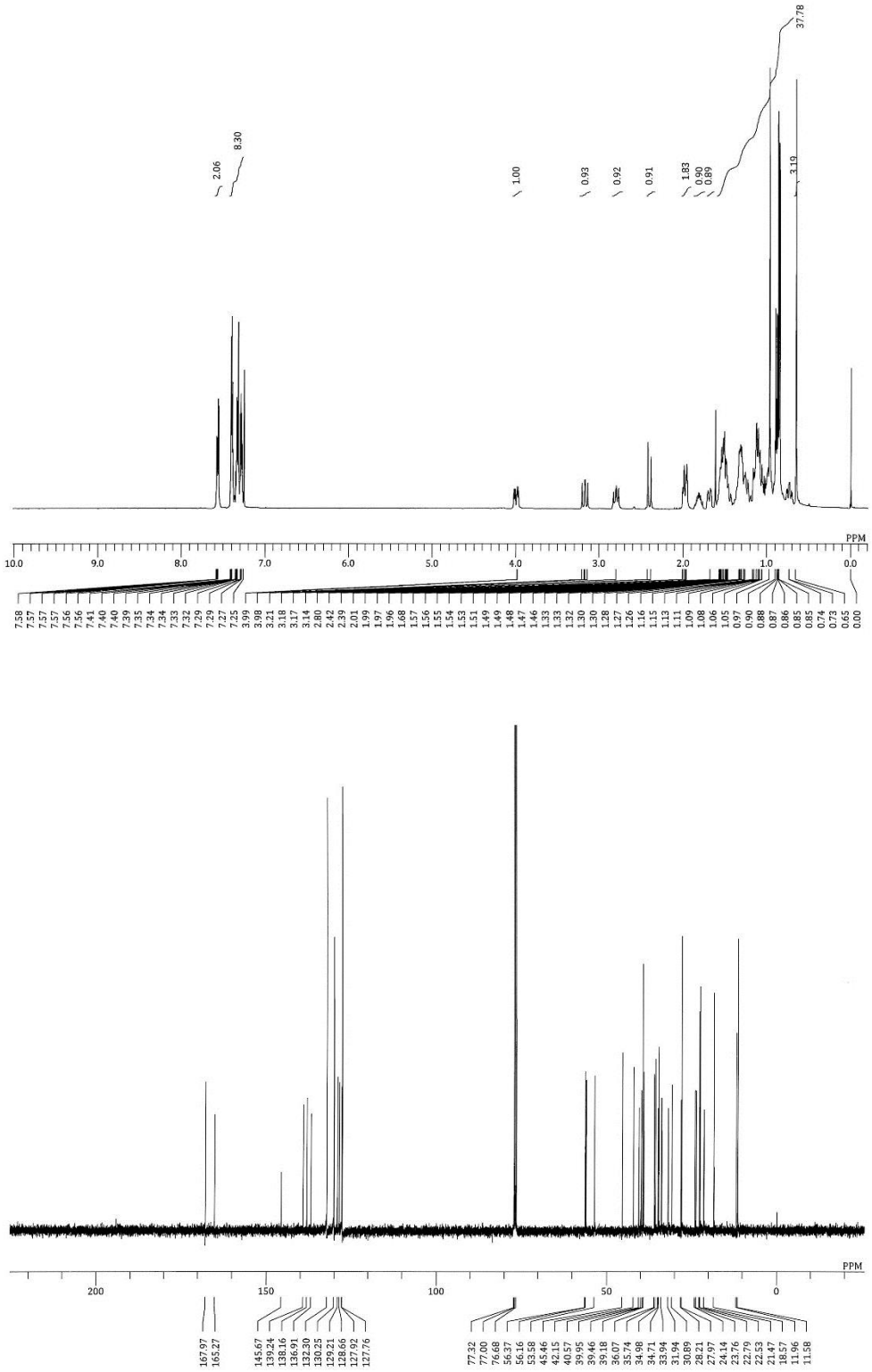

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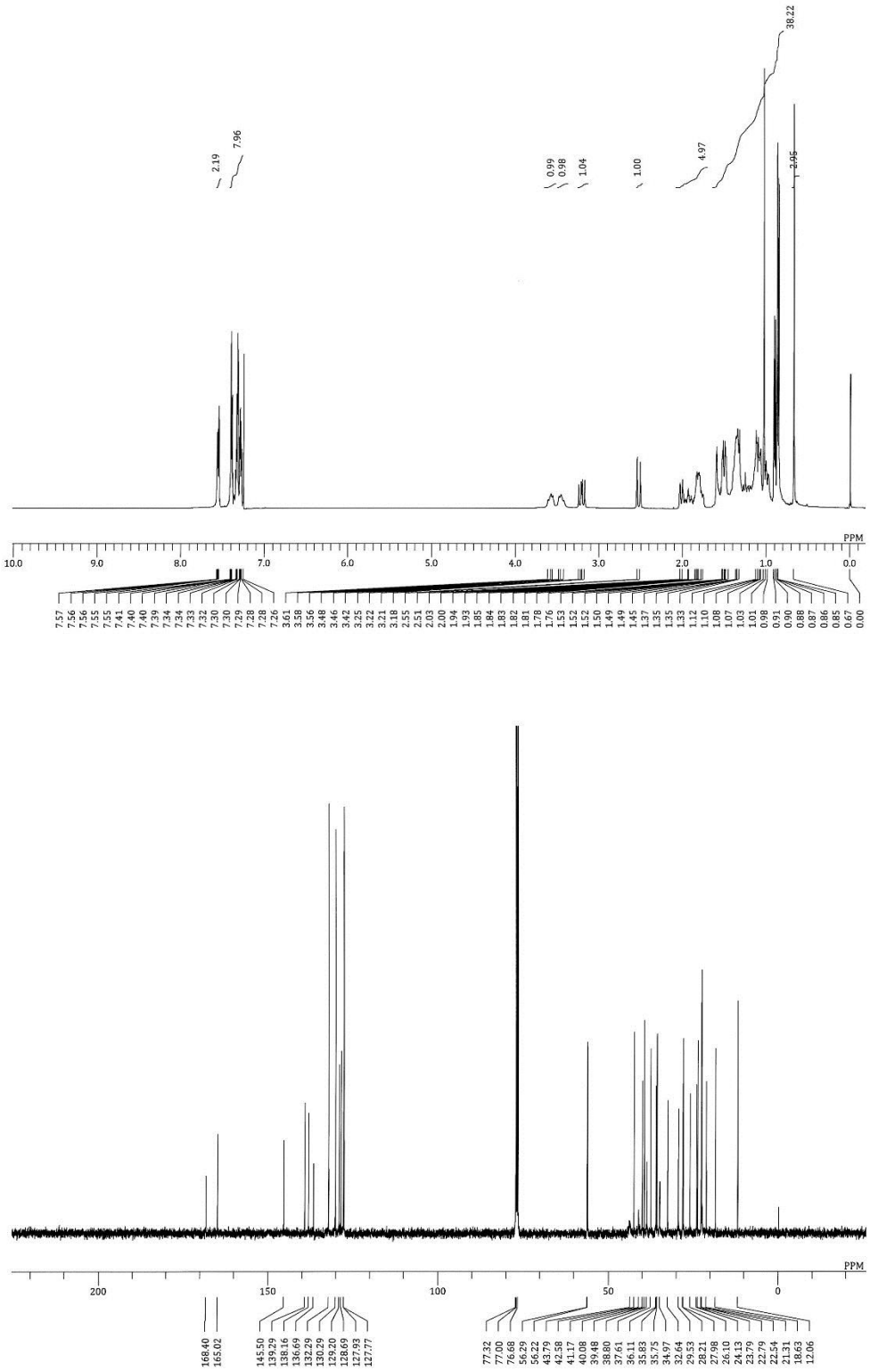
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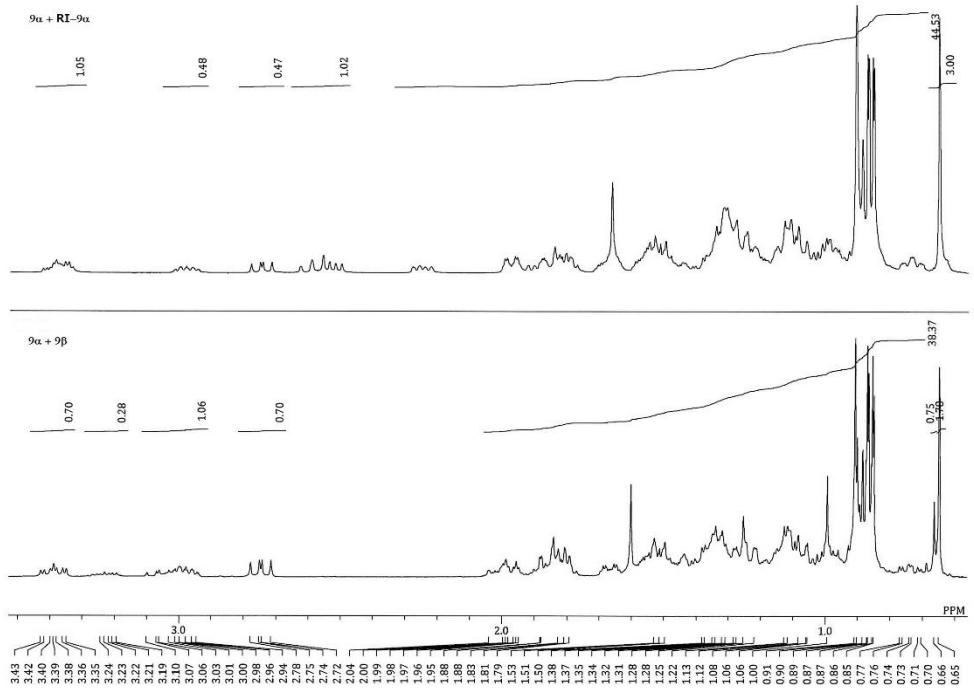
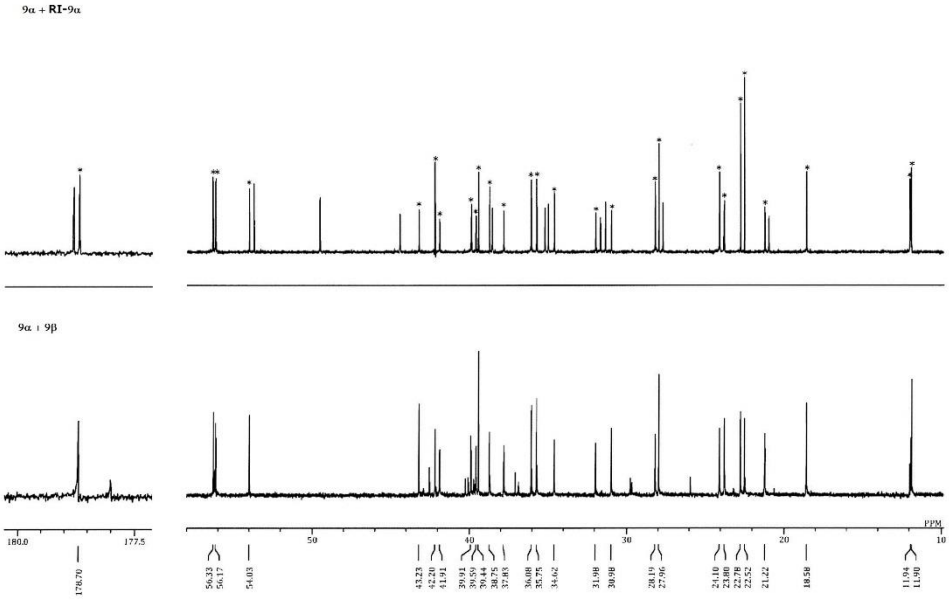
Compound **9α** + RI-**9α** (comparison with **9**)





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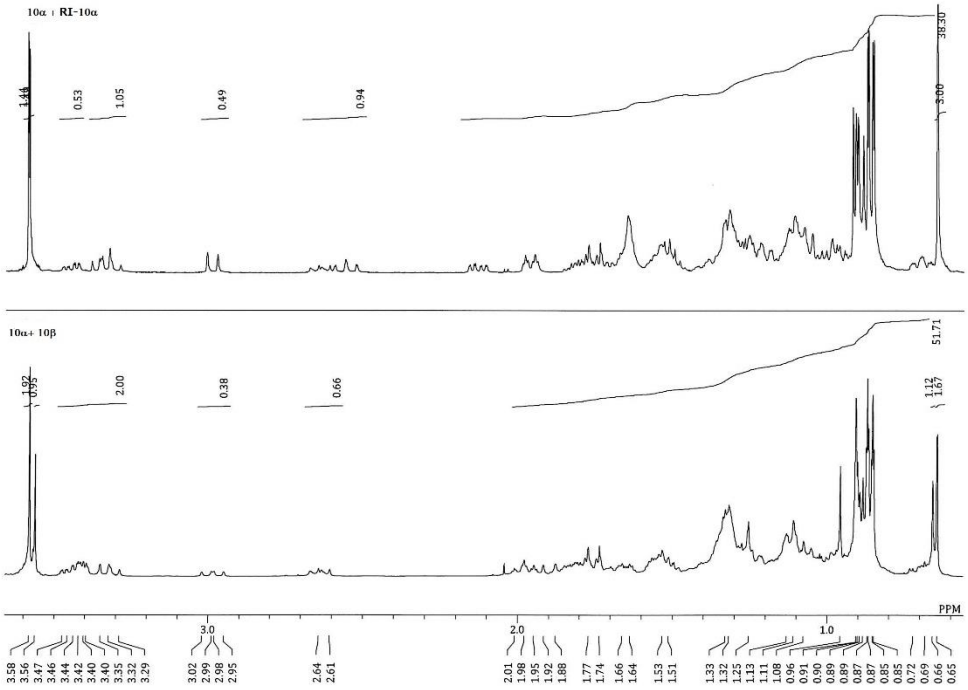
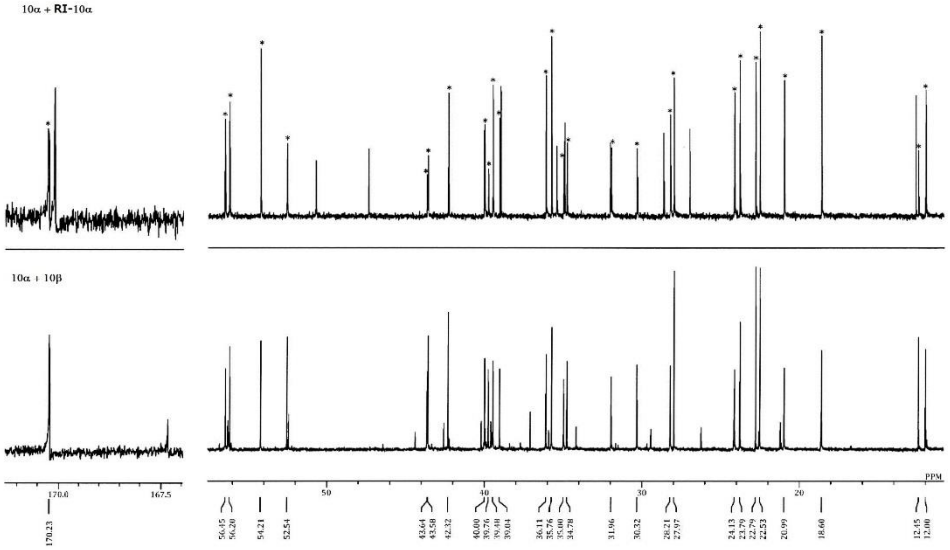
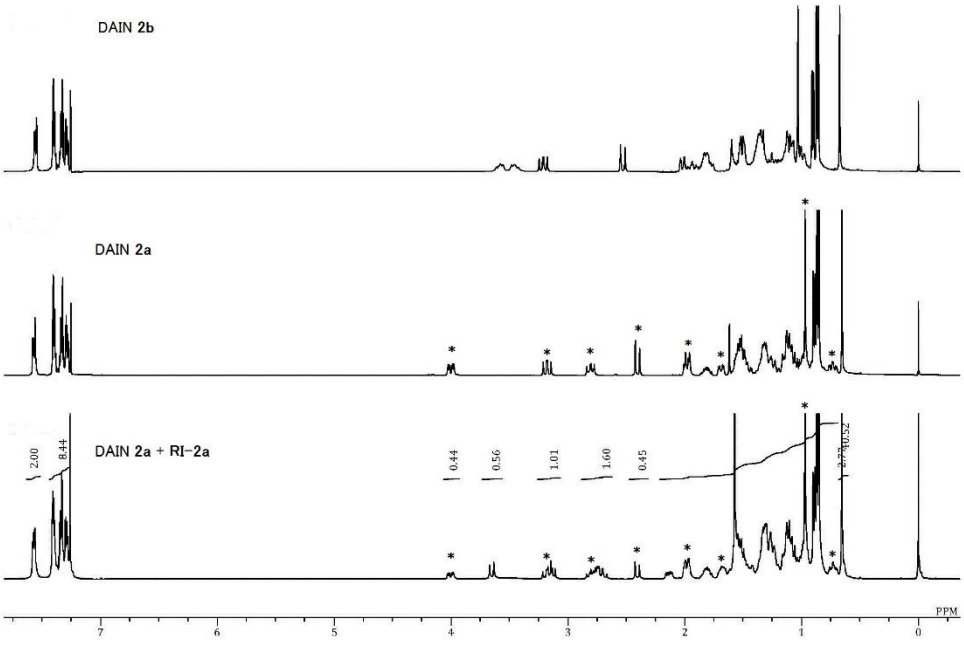
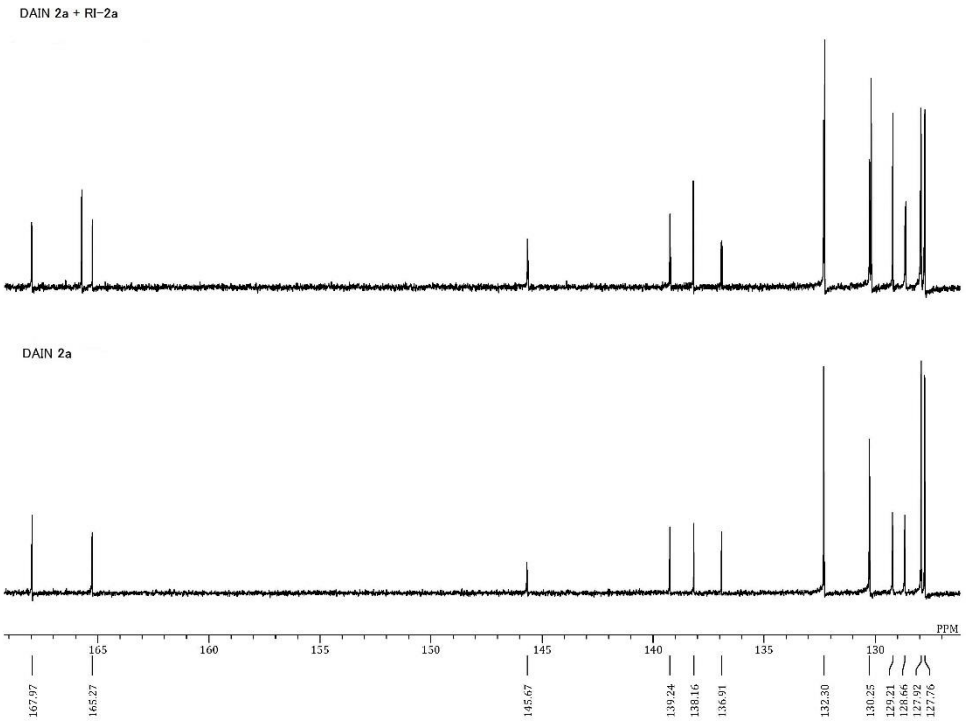


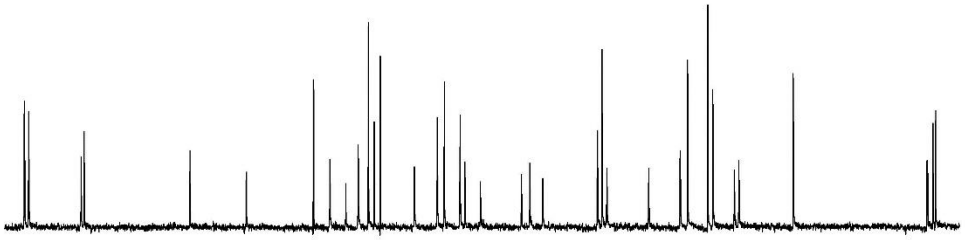


Compound **2a** + RI-**2a** (comparison with **2a**)

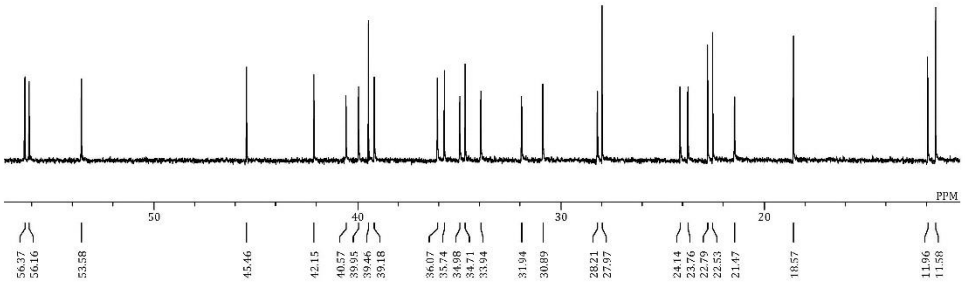




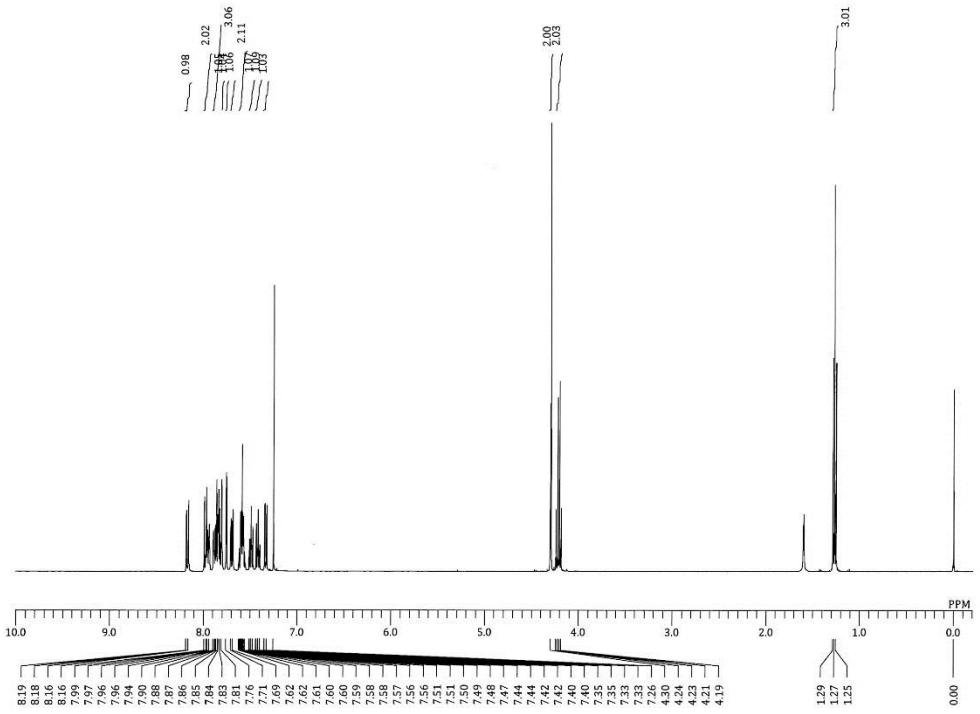
DAIN 2a + RI-2a



DAIN 2a



Compound **8**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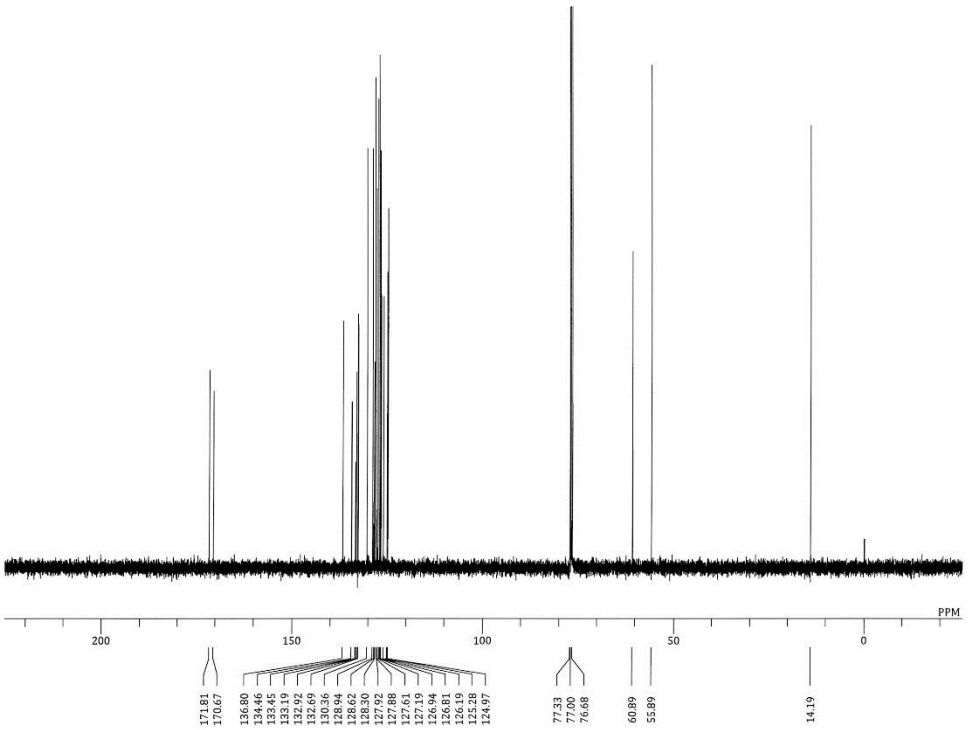
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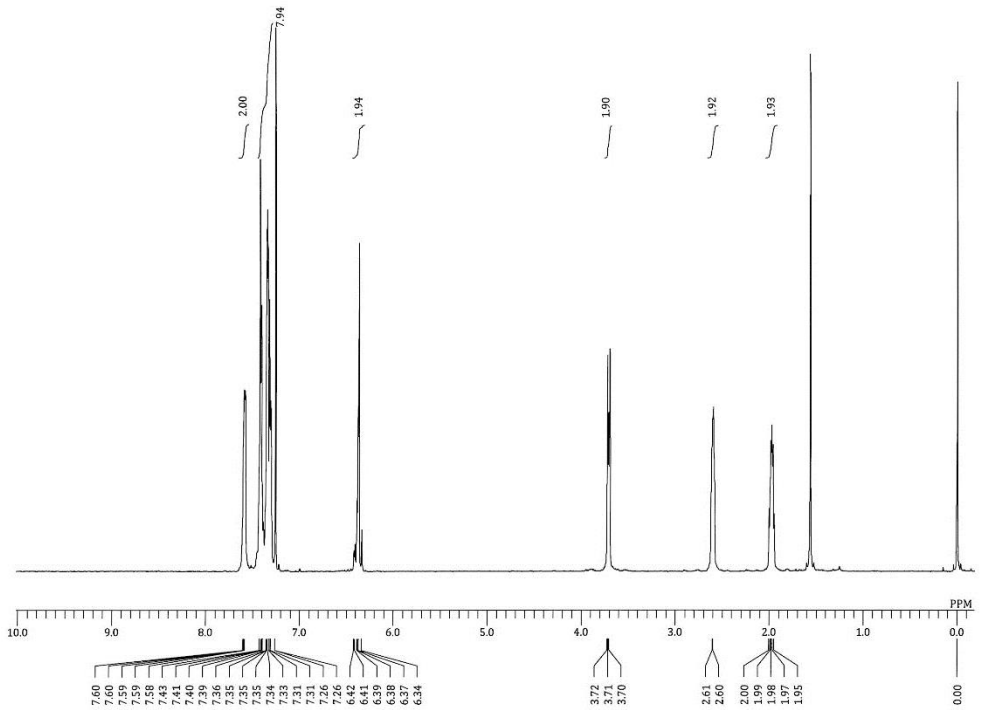
Compound **13**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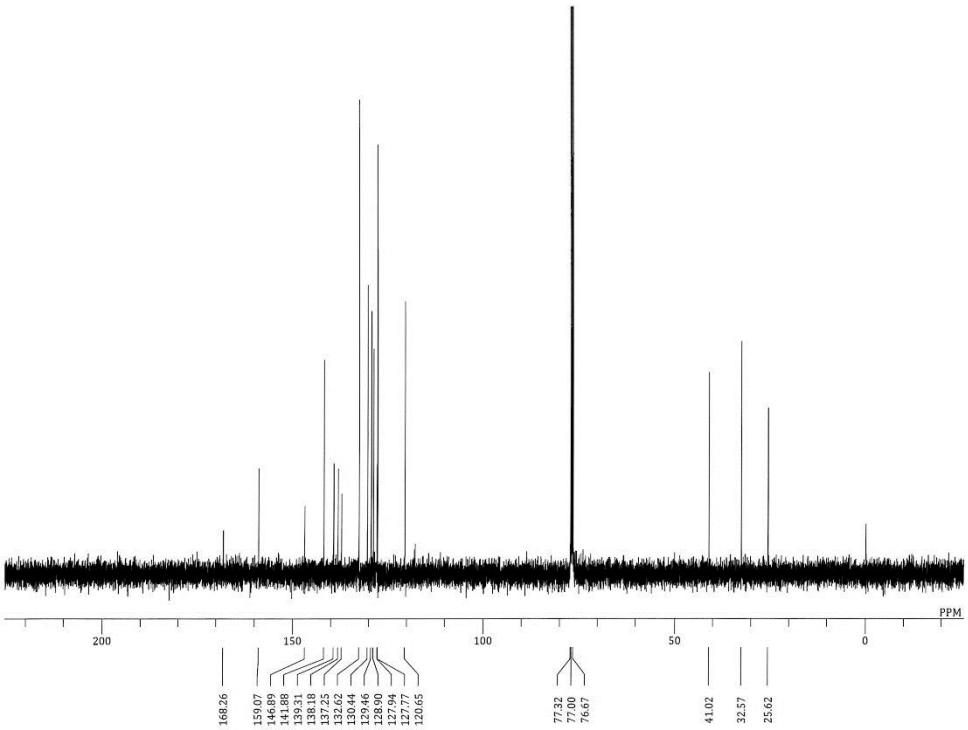
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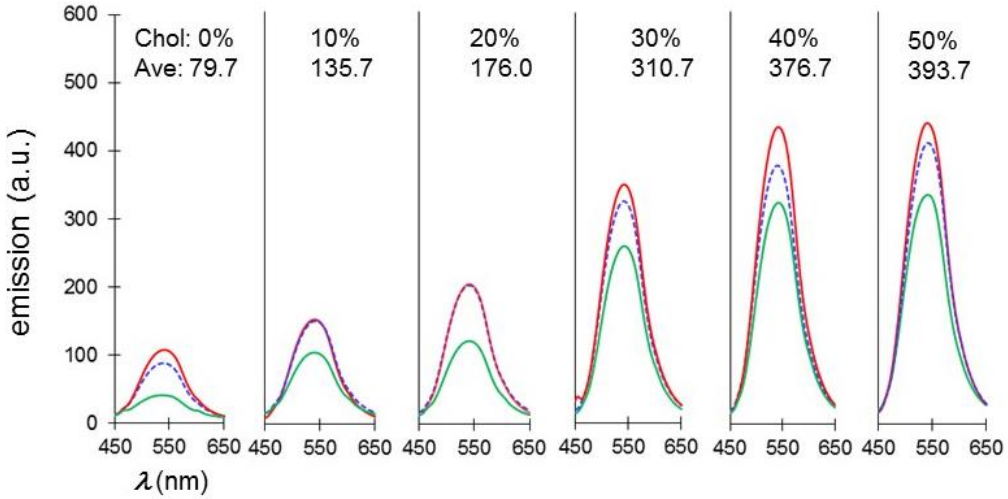
4. Figures S1—S3.



$y = 6.9362x + 71.984$, $R^2 = 0.9589$ (from 0 to 50%)

$y = 7.69x + 61.933$, $R^2 = 0.9629$ (from 0 to 40%)

Fig. S1. Fluorescence spectra of DAIN **1** in Fig. 10. Experiments were repeated three times.

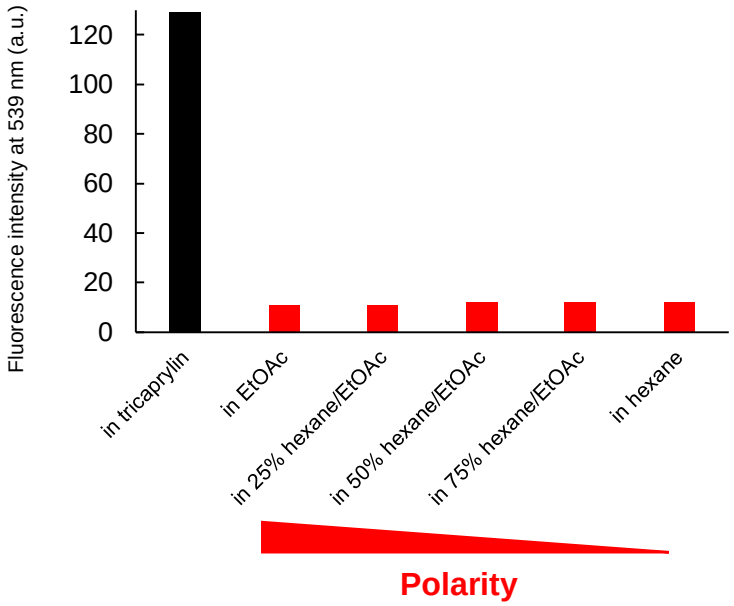


Fig. S2. Fluorescence of Ch-DAIN **1** in EtOAc/hexane and tricaprylin.

The fluorescence intensity of Ch-DAIN **1** was not enhanced by decreasing the solvent polarity. Therefore, the fluorescence enhancement of Ch-DAIN **1** was not due to the low polarity of the solvent.

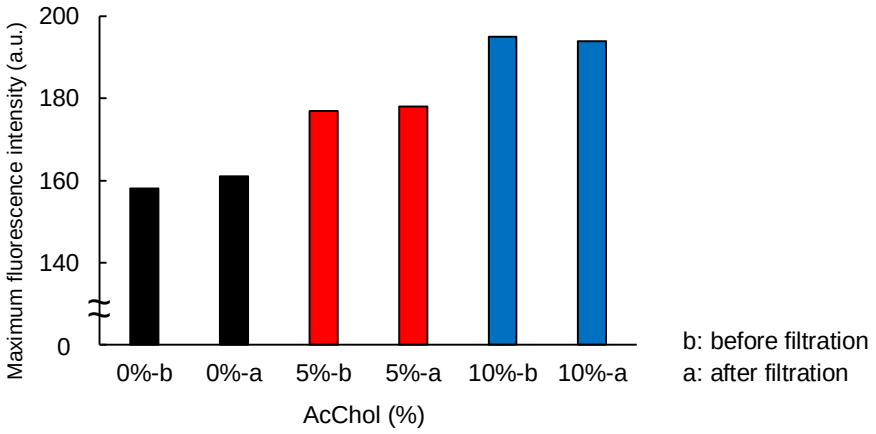


Fig. S3. Fluorescence of Ch-DAIN **1** in tricaprylin containing 0, 5, 10% cholesterol acetate (AcChol) before and after filtration (0.2 μm, PTFE filter).

The fluorescence intensity of Ch-DAIN **1** was not decreased after filtration. In addition, Tyndall effect was not observed for every solution. Therefore, the fluorescence enhancement of Ch-DAIN **1** was not due to the aggregation-induced emission mechanism.

5. Mol2 files, energies and number of imaginary frequencies for computed structure

Ch(en)-DAIN **1'**:
E = -1542.60389023 A.U.
No imaginary frequencies

@<TRIPOS>MOLECULE
Molecule Name
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SMALL
NO_CHARGES

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3 C3 -1.3897 0.9376 1.1593 C
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5 C5 -2.0809 -0.4347 1.2000 C
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8 C8 1.0980 0.4299 0.7133 C
9 C9 -0.0894 1.2347 0.9228 C
10 N10 2.2199 0.9669 0.2975 N
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12 C12 2.4910 -1.3523 0.6194 C
13 O13 2.8878 -2.5020 0.7292 O
14 C14 4.4676 0.1049 -0.1563 C
15 C15 0.1644 -1.8077 1.4579 C
16 C16 -1.1769 -1.6128 0.7469 C
17 C17 -5.3785 0.8036 -0.6261 C
18 C18 -6.2291 -0.4923 -0.6244 C
19 C19 -5.2793 -1.6686 -0.8953 C
20 C20 -4.1090 -1.7096 0.1109 C
21 C21 -7.2280 -0.1560 -1.7691 C
22 C22 -7.5888 1.3392 -1.5138 C
23 C23 -6.4211 1.9382 -0.6714 C
24 C24 -6.9895 -0.7135 0.7022 C
25 C25 -2.5502 -0.7062 2.6559 C
26 C26 -8.4441 -1.0695 -1.9343 C
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37 H37 -1.7433 -2.5363 0.8967 H
38 H38 -0.9828 -1.5379 -0.3312 H
39 H39 -5.8124 -2.6286 -0.8627 H
40 H40 -4.8733 -1.5712 -1.9131 H
41 H41 -4.4947 -1.9766 1.1024 H
42 H42 -3.4457 -2.5272 -0.1866 H
43 H43 -6.6501 -0.2070 -2.7042 H
44 H44 -8.5398 1.4159 -0.9730 H
45 H45 -7.7285 1.8747 -2.4591 H
46 H46 -6.7597 2.1988 0.3392 H
47 H47 -6.0178 2.8548 -1.1136 H
48 H48 -7.7053 0.0890 0.9085 H
49 H49 -7.5535 -1.6523 0.6641 H
50 H50 -6.3188 -0.7767 1.5637 H
51 H51 -3.3112 0.0037 2.9892 H
52 H52 -2.9725 -1.7122 2.7480 H
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54 H54 -9.1068 -1.0315 -1.0622 H
55 H55 -8.1469 -2.1144 -2.0863 H
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59 C59 6.6320 -1.1003 0.2209 C
60 C60 5.0176 -2.0890 -1.2772 C
61 C61 5.8950 -3.1418 -1.5251 C
62 C62 7.5020 -2.1636 -0.0123 C
63 H63 6.9228 -0.3012 0.8966 H
64 H64 4.0532 -2.0595 -1.7733 H
65 H65 5.6062 -3.9306 -2.2146 H
66 H66 8.4666 -2.1899 0.4877 H
67 H67 7.8194 -4.0113 -1.0806 H
68 C68 5.0566 1.4545 -0.3335 C
69 C69 6.2412 3.9893 -0.6970 C
70 C70 4.6906 2.5469 0.4773 C
71 C71 6.0362 1.6644 -1.3248 C
72 C72 6.6128 2.9183 -1.5117 C
73 C73 5.2819 3.7950 0.2995 C
74 H74 3.9411 2.4070 1.2456 H
75 H75 6.3335 0.8370 -1.9610 H
76 H76 7.3556 3.0574 -2.2928 H
77 H77 4.9928 4.6205 0.9447 H
78 H78 6.6971 4.9663 -0.8350 H
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Ch(an)-DAIN **2a'**:
E = -1543.82394874 A.U.
No imaginary frequencies.

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Molecule Name
80 86
SMALL
NO_CHARGES

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2 C2 -3.3821 2.1384 -0.3478 C
3 C3 -2.1427 2.3539 0.5209 C
4 C4 -2.0448 -0.1591 1.1244 C
5 C5 -4.2040 0.9231 0.0998 C
6 N6 1.2203 -0.7420 1.2449 N
7 C7 1.2330 0.6268 1.0484 C
8 N8 2.3382 1.0796 0.5342 N
9 C9 3.1747 -0.0350 0.3392 C
10 C10 2.4417 -1.2675 0.7923 C
11 O11 2.7406 -2.4504 0.8356 O
12 C12 4.4653 0.0365 -0.1141 C
13 C13 0.1393 -1.5423 1.7900 C
14 C14 -1.1785 -1.4495 1.0070 C
15 C15 -5.3741 0.6547 -0.8564 C
16 C16 -6.2600 -0.5543 -0.4637 C
17 C17 -5.3609 -1.7978 -0.4528 C
18 C18 -4.1415 -1.6187 0.4774 C
19 C19 -7.3113 -0.4967 -1.6095 C
20 C20 -7.6139 1.0255 -1.7556 C
21 C21 -6.3847 1.7784 -1.1618 C
22 C22 -6.9501 -0.3777 0.9071 C
23 C23 -2.4860 0.0171 2.5951 C
24 C24 -8.5613 -1.3675 -1.4671 C
25 H25 -2.8891 -0.4811 -0.8336 H
26 H26 -4.6105 1.1403 1.0982 H

27 H27	-4.9172	0.3800	-1.8230 H
28 H28	-4.0057	3.0410	-0.3382 H
29 H29	-3.0674	1.9901	-1.3925 H
30 H30	-2.4410	2.6666	1.5315 H
31 H31	-1.5478	3.1807	0.1123 H
32 H32	-0.0080	-1.2908	2.8477 H
33 H33	0.5086	-2.5714	1.7546 H
34 H34	-1.7806	-2.2945	1.3567 H
35 H35	-0.9585	-1.6434	-0.0520 H
36 H36	-5.9189	-2.6926	-0.1441 H
37 H37	-5.0067	-1.9890	-1.4767 H
38 H38	-4.4849	-1.6059	1.5189 H
39 H39	-3.5160	-2.5112	0.3774 H
40 H40	-6.7876	-0.8227	-2.5209 H
41 H41	-8.5315	1.2873	-1.2148 H
42 H42	-7.7895	1.2900	-2.8041 H
43 H43	-6.6604	2.3157	-0.2456 H
44 H44	-5.9799	2.5242	-1.8533 H
45 H45	-6.2336	-0.2310	1.7203 H
46 H46	-7.5394	-1.2683	1.1537 H
47 H47	-7.6324	0.4787	0.9196 H
48 H48	-3.1562	0.8703	2.7315 H
49 H49	-3.0122	-0.8736	2.9541 H
50 H50	-1.6354	0.1706	3.2663 H
51 H51	-9.1735	-1.0688	-0.6084 H
52 H52	-8.3046	-2.4272	-1.3454 H
53 H53	-9.1918	-1.2842	-2.3607 H
54 C54	5.1522	1.3345	-0.3297 C
55 C55	6.5153	3.7642	-0.7749 C
56 C56	4.9360	2.4484	0.5050 C
57 C57	6.0749	1.4677	-1.3864 C
58 C58	6.7397	2.6706	-1.6129 C
59 C59	5.6147	3.6445	0.2858 C
60 H60	4.2325	2.3671	1.3234 H
61 H61	6.2583	0.6219	-2.0410 H
62 H62	7.4361	2.7517	-2.4434 H
63 H63	5.4404	4.4876	0.9493 H
64 H64	7.0402	4.7008	-0.9445 H
65 C65	5.2485	-1.1901	-0.4313 C
66 C66	6.7896	-3.4562	-1.0656 C
67 C67	4.7579	-2.1674	-1.3109 C
68 C68	6.5321	-1.3628	0.1148 C
69 C69	7.2902	-2.4922	-0.1886 C
70 C70	5.5236	-3.2865	-1.6298 C
71 H71	3.7733	-2.0414	-1.7492 H
72 H72	6.9290	-0.6087	0.7883 H
73 H73	8.2744	-2.6158	0.2556 H
74 H74	5.1291	-4.0293	-2.3179 H
75 H75	7.3839	-4.3325	-1.3111 H
76 C76	-1.2546	1.0974	0.6018 C
77 H77	-0.9489	0.8608	-0.4291 H
78 C78	0.0427	1.4642	1.3783 C
79 H79	0.3257	2.4923	1.1354 H
80 H80	-0.1409	1.4385	2.4609 H

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11 3 76 1
12 4 14 1
13 4 23 1
14 4 76 1
15 5 15 1
16 5 26 1
17 6 7 1
18 6 10 1
19 6 13 1
20 7 8 2
21 7 78 1
22 8 9 1
23 9 10 1
24 9 12 2
25 10 11 2
26 12 54 1
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28 13 14 1
29 13 32 1
30 13 33 1
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76 66 75 1
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Ch(an)-DAIN **2b'**:
E = -1543.82114804 A.U.
No imaginary frequencies.

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Molecule Name
80 86
SMALL
NO_CHARGES

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1 C1	-3.2944	-0.5645	0.1360 C
2 C2	-3.3352	1.7820	1.1164 C
3 C3	-2.2150	1.3905	2.0842 C
4 C4	-2.1150	-0.9865	1.0858 C
5 C5	-4.1896	0.5672	0.7231 C
6 N6	1.1660	-1.1687	0.5238 N
7 C7	0.9737	0.1936	0.3374 C
8 N8	2.0640	0.8459	0.0595 N
9 C9	3.1040	-0.0980	0.0179 C
10 C10	2.5278	-1.4503	0.3207 C
11 O11	3.0170	-2.5643	0.4264 O
12 C12	4.4231	0.2094	-0.1879 C
13 C13	0.2104	-2.2073	0.8917 C
14 C14	-1.1944	-1.9853	0.3193 C
15 C15	-5.2678	0.9302	-0.3073 C
16 C16	-6.1715	-0.2580	-0.7294 C
17 C17	-5.2679	-1.3398	-1.3432 C
18 C18	-4.1390	-1.7572	-0.3774 C
19 C19	-7.1193	0.4692	-1.7261 C
20 C20	-7.4224	1.8278	-1.0230 C
21 C21	-6.2613	2.0705	-0.0109 C
22 C22	-6.9809	-0.8446	0.4490 C
23 C23	-2.6337	-1.6969	2.3580 C
24 C24	-8.3703	-0.2828	-2.1856 C
25 H25	-2.8211	-0.1262	-0.7591 H
26 H26	-4.6829	0.1992	1.6351 H
27 H27	-4.7246	1.2250	-1.2222 H
28 H28	-3.9669	2.5524	1.5755 H
29 H29	-2.9100	2.2355	0.2083 H
30 H30	-2.6615	1.0521	3.0279 H
31 H31	-1.6032	2.2661	2.3372 H
32 H32	0.1809	-2.3121	1.9845 H
33 H33	0.6365	-3.1379	0.5057 H
34 H34	-1.6875	-2.9633	0.2984 H
35 H35	-1.0902	-1.6795	-0.7300 H
36 H36	-5.8479	-2.2284	-1.6279 H
37 H37	-4.8226	-0.9477	-2.2697 H
38 H38	-4.5747	-2.2986	0.4706 H
39 H39	-3.4930	-2.4759	-0.8940 H
40 H40	-6.5162	0.6812	-2.6218 H
41 H41	-8.3891	1.7848	-0.5070 H
42 H42	-7.5018	2.6377	-1.7565 H
43 H43	-6.6242	2.0135	1.0231 H
44 H44	-5.8065	3.0593	-0.1297 H
45 H45	-6.3401	-1.1960	1.2625 H
46 H46	-7.5744	-1.7025	0.1133 H
47 H47	-7.6758	-0.1153	0.8786 H
48 H48	-3.3076	-1.0674	2.9458 H
49 H49	-3.1726	-2.6182	2.1137 H
50 H50	-1.8005	-1.9746	3.0143 H
51 H51	-9.0532	-0.4869	-1.3531 H
52 H52	-8.1170	-1.2408	-2.6562 H
53 H53	-8.9250	0.3082	-2.9246 H
54 C54	4.9010	1.6126	-0.2568 C
55 C55	5.8785	4.2546	-0.4062 C
56 C56	4.3511	2.6332	0.5431 C
57 C57	5.9576	1.9487	-1.1264 C
58 C58	6.4327	3.2555	-1.2083 C
59 C59	4.8400	3.9351	0.4714 C
60 H60	3.5394	2.3956	1.2185 H
61 H61	6.3970	1.1777	-1.7509 H
62 H62	7.2394	3.4919	-1.8972 H
63 H63	4.4084	4.7044	1.1065 H
64 H64	6.2546	5.2728	-0.4618 H

65 C65 5.4496 -0.8536 -0.3724 C
66 C66 7.4434 -2.8028 -0.7459 C
67 C67 5.2953 -1.8618 -1.3367 C
68 C68 6.6288 -0.8321 0.3923 C
69 C69 7.6105 -1.8057 0.2169 C
70 C70 6.2851 -2.8234 -1.5255 C
71 H71 4.3962 -1.8832 -1.9438 H
72 H72 6.7671 -0.0510 1.1342 H
73 H73 8.5086 -1.7817 0.8286 H
74 H74 6.1500 -3.5924 -2.2814 H
75 H75 8.2127 -3.5567 -0.8909 H
76 C76 -1.3003 0.2819 1.5241 C
77 H77 -0.6450 -0.0265 2.3507 H
78 C78 -0.3769 0.8404 0.4090 C
79 H79 -0.1873 1.9072 0.5628 H
80 H80 -0.8592 0.7629 -0.5747 H
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DAIN **1”** (optimized):
$E(S_0)$ = -1191.20182558 A.U.
No imaginary frequencies.

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Molecule Name
55 59
SMALL
NO_CHARGES

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3 C3 -3.6955 0.7169 0.1435 C
4 C4 -4.7043 1.8542 0.2091 C
5 C5 -4.3026 -0.6895 0.1348 C
6 C6 -6.4882 0.4004 -0.8107 C
7 N7 -1.0431 -1.0810 0.3264 N
8 C8 -1.1572 0.2889 0.1350 C
9 C9 -2.3867 1.0591 0.1174 C
10 N10 0.0007 0.8851 -0.0231 N
11 C11 0.9831 -0.1041 0.0365 C
12 C12 0.3131 -1.4296 0.2597 C
13 O13 0.7342 -2.5677 0.3988 O
14 C14 -2.0892 -2.0540 0.5732 C
15 C15 -3.3260 -1.8133 -0.2911 C
16 C16 2.3335 0.1404 -0.0168 C
17 C17 2.8779 1.5198 -0.0188 C
18 C18 3.9833 4.1151 -0.0401 C
19 C19 4.0396 1.8093 -0.7623 C
20 C20 2.2878 2.5632 0.7214 C
21 C21 2.8397 3.8415 0.7138 C
22 C22 4.5785 3.0933 -0.7820 C
23 C23 3.3254 -0.9664 -0.0835 C
24 C24 5.2653 -3.0005 -0.2105 C
25 C25 3.2330 -1.9867 -1.0435 C
26 C26 4.4160 -0.9786 0.8040 C
27 C27 5.3697 -1.9929 0.7501 C
28 C28 4.1972 -2.9896 -1.1102 C
29 C29 -4.8734 -1.0066 1.5422 C
30 H30 -7.2203 0.3026 -1.6224 H
31 H31 -7.0571 0.3220 0.1261 H
32 H32 -6.5117 2.5777 -0.7469 H
33 H33 -5.3296 1.8937 -1.8636 H
34 H34 -5.9620 -1.7070 -0.8295 H
35 H35 -5.0131 -0.7000 -1.9168 H
36 H36 -4.1811 2.8137 0.1446 H
37 H37 -5.1991 1.8390 1.1927 H
38 H38 -5.6824 -0.3256 1.8197 H
39 H39 -5.2787 -2.0257 1.5616 H
40 H40 -4.1038 -0.9306 2.3166 H
41 H41 -3.9044 -2.7461 -0.3097 H
42 H42 -2.9939 -1.6352 -1.3220 H
43 H43 -2.1484 2.1200 0.0895 H
44 H44 -2.3421 -2.0721 1.6411 H
45 H45 -1.6431 -3.0248 0.3389 H
46 H46 4.5049 -0.1906 1.5460 H
47 H47 6.1967 -1.9930 1.4553 H
48 H48 6.0133 -3.7874 -0.2608 H
49 H49 4.1124 -3.7664 -1.8655 H
50 H50 2.4044 -1.9834 -1.7438 H
51 H51 1.3951 2.3614 1.2992 H
52 H52 2.3745 4.6282 1.3021 H
53 H53 4.4087 5.1153 -0.0466 H
54 H54 5.4672 3.2942 -1.3747 H
55 H55 4.5112 1.0205 -1.3394 H
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DAIN **1”** (0 °):
$E(S_0)$ = -1191.20102850 A.U.
$E(S_1)$ = -1191.09228404 A.U.

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SMALL
NO_CHARGES

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2 C2 5.7171 1.8730 0.6867 C
3 C3 3.7067 0.6647 -0.3021 C
4 C4 4.7251 1.7799 -0.4857 C
5 C5 4.3116 -0.7198 -0.0470 C
6 C6 6.4125 0.5269 0.9031 C
7 N7 1.0530 -1.1248 -0.3066 N
8 C8 1.1676 0.2564 -0.2775 C
9 C9 2.4012 1.0143 -0.3642 C
10 N10 0.0131 0.8689 -0.1754 N
11 C11 -0.9719 -0.1187 -0.1127 C
12 C12 -0.3025 -1.4629 -0.1893 C
13 O13 -0.7217 -2.6099 -0.1758 O
14 C14 2.1071 -2.1108 -0.4389 C
15 C15 3.3101 -1.7920 0.4492 C
16 C16 -2.3166 0.1385 -0.0134 C
17 C17 -2.8518 1.5223 0.0371 C
18 C18 -3.9479 4.1186 0.1863 C
19 C19 -3.9865 1.7893 0.8297 C
20 C20 -2.2866 2.5889 -0.6895 C
21 C21 -2.8348 3.8672 -0.6187 C
22 C22 -4.5191 3.0733 0.9141 C
23 C23 -3.3307 -0.9533 0.0327 C
24 C24 -5.3293 -2.9326 0.0986 C
25 C25 -3.3022 -1.9678 1.0018 C
26 C26 -4.3876 -0.9411 -0.8943 C
27 C27 -5.3694 -1.9295 -0.8714 C
28 C28 -4.2965 -2.9436 1.0379 C
29 C29 4.9970 -1.2252 -1.3445 C
30 H30 7.0631 0.5677 1.7859 H
31 H31 7.0695 0.3102 0.0495 H
32 H32 6.4500 2.6653 0.4908 H
33 H33 5.1723 2.1592 1.5970 H
34 H34 5.8856 -1.5601 1.1947 H
35 H35 4.8480 -0.4135 2.0336 H
36 H36 4.2053 2.7337 -0.6229 H
37 H37 5.2974 1.6049 -1.4093 H
38 H38 5.8123 -0.5703 -1.6614 H
39 H39 5.4199 -2.2243 -1.1827 H
40 H40 4.2880 -1.2866 -2.1762 H
41 H41 3.8820 -2.7190 0.5866 H
42 H42 2.9341 -1.5116 1.4416 H
43 H43 2.1746 2.0694 -0.4987 H
44 H44 2.3987 -2.2117 -1.4923 H
45 H45 1.6528 -3.0606 -0.1424 H
46 H46 -4.4304 -0.1536 -1.6412 H
47 H47 -6.1695 -1.9111 -1.6069 H
48 H48 -6.0999 -3.6987 0.1250 H
49 H49 -4.2611 -3.7170 1.8007 H
50 H50 -2.4999 -1.9873 1.7312 H
51 H51 -1.4154 2.4064 -1.3044 H
52 H52 -2.3891 4.6719 -1.1978 H
53 H53 -4.3688 5.1192 0.2426 H
54 H54 -5.3848 3.2553 1.5456 H
55 H55 -4.4425 0.9819 1.3936 H
@<TRIPOS>BOND
1 1 5 1
2 1 6 1
3 1 34 1
4 1 35 1
5 2 4 1
6 2 6 1
7 2 32 1
8 2 33 1
9 3 4 1
10 3 5 1
11 3 9 2
12 4 36 1
13 4 37 1
14 5 15 1
15 5 29 1
16 6 30 1
17 6 31 1
18 7 8 1
19 7 12 1
20 7 14 1
21 8 9 1
22 8 10 2
23 9 43 1
24 10 11 1
25 11 12 1
26 11 16 2
27 12 13 2
28 14 15 1
29 14 44 1
30 14 45 1
31 15 41 1
32 15 42 1
33 16 17 1
34 16 23 1
35 17 19 Ar
36 17 20 Ar
37 18 21 Ar
38 18 22 Ar
39 18 53 1
40 19 22 Ar
41 19 55 1
42 20 21 Ar
43 20 51 1
44 21 52 1
45 22 54 1
46 23 25 Ar
47 23 26 Ar
48 24 27 Ar
49 24 28 Ar
50 24 48 1
51 25 28 Ar
52 25 50 1
53 26 27 Ar
54 26 46 1
55 27 47 1
56 28 49 1
57 29 38 1
58 29 39 1
59 29 40 1

DAIN **1”** (15 °):
$E(S_0)$ = -1191.20140998 A.U.
$E(S_1)$ = -1191.09737350 A.U.

@<TRIPOS>MOLECULE
Molecule Name
55 59
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 5.3727 -0.7844 0.9649 C
2 C2 5.7187 1.7053 1.1059 C
3 C3 3.6889 0.7456 -0.0999 C
4 C4 4.7031 1.8771 -0.0381 C
5 C5 4.2949 -0.6604 -0.1607 C
6 C6 6.4095 0.3433 1.0052 C
7 N7 1.0387 -1.0099 -0.5118 N
8 C8 1.1493 0.3364 -0.1962 C
9 C9 2.3813 1.0949 -0.0948 C
10 N10 -0.0101 0.9149 0.0134 N
11 C11 -0.9871 -0.0710 -0.1259 C
12 C12 -0.3162 -1.3697 -0.4684 C
13 O13 -0.7388 -2.4880 -0.7177 O
14 C14 2.0958 -1.9456 -0.8397 C
15 C15 3.2952 -1.8151 0.0988 C
16 C16 -2.3381 0.1456 0.0091 C
17 C17 -2.9131 1.5093 -0.0031 C
18 C18 -4.0650 4.0845 -0.0225 C
19 C19 -4.0745 1.7925 0.7441 C
20 C20 -2.3456 2.5505 -0.7646 C
21 C21 -2.9197 3.8184 -0.7769 C
22 C22 -4.6379 3.0660 0.7413 C
23 C23 -3.2844 -0.9927 0.1449 C
24 C24 -5.1116 -3.1123 0.4371 C
25 C25 -3.0750 -1.9945 1.1064 C
26 C26 -4.4352 -1.0670 -0.6598 C
27 C27 -5.3338 -2.1231 -0.5231 C
28 C28 -3.9817 -3.0405 1.2549 C
29 C29 4.9650 -0.8721 -1.5439 C
30 H30 7.0815 0.1873 1.8583 H
31 H31 7.0406 0.3143 0.1070 H
32 H32 6.4529 2.5200 1.0781 H
33 H33 5.1935 1.7813 2.0682 H
34 H34 5.8726 -1.7562 0.8562 H
35 H35 4.8494 -0.8094 1.9311 H
36 H36 4.1814 2.8350 0.0557 H
37 H37 5.2582 1.9204 -0.9877 H
38 H38 5.7722 -0.1585 -1.7288 H
39 H39 5.3952 -1.8795 -1.6006 H
40 H40 4.2442 -0.7637 -2.3606 H
41 H41 3.8680 -2.7498 0.0405 H
42 H42 2.9162 -1.7489 1.1268 H
43 H43 2.1487 2.1531 0.0024 H
44 H44 2.3911 -1.8272 -1.8903 H
45 H45 1.6422 -2.9371 -0.7495 H
46 H46 -4.6131 -0.2960 -1.4037 H
47 H47 -6.2093 -2.1719 -1.1652 H
48 H48 -5.8163 -3.9319 0.5499 H
49 H49 -3.8049 -3.8024 2.0093 H
50 H50 -2.1995 -1.9398 1.7455 H
51 H51 -1.4534 2.3544 -1.3456 H
52 H52 -2.4713 4.6030 -1.3809 H
53 H53 -4.5086 5.0768 -0.0319 H
54 H54 -5.5266 3.2623 1.3354 H
55 H55 -4.5263 1.0071 1.3414 H
@<TRIPOS>BOND
1 1 5 1
2 1 6 1
3 1 34 1
4 1 35 1
5 2 4 1

6 2 6 1
7 2 32 1
8 2 33 1
9 3 4 1
10 3 5 1
11 3 9 2
12 4 36 1
13 4 37 1
14 5 15 1
15 5 29 1
16 6 30 1
17 6 31 1
18 7 8 1
19 7 12 1
20 7 14 1
21 8 9 1
22 8 10 2
23 9 43 1
24 10 11 1
25 11 12 1
26 11 16 2
27 12 13 2
28 14 15 1
29 14 44 1
30 14 45 1
31 15 41 1
32 15 42 1
33 16 17 1
34 16 23 1
35 17 19 Ar
36 17 20 Ar
37 18 21 Ar
38 18 22 Ar
39 18 53 1
40 19 22 Ar
41 19 55 1
42 20 21 Ar
43 20 51 1
44 21 52 1
45 22 54 1
46 23 25 Ar
47 23 26 Ar
48 24 27 Ar
49 24 28 Ar
50 24 48 1
51 25 28 Ar
52 25 50 1
53 26 27 Ar
54 26 46 1
55 27 47 1
56 28 49 1
57 29 38 1
58 29 39 1
59 29 40 1

DAIN **1”** (30 °):
$E(S_0)$ = -1191.19673202 A.U.
$E(S_1)$ = -1191.10095332 A.U.

@<TRIPOS>MOLECULE
Molecule Name
55 59
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 -5.4034 -0.9402 -0.7293 C
2 C2 -5.7281 1.4416 -1.4684 C
3 C3 -3.6640 0.7748 -0.1207 C
4 C4 -4.6683 1.8719 -0.4412 C
5 C5 -4.2777 -0.5676 0.2900 C
6 C6 -6.4301 0.1624 -1.0060 C
7 N7 -1.0217 -0.8612 0.6766 N
8 C8 -1.1280 0.3812 0.0703 C
9 C9 -2.3534 1.0996 -0.2180 C
10 N10 0.0376 0.8991 -0.2541 N
11 C11 1.0042 -0.0372 0.0969 C
12 C12 0.3336 -1.2297 0.7053 C
13 O13 0.7597 -2.2613 1.2020 O
14 C14 -2.0789 -1.7058 1.1966 C
15 C15 -3.2911 -1.7623 0.2687 C
16 C16 2.3657 0.1392 -0.0564 C
17 C17 2.9773 1.4793 0.0164 C
18 C18 4.1711 4.0302 0.1803 C
19 C19 4.1717 1.7696 -0.6752 C
20 C20 2.3948 2.5044 0.7897 C
21 C21 2.9875 3.7603 0.8724 C
22 C22 4.7591 3.0295 -0.5959 C
23 C23 3.2411 -1.0385 -0.2465 C
24 C24 4.8935 -3.2786 -0.6649 C
25 C25 2.8739 -2.0464 -1.1563 C
26 C26 4.4611 -1.1740 0.4434 C
27 C27 5.2741 -2.2864 0.2415 C
28 C28 3.6921 -3.1527 -1.3656 C
29 C29 -4.8926 -0.4356 1.7085 C
30 H30 -7.1405 -0.1849 -1.7671 H
31 H31 -7.0227 0.3714 -0.1048 H
32 H32 -6.4512 2.2532 -1.6163 H
33 H33 -5.2426 1.2658 -2.4386 H
34 H34 -5.9057 -1.8463 -0.3653 H
35 H35 -4.9242 -1.2121 -1.6809 H
36 H36 -4.1373 2.7628 -0.7926 H
37 H37 -5.1856 2.1698 0.4839 H
38 H38 -5.6843 0.3176 1.7492 H
39 H39 -5.3310 -1.3922 2.0188 H
40 H40 -4.1378 -0.1512 2.4484 H
41 H41 -3.8704 -2.6568 0.5336 H
42 H42 -2.9324 -1.9193 -0.7566 H
43 H43 -2.1144 2.1009 -0.5686 H
44 H44 -2.3615 -1.3773 2.2050 H
45 H45 -1.6301 -2.6978 1.3028 H
46 H46 4.7563 -0.4099 1.1563 H
47 H47 6.2046 -2.3815 0.7951 H
48 H48 5.5317 -4.1435 -0.8264 H
49 H49 3.3931 -3.9170 -2.0778 H
50 H50 1.9467 -1.9417 -1.7114 H
51 H51 1.4774 2.3016 1.3292 H
52 H52 2.5260 4.5316 1.4833 H
53 H53 4.6315 5.0125 0.2463 H
54 H54 5.6751 3.2318 -1.1448 H
55 H55 4.6290 1.0015 -1.2904 H
@<TRIPOS>BOND
1 1 5 1
2 1 6 1
3 1 34 1
4 1 35 1
5 2 4 1
6 2 6 1
7 2 32 1
8 2 33 1
9 3 4 1
10 3 5 1
11 3 9 2
12 4 36 1
13 4 37 1
14 5 15 1
15 5 29 1
16 6 30 1
17 6 31 1
18 7 8 1
19 7 12 1
20 7 14 1
21 8 9 1
22 8 10 2
23 9 43 1
24 10 11 1
25 11 12 1
26 11 16 2
27 12 13 2
28 14 15 1
29 14 44 1
30 14 45 1
31 15 41 1
32 15 42 1
33 16 17 1
34 16 23 1
35 17 19 Ar
36 17 20 Ar
37 18 21 Ar
38 18 22 Ar
39 18 53 1
40 19 22 Ar
41 19 55 1
42 20 21 Ar
43 20 51 1
44 21 52 1
45 22 54 1
46 23 25 Ar
47 23 26 Ar
48 24 27 Ar
49 24 28 Ar
50 24 48 1
51 25 28 Ar
52 25 50 1
53 26 27 Ar
54 26 46 1
55 27 47 1
56 28 49 1
57 29 38 1
58 29 39 1
59 29 40 1

DAIN **1”** (45 °):
$E(S_0)$ = -1191.18669796 A.U.
$E(S_1)$ = -1191.10271099 A.U.

@<TRIPOS>MOLECULE
Molecule Name
55 59
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 -5.4204 -1.0426 -0.4276 C
2 C2 -5.7365 1.0423 -1.7972 C
3 C3 -3.6473 0.7449 -0.3536 C
4 C4 -4.6447 1.7238 -0.9539 C
5 C5 -4.2638 -0.4235 0.4224 C
6 C6 -6.4410 -0.0423 -0.9801 C
7 N7 -1.0091 -0.6469 0.8385 N
8 C8 -1.1142 0.4019 -0.0595 C
9 C9 -2.3335 1.0194 -0.5364 C
10 N10 0.0589 0.8175 -0.5033 N
11 C11 1.0130 -0.0124 0.0587 C
12 C12 0.3458 -1.0144 0.9400 C
13 O13 0.7758 -1.8917 1.6749 O
14 C14 -2.0614 -1.3244 1.5692 C
15 C15 -3.2941 -1.5974 0.7086 C
16 C16 2.3897 0.1155 -0.1163 C
17 C17 3.0426 1.4277 -0.0175 C
18 C18 4.3017 3.9405 0.2348 C
19 C19 4.2529 1.7068 -0.6882 C
20 C20 2.4746 2.4497 0.7724 C
21 C21 3.0981 3.6865 0.8980 C
22 C22 4.8746 2.9454 -0.5608 C

23 C23 3.1917 -1.1016 -0.3215 C
24 C24 4.6806 -3.4507 -0.7722 C
25 C25 2.6814 -2.1399 -1.1261 C
26 C26 4.4695 -1.2711 0.2521 C
27 C27 5.2023 -2.4325 0.0312 C
28 C28 3.4183 -3.2997 -1.3494 C
29 C29 -4.8419 0.1080 1.7599 C
30 H30 -7.1737 -0.5765 -1.5980 H
31 H31 -7.0093 0.4225 -0.1624 H
32 H32 -6.4528 1.7936 -2.1525 H
33 H33 -5.2781 0.5929 -2.6894 H
34 H34 -5.9268 -1.8017 0.1839 H
35 H35 -4.9714 -1.5784 -1.2763 H
36 H36 -4.1096 2.4686 -1.5524 H
37 H37 -5.1376 2.2823 -0.1421 H
38 H38 -5.6248 0.8518 1.5936 H
39 H39 -5.2803 -0.7148 2.3381 H
40 H40 -4.0673 0.5806 2.3712 H
41 H41 -3.8808 -2.3766 1.2125 H
42 H42 -2.9556 -2.0305 -0.2414 H
43 H43 -2.0865 1.8857 -1.1461 H
44 H44 -2.3159 -0.7566 2.4737 H
45 H45 -1.6183 -2.2661 1.9068 H
46 H46 4.8693 -0.4955 0.8976 H
47 H47 6.1783 -2.5506 0.4945 H
48 H48 5.2564 -4.3557 -0.9477 H
49 H49 3.0102 -4.0843 -1.9809 H
50 H50 1.7112 -2.0096 -1.5951 H
51 H51 1.5479 2.2530 1.3000 H
52 H52 2.6480 4.4536 1.5226 H
53 H53 4.7892 4.9064 0.3374 H
54 H54 5.8034 3.1389 -1.0911 H
55 H55 4.6928 0.9473 -1.3264 H
@<TRIPOS>BOND
1 1 5 1
2 1 6 1
3 1 34 1
4 1 35 1
5 2 4 1
6 2 6 1
7 2 32 1
8 2 33 1
9 3 4 1
10 3 5 1
11 3 9 2
12 4 36 1
13 4 37 1
14 5 15 1
15 5 29 1
16 6 30 1
17 6 31 1
18 7 8 1
19 7 12 1
20 7 14 1
21 8 9 Ar
22 8 10 2
23 9 43 1
24 10 11 1
25 11 12 1
26 11 16 Ar
27 12 13 2
28 14 15 1
29 14 44 1
30 14 45 1
31 15 41 1
32 15 42 1
33 16 17 1
34 16 23 1
35 17 19 Ar
36 17 20 Ar
37 18 21 Ar
38 18 22 Ar
39 18 53 1
40 19 22 Ar
41 19 55 1
42 20 21 Ar
43 20 51 1
44 21 52 1
45 22 54 1
46 23 25 Ar
47 23 26 Ar
48 24 27 Ar
49 24 28 Ar
50 24 48 1
51 25 28 Ar
52 25 50 1
53 26 27 Ar
54 26 46 1
55 27 47 1
56 28 49 1
57 29 38 1
58 29 39 1
59 29 40 1

DAIN **1”** (60 °):
$E(S_0)$ = -1191.17215637 A.U.
$E(S_1)$ = -1191.10370145 A.U.

@<TRIPOS>MOLECULE
Molecule Name
55 59
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 -5.3582 -1.0939 -0.2202 C
2 C2 -5.6453 0.6040 -2.0601 C
3 C3 -3.6263 0.7044 -0.5124 C
4 C4 -4.6190 1.4987 -1.3443 C
5 C5 -4.2555 -0.2540 0.5039 C
6 C6 -6.3672 -0.2871 -1.0464 C
7 N7 -1.0049 -0.3075 1.0299 N
8 C8 -1.1008 0.4420 -0.1246 C
9 C9 -2.3099 0.9228 -0.7511 C
10 N10 0.0838 0.6933 -0.6712 N
11 C11 1.0170 0.0330 0.0910 C
12 C12 0.3484 -0.6600 1.2225 C
13 O13 0.7749 -1.2942 2.1789 O
14 C14 -2.0731 -0.7734 1.8923 C
15 C15 -3.2761 -1.2935 1.1051 C
16 C16 2.4128 0.0671 -0.1300 C
17 C17 3.1345 1.3376 -0.0863 C
18 C18 4.5012 3.8041 0.0575 C
19 C19 4.3343 1.5513 -0.8037 C
20 C20 2.6335 2.4054 0.6913 C
21 C21 3.3080 3.6193 0.7612 C
22 C22 5.0099 2.7643 -0.7262 C
23 C23 3.1067 -1.2053 -0.3214 C
24 C24 4.3659 -3.6961 -0.7342 C
25 C25 2.4296 -2.2672 -0.9613 C
26 C26 4.4352 -1.4314 0.1094 C
27 C27 5.0549 -2.6573 -0.0981 C
28 C28 3.0517 -3.4963 -1.1607 C
29 C29 -4.9017 0.5636 1.6531 C
30 H30 -7.0497 -0.9782 -1.5573 H
31 H31 -6.9927 0.3321 -0.3890 H
32 H32 -6.3600 1.2247 -2.6145 H
33 H33 -5.1253 -0.0230 -2.7977 H
34 H34 -5.8810 -1.6943 0.5365 H
35 H35 -4.8543 -1.8057 -0.8886 H
36 H36 -4.0818 2.1196 -2.0691 H
37 H37 -5.1682 2.1942 -0.6911 H
38 H38 -5.6841 1.2396 1.2958 H
39 H39 -5.3610 -0.1149 2.3828 H
40 H40 -4.1608 1.1758 2.1775 H
41 H41 -3.8623 -1.9324 1.7795 H
42 H42 -2.9053 -1.9469 0.3051 H
43 H43 -2.0587 1.6084 -1.5575 H
44 H44 -2.3645 0.0215 2.5910 H
45 H45 -1.6308 -1.5741 2.4923 H
46 H46 4.9599 -0.6455 0.6430 H
47 H47 6.0714 -2.8137 0.2529 H
48 H48 4.8526 -4.6542 -0.8961 H
49 H49 2.5141 -4.2968 -1.6618 H
50 H50 1.4239 -2.0968 -1.3314 H
51 H51 1.7231 2.2560 1.2620 H
52 H52 2.9083 4.4214 1.3758 H
53 H53 5.0307 4.7512 0.1184 H
54 H54 5.9272 2.9073 -1.2914 H
55 H55 4.7141 0.7638 -1.4467 H
@<TRIPOS>BOND
1 1 5 1
2 1 6 1
3 1 34 1
4 1 35 1
5 2 4 1
6 2 6 1
7 2 32 1
8 2 33 1
9 3 4 1
10 3 5 1
11 3 9 2
12 4 36 1
13 4 37 1
14 5 15 1
15 5 29 1
16 6 30 1
17 6 31 1
18 7 8 Ar
19 7 12 1
20 7 14 1
21 8 9 Ar
22 8 10 Ar
23 9 43 1
24 10 11 Ar
25 11 12 1
26 11 16 Ar
27 12 13 2
28 14 15 1
29 14 44 1
30 14 45 1
31 15 41 1
32 15 42 1
33 16 17 1
34 16 23 1
35 17 19 Ar
36 17 20 Ar
37 18 21 Ar
38 18 22 Ar
39 18 53 1
40 19 22 Ar
41 19 55 1
42 20 21 Ar
43 20 51 1
44 21 52 1
45 22 54 1
46 23 25 Ar
47 23 26 Ar
48 24 27 Ar
49 24 28 Ar
50 24 48 1
51 25 28 Ar
52 25 50 1
53 26 27 Ar
54 26 46 1
55 27 47 1
56 28 49 1

57 29 38 1
58 29 39 1
59 29 40 1

DAIN **1”** (75 °):
$E(S_0)$ = -1191.15589306 A.U.
$E(S_1)$ = -1191.10645859 A.U.

@<TRIPOS>MOLECULE
Molecule Name
55 59
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 5.4299 0.9922 0.2271 C
2 C2 5.7241 0.0849 -2.1005 C
3 C3 3.6191 -0.4555 -0.7524 C
4 C4 4.5993 -0.9250 -1.8146 C
5 C5 4.2480 0.0251 0.5576 C
6 C6 6.4380 0.4681 -0.8017 C
7 N7 0.9990 -0.0083 1.0536 N
8 C8 1.0997 -0.3241 -0.2808 C
9 C9 2.2975 -0.5458 -1.0486 C
10 N10 -0.0993 -0.3850 -0.8752 N
11 C11 -1.0209 -0.0275 0.0611 C
12 C12 -0.3608 0.2465 1.3526 C
13 O13 -0.7937 0.5036 2.4720 O
14 C14 2.0581 0.1426 2.0330 C
15 C15 3.2940 0.8417 1.4671 C
16 C16 -2.4430 -0.0060 -0.1623 C
17 C17 -3.1813 -1.2573 -0.2124 C
18 C18 -4.5780 -3.7134 -0.2419 C
19 C19 -4.3847 -1.4083 -0.9457 C
20 C20 -2.6950 -2.3854 0.4909 C
21 C21 -3.3839 -3.5931 0.4735 C
22 C22 -5.0736 -2.6142 -0.9521 C
23 C23 -3.0898 1.2906 -0.2350 C
24 C24 -4.2531 3.8591 -0.4050 C
25 C25 -2.3412 2.4064 -0.6842 C
26 C26 -4.4415 1.5096 0.1367 C
27 C27 -5.0121 2.7707 0.0453 C
28 C28 -2.9171 3.6710 -0.7630 C
29 C29 4.7902 -1.1971 1.3432 C
30 H30 7.1975 1.2371 -0.9907 H
31 H31 6.9736 -0.4041 -0.4032 H
32 H32 6.4295 -0.3426 -2.8240 H
33 H33 5.2973 0.9850 -2.5649 H
34 H34 5.9419 1.2420 1.1662 H
35 H35 5.0046 1.9313 -0.1550 H
36 H36 4.0559 -1.1630 -2.7353 H
37 H37 5.0649 -1.8674 -1.4834 H
38 H38 5.5702 -1.7302 0.7925 H
39 H39 5.2248 -0.8708 2.2965 H
40 H40 3.9966 -1.9192 1.5578 H
41 H41 3.8896 1.1903 2.3212 H
42 H42 2.9650 1.7419 0.9323 H
43 H43 2.0356 -0.8828 -2.0491 H
44 H44 2.3140 -0.8350 2.4610 H
45 H45 1.6228 0.7341 2.8439 H
46 H46 -5.0208 0.6852 0.5393 H
47 H47 -6.0459 2.9175 0.3465 H
48 H48 -4.7035 4.8456 -0.4741 H
49 H49 -2.3252 4.5102 -1.1183 H
50 H50 -1.3195 2.2491 -1.0121 H
51 H51 -1.7938 -2.2828 1.0854 H
52 H52 -2.9962 -4.4406 1.0324 H
53 H53 -5.1195 -4.6555 -0.2474 H
54 H54 -5.9901 -2.7085 -1.5288 H
55 H55 -4.7491 -0.5769 -1.5405 H
@<TRIPOS>BOND
1 1 5 1
2 1 6 1
3 1 34 1
4 1 35 1
5 2 4 1
6 2 6 1
7 2 32 1
8 2 33 1
9 3 4 1
10 3 5 1
11 3 9 2
12 4 36 1
13 4 37 1
14 5 15 1
15 5 29 1
16 6 30 1
17 6 31 1
18 7 8 Ar
19 7 12 1
20 7 14 1
21 8 9 Ar
22 8 10 Ar
23 9 43 1
24 10 11 Ar
25 11 12 1
26 11 16 Ar
27 12 13 2
28 14 15 1
29 14 44 1
30 14 45 1
31 15 41 1
32 15 42 1
33 16 17 1
34 16 23 1
35 17 19 Ar
36 17 20 Ar
37 18 21 Ar
38 18 22 Ar
39 18 53 1
40 19 22 Ar
41 19 55 1
42 20 21 Ar
43 20 51 1
44 21 52 1
45 22 54 1
46 23 25 Ar
47 23 26 Ar
48 24 27 Ar
49 24 28 Ar
50 24 48 1
51 25 28 Ar
52 25 50 1
53 26 27 Ar
54 26 46 1
55 27 47 1
56 28 49 1
57 29 38 1
58 29 39 1
59 29 40 1

DAIN **1”** (90 °):
$E(S_0)$ = -1191.13262730 A.U.
$E(S_1)$ = -1191.12492080 A.U.

@<TRIPOS>MOLECULE
Molecule Name
55 59
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 5.4215 0.8976 0.3895 C
2 C2 5.6525 0.4370 -2.0735 C
3 C3 3.5865 -0.3491 -0.8004 C
4 C4 4.5429 -0.6214 -1.9483 C
5 C5 4.2452 -0.1190 0.5629 C
6 C6 6.3997 0.5805 -0.7456 C
7 N7 1.0015 -0.1561 1.0864 N
8 C8 1.0872 -0.1827 -0.2757 C
9 C9 2.2561 -0.3456 -1.0875 C
10 N10 -0.1451 -0.1436 -0.8466 N
11 C11 -1.0395 -0.1302 0.1564 C
12 C12 -0.3696 -0.1577 1.4605 C
13 O13 -0.7734 -0.0962 2.6206 O
14 C14 2.0733 -0.2739 2.0564 C
15 C15 3.3173 0.5068 1.6357 C
16 C16 -2.4866 -0.0061 -0.0421 C
17 C17 -3.2755 -1.1925 -0.2071 C
18 C18 -4.7404 -3.5874 -0.6086 C
19 C19 -4.6210 -1.1695 -0.6774 C
20 C20 -2.6891 -2.4730 0.0157 C
21 C21 -3.4177 -3.6394 -0.1539 C
22 C22 -5.3255 -2.3454 -0.8848 C
23 C23 -3.0209 1.3509 -0.1635 C
24 C24 -3.9833 4.0080 -0.2431 C
25 C25 -2.2864 2.3759 -0.8087 C
26 C26 -4.2411 1.7048 0.4568 C
27 C27 -4.7048 3.0185 0.4245 C
28 C28 -2.7716 3.6748 -0.8618 C
29 C29 4.8084 -1.4640 1.0937 C
30 H30 7.1507 1.3781 -0.8102 H
31 H31 6.9516 -0.3447 -0.5306 H
32 H32 6.3404 0.1621 -2.8829 H
33 H33 5.2032 1.4013 -2.3496 H
34 H34 5.9594 0.9681 1.3448 H
35 H35 4.9875 1.8904 0.2033 H
36 H36 3.9808 -0.6985 -2.8852 H
37 H37 5.0235 -1.6016 -1.7985 H
38 H38 4.0168 -2.2100 1.2157 H
39 H39 5.5551 -1.8928 0.4195 H
40 H40 5.2908 -1.3126 2.0677 H
41 H41 3.9291 0.6594 2.5341 H
42 H42 2.9991 1.5039 1.3056 H
43 H43 1.9732 -0.4818 -2.1293 H
44 H44 2.3049 -1.3314 2.2384 H
45 H45 1.6659 0.1247 2.9905 H
46 H46 -4.7914 0.9560 1.0163 H
47 H47 -5.6332 3.2679 0.9316 H
48 H48 -4.3515 5.0297 -0.2731 H
49 H49 -2.2009 4.4381 -1.3845 H
50 H50 -1.3442 2.1224 -1.2840 H
51 H51 -1.6483 -2.5260 0.3136 H
52 H52 -2.9468 -4.5992 0.0406 H
53 H53 -5.3000 -4.5039 -0.7730 H
54 H54 -6.3418 -2.2981 -1.2668 H
55 H55 -5.0870 -0.2218 -0.9175 H
@<TRIPOS>BOND
1 1 5 1
2 1 6 1
3 1 34 1
4 1 35 1
5 2 4 1
6 2 6 1
7 2 32 1
8 2 33 1
9 3 4 1
10 3 5 1
11 3 9 2
12 4 36 1
13 4 37 1
14 5 15 1
15 5 29 1
16 6 30 1
17 6 31 1

18 7 8 Ar
19 7 12 1
20 7 14 1
21 8 9 Ar
22 8 10 Ar
23 9 43 1
24 10 11 Ar
25 11 12 1
26 11 16 1
27 12 13 2
28 14 15 1
29 14 44 1
30 14 45 1
31 15 41 1
32 15 42 1
33 16 17 Ar
34 16 23 1
35 17 19 Ar
36 17 20 Ar
37 18 21 Ar
38 18 22 Ar
39 18 53 1
40 19 22 Ar
41 19 55 1
42 20 21 2
43 20 51 1
44 21 52 1
45 22 54 1
46 23 25 Ar
47 23 26 Ar
48 24 27 Ar
49 24 28 Ar
50 24 48 1
51 25 28 Ar
52 25 50 1
53 26 27 Ar
54 26 46 1
55 27 47 1
56 28 49 1
57 29 38 1
58 29 39 1
59 29 40 1

DAIN **1"** (-15 °):
$E(S_0)$ = -1191.20160978 A.U.
$E(S_1)$ = -1191.09678436 A.U.

@<TRIPOS>MOLECULE
Molecule Name
55 59
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 -5.4449 -0.3418 -1.0724 C
2 C2 -5.7939 1.9109 -0.0072 C
3 C3 -3.6850 0.5576 0.4834 C
4 C4 -4.6989 1.5588 1.0145 C
5 C5 -4.2838 -0.7252 -0.0999 C
6 C6 -6.4804 0.6388 -0.5107 C
7 N7 -1.0216 -1.1460 -0.0730 N
8 C8 -1.1465 0.1908 0.2800 C
9 C9 -2.3782 0.8910 0.5905 C
10 N10 0.0074 0.8093 0.3741 N
11 C11 0.9983 -0.1291 0.0879 C
12 C12 0.3423 -1.4491 -0.1966 C
13 O13 0.7752 -2.5454 -0.5166 O
14 C14 -2.0624 -2.1397 -0.2585 C
15 C15 -3.2985 -1.5662 -0.9492 C
16 C16 2.3435 0.1515 0.0526 C
17 C17 2.8360 1.5470 -0.0035 C
18 C18 3.8243 4.1858 -0.1088 C
19 C19 4.0375 1.8990 0.6429 C
20 C20 2.1436 2.5503 -0.7093 C
21 C21 2.6376 3.8506 -0.7652 C
22 C22 4.5209 3.2045 0.5990 C
23 C23 3.3600 -0.9302 0.0353 C
24 C24 5.3350 -2.9354 0.0332 C
25 C25 4.4202 -0.8971 -0.8886 C
26 C26 3.3175 -1.9828 0.9649 C
27 C27 4.2977 -2.9714 0.9674 C
28 C28 5.3911 -1.8963 -0.8975 C
29 C29 -4.8447 -1.5977 1.0533 C
30 H30 -7.2125 0.8789 -1.2918 H
31 H31 -7.0455 0.1748 0.3092 H
32 H32 -6.5205 2.5937 0.4504 H
33 H33 -5.3427 2.4465 -0.8542 H
34 H34 -5.9372 -1.2677 -1.3983 H
35 H35 -4.9992 0.1065 -1.9719 H
36 H36 -4.1818 2.4640 1.3499 H
37 H37 -5.1869 1.1359 1.9066 H
38 H38 -5.6510 -1.0974 1.5963 H
39 H39 -5.2499 -2.5355 0.6534 H
40 H40 -4.0683 -1.8434 1.7840 H
41 H41 -3.8692 -2.4118 -1.3545 H
42 H42 -2.9651 -0.9752 -1.8117 H
43 H43 -2.1460 1.8728 0.9963 H
44 H44 -2.3182 -2.6062 0.7019 H
45 H45 -1.6095 -2.9216 -0.8754 H
46 H46 2.5162 -2.0137 1.6964 H
47 H47 4.2509 -3.7728 1.7000 H
48 H48 6.0974 -3.7102 0.0336 H
49 H49 6.1934 -1.8613 -1.6299 H
50 H50 4.4714 -0.0876 -1.6109 H
51 H51 1.2195 2.2987 -1.2146 H
52 H52 2.0938 4.6063 -1.3261 H
53 H53 4.2044 5.2032 -0.1519 H
54 H54 5.4428 3.4546 1.1172 H
55 H55 4.5831 1.1410 1.1958 H
@<TRIPOS>BOND
1 1 5 1
2 1 6 1
3 1 34 1
4 1 35 1
5 2 4 1
6 2 6 1
7 2 32 1
8 2 33 1
9 3 4 1
10 3 5 1
11 3 9 2
12 4 36 1
13 4 37 1
14 5 15 1
15 5 29 1
16 6 30 1
17 6 31 1
18 7 8 1
19 7 12 1
20 7 14 1
21 8 9 1
22 8 10 2
23 9 43 1
24 10 11 1
25 11 12 1
26 11 16 2
27 12 13 2
28 14 15 1
29 14 44 1
30 14 45 1
31 15 41 1
32 15 42 1
33 16 17 1
34 16 23 1
35 17 19 Ar
36 17 20 Ar
37 18 21 Ar
38 18 22 Ar
39 18 53 1
40 19 22 Ar
41 19 55 1
42 20 21 Ar
43 20 51 1
44 21 52 1
45 22 54 1
46 23 25 Ar
47 23 26 Ar
48 24 27 Ar
49 24 28 Ar
50 24 48 1
51 25 28 Ar
52 25 50 1
53 26 27 Ar
54 26 46 1
55 27 47 1
56 28 49 1
57 29 38 1
58 29 39 1
59 29 40 1

DAIN **1"** (-30 °):
$E(S_0)$ = -1191.19685665 A.U.
$E(S_1)$ = -1191.10057302 A.U.

@<TRIPOS>MOLECULE
Molecule Name
55 59
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 -5.3846 -0.1214 -1.1268 C
2 C2 -5.7509 1.8836 0.3470 C
3 C3 -3.6729 0.4329 0.6372 C
4 C4 -4.7018 1.3201 1.3218 C
5 C5 -4.2581 -0.7027 -0.2120 C
6 C6 -6.4297 0.7449 -0.4176 C
7 N7 -0.9933 -1.1060 -0.2240 N
8 C8 -1.1288 0.1208 0.4069 C
9 C9 -2.3686 0.7295 0.8479 C
10 N10 0.0235 0.7190 0.6242 N
11 C11 1.0142 -0.1280 0.1388 C
12 C12 0.3737 -1.3649 -0.4126 C
13 O13 0.8175 -2.3554 -0.9734 O
14 C14 -2.0271 -2.0582 -0.5753 C
15 C15 -3.2547 -1.3781 -1.1777 C
16 C16 2.3634 0.1685 0.1167 C
17 C17 2.8362 1.5597 -0.0175 C
18 C18 3.7648 4.2076 -0.3062 C
19 C19 2.0773 2.5215 -0.7143 C
20 C20 4.0692 1.9628 0.5352 C
21 C21 4.5264 3.2705 0.3950 C
22 C22 2.5400 3.8255 -0.8599 C
23 C23 3.3603 -0.9239 0.1532 C
24 C24 5.2543 -3.0053 0.2488 C
25 C25 4.4900 -0.9129 -0.6876 C
26 C26 3.2069 -1.9982 1.0482 C
27 C27 4.1447 -3.0257 1.0969 C
28 C28 5.4227 -1.9455 -0.6453 C
29 C29 -4.8681 -1.7760 0.7280 C
30 H30 -7.1358 1.1421 -1.1577 H
31 H31 -7.0248 0.1389 0.2801 H
32 H32 -6.4881 2.4793 0.8994 H
33 H33 -5.2576 2.5630 -0.3620 H

34 H34 -5.8736 -0.9593 -1.6413 H
35 H35 -4.9075 0.4855 -1.9094 H
36 H36 -4.1921 2.1349 1.8467 H
37 H37 -5.2292 0.7406 2.0955 H
38 H38 -5.6815 -1.3692 1.3338 H
39 H39 -5.2749 -2.6069 0.1382 H
40 H40 -4.1207 -2.1811 1.4173 H
41 H41 -3.8153 -2.1389 -1.7364 H
42 H42 -2.9088 -0.6455 -1.9186 H
43 H43 -2.1485 1.6055 1.4539 H
44 H44 -2.2921 -2.6714 0.2962 H
45 H45 -1.5651 -2.7297 -1.3050 H
46 H46 2.3503 -2.0094 1.7151 H
47 H47 4.0110 -3.8436 1.7997 H
48 H48 5.9847 -3.8092 0.2863 H
49 H49 6.2786 -1.9265 -1.3147 H
50 H50 4.6191 -0.0975 -1.3927 H
51 H51 4.6603 1.2427 1.0917 H
52 H52 5.4758 3.5591 0.8383 H
53 H53 4.1224 5.2274 -0.4216 H
54 H54 1.9440 4.5471 -1.4124 H
55 H55 1.1270 2.2324 -1.1473 H
@<TRIPOS>BOND
1 1 5 1
2 1 6 1
3 1 34 1
4 1 35 1
5 2 4 1
6 2 6 1
7 2 32 1
8 2 33 1
9 3 4 1
10 3 5 1
11 3 9 2
12 4 36 1
13 4 37 1
14 5 15 1
15 5 29 1
16 6 30 1
17 6 31 1
18 7 8 1
19 7 12 1
20 7 14 1
21 8 9 1
22 8 10 2
23 9 43 1
24 10 11 1
25 11 12 1
26 11 16 2
27 12 13 2
28 14 15 1
29 14 44 1
30 14 45 1
31 15 41 1
32 15 42 1
33 16 17 1
34 16 23 1
35 17 19 Ar
36 17 20 Ar
37 18 21 Ar
38 18 22 Ar
39 18 53 1
40 19 22 Ar
41 19 55 1
42 20 21 Ar
43 20 51 1
44 21 52 1
45 22 54 1
46 23 25 Ar
47 23 26 Ar
48 24 27 Ar
49 24 28 Ar
50 24 48 1
51 25 28 Ar
52 25 50 1
53 26 27 Ar
54 26 46 1
55 27 47 1
56 28 49 1
57 29 38 1
58 29 39 1
59 29 40 1

DAIN **1”** (-45 °):
$E(S_0)$ = -1191.18679423 A.U.
$E(S_1)$ = -1191.10173449 A.U.

@<TRIPOS>MOLECULE
Molecule Name
55 59
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 -5.3755 0.2196 -1.0536 C
2 C2 -5.7333 1.7108 0.9461 C
3 C3 -3.6496 0.2579 0.7710 C
4 C4 -4.6674 0.8988 1.7004 C
5 C5 -4.2491 -0.6030 -0.3461 C
6 C6 -6.4147 0.8453 -0.1179 C
7 N7 -0.9829 -0.9731 -0.5040 N
8 C8 -1.1148 0.0687 0.3977 C
9 C9 -2.3436 0.5227 1.0125 C
10 N10 0.0435 0.6052 0.7379 N
11 C11 1.0242 -0.1174 0.0820 C
12 C12 0.3879 -1.1956 -0.7327 C
13 O13 0.8373 -2.0285 -1.5063 O
14 C14 -2.0224 -1.8053 -1.0775 C
15 C15 -3.2562 -0.9936 -1.4696 C
16 C16 2.3890 0.1619 0.1225 C
17 C17 2.8792 1.5381 -0.0335 C
18 C18 3.8131 4.1768 -0.3950 C
19 C19 2.1238 2.4842 -0.7580 C
20 C20 4.1100 1.9573 0.5161 C
21 C21 4.5714 3.2580 0.3344 C
22 C22 2.5866 3.7831 -0.9373 C
23 C23 3.3351 -0.9588 0.2468 C
24 C24 5.1066 -3.1281 0.5597 C
25 C25 4.5684 -0.9920 -0.4376 C
26 C26 3.0155 -2.0404 1.0918 C
27 C27 3.8907 -3.1115 1.2460 C
28 C28 5.4409 -2.0645 -0.2838 C
29 C29 -4.8606 -1.8919 0.2640 C
30 H30 -7.1200 1.4446 -0.7077 H
31 H31 -7.0110 0.0618 0.3684 H
32 H32 -6.4696 2.1088 1.6556 H
33 H33 -5.2534 2.5746 0.4654 H
34 H34 -5.8680 -0.4340 -1.7858 H
35 H35 -4.8942 1.0238 -1.6284 H
36 H36 -4.1519 1.5327 2.4293 H
37 H37 -5.1755 0.1133 2.2802 H
38 H38 -5.6482 -1.6763 0.9916 H
39 H39 -5.3042 -2.5076 -0.5282 H
40 H40 -4.1048 -2.4938 0.7792 H
41 H41 -3.8235 -1.5810 -2.2033 H
42 H42 -2.9203 -0.0883 -1.9916 H
43 H43 -2.1172 1.2160 1.8197 H
44 H44 -2.2841 -2.6178 -0.3871 H
45 H45 -1.5692 -2.2707 -1.9579 H
46 H46 2.0828 -2.0133 1.6462 H
47 H47 3.6276 -3.9305 1.9101 H
48 H48 5.7916 -3.9628 0.6822 H
49 H49 6.3794 -2.0783 -0.8316 H
50 H50 4.8218 -0.1820 -1.1143 H
51 H51 4.6932 1.2568 1.1052 H
52 H52 5.5197 3.5585 0.7720 H
53 H53 4.1744 5.1913 -0.5404 H
54 H54 1.9926 4.4901 -1.5105 H
55 H55 1.1789 2.1808 -1.1947 H
@<TRIPOS>BOND
1 1 5 1
2 1 6 1
3 1 34 1
4 1 35 1
5 2 4 1
6 2 6 1
7 2 32 1
8 2 33 1
9 3 4 1
10 3 5 1
11 3 9 2
12 4 36 1
13 4 37 1
14 5 15 1
15 5 29 1
16 6 30 1
17 6 31 1
18 7 8 1
19 7 12 1
20 7 14 1
21 8 9 Ar
22 8 10 2
23 9 43 1
24 10 11 1
25 11 12 1
26 11 16 Ar
27 12 13 2
28 14 15 1
29 14 44 1
30 14 45 1
31 15 41 1
32 15 42 1
33 16 17 1
34 16 23 1
35 17 19 Ar
36 17 20 Ar
37 18 21 Ar
38 18 22 Ar
39 18 53 1
40 19 22 Ar
41 19 55 1
42 20 21 Ar
43 20 51 1
44 21 52 1
45 22 54 1
46 23 25 Ar
47 23 26 Ar
48 24 27 Ar
49 24 28 Ar
50 24 48 1
51 25 28 Ar
52 25 50 1
53 26 27 Ar
54 26 46 1
55 27 47 1
56 28 49 1
57 29 38 1
58 29 39 1
59 29 40 1

DAIN **1”** (-60 °):
$E(S_0)$ = -1191.17241609 A.U.
$E(S_1)$ = -1191.10323327 A.U.

@<TRIPOS>MOLECULE
Molecule Name

55 59
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 5.4587 0.3778 0.9038 C
2 C2 5.7718 1.4810 -1.3337 C
3 C3 3.6332 0.1772 -0.8223 C
4 C4 4.6283 0.6121 -1.8868 C
5 C5 4.2459 -0.4804 0.4176 C
6 C6 6.4723 0.7622 -0.1795 C
7 N7 0.9879 -0.7164 0.7624 N
8 C8 1.1071 0.0632 -0.3701 C
9 C9 2.3196 0.3860 -1.0846 C
10 N10 -0.0701 0.4716 -0.8342 N
11 C11 -1.0302 -0.0900 -0.0295 C
12 C12 -0.3850 -0.9042 1.0331 C
13 O13 -0.8252 -1.5160 1.9976 O
14 C14 2.0245 -1.4023 1.5092 C
15 C15 3.2979 -0.5704 1.6399 C
16 C16 -2.4214 0.1328 -0.1421 C
17 C17 -2.9703 1.4803 -0.0036 C
18 C18 -3.9970 4.0922 0.3125 C
19 C19 -4.1905 1.8645 -0.6062 C
20 C20 -2.2744 2.4518 0.7500 C
21 C21 -2.7817 3.7371 0.9043 C
22 C22 -4.6982 3.1490 -0.4443 C
23 C23 -3.2856 -1.0352 -0.3113 C
24 C24 -4.8745 -3.3369 -0.6770 C
25 C25 -4.5909 -1.1128 0.2288 C
26 C26 -2.8023 -2.1471 -1.0362 C
27 C27 -3.5872 -3.2829 -1.2141 C
28 C28 -5.3725 -2.2465 0.0452 C
29 C29 4.7445 -1.9001 0.0402 C
30 H30 7.2482 1.4014 0.2602 H
31 H31 6.9882 -0.1304 -0.5596 H
32 H32 6.4796 1.7183 -2.1376 H
33 H33 5.3616 2.4365 -0.9774 H
34 H34 5.9612 -0.1664 1.7150 H
35 H35 5.0660 1.3031 1.3491 H
36 H36 4.0998 1.1401 -2.6876 H
37 H37 5.0738 -0.2815 -2.3530 H
38 H38 5.5099 -1.8667 -0.7399 H
39 H39 5.1830 -2.3940 0.9163 H
40 H40 3.9274 -2.5256 -0.3317 H
41 H41 3.8834 -0.9981 2.4642 H
42 H42 3.0141 0.4422 1.9540 H
43 H43 2.0719 0.9016 -2.0098 H
44 H44 2.2276 -2.3842 1.0613 H
45 H45 1.5933 -1.5935 2.4967 H
46 H46 -1.8164 -2.0878 -1.4856 H
47 H47 -3.1977 -4.1235 -1.7821 H
48 H48 -5.4888 -4.2223 -0.8185 H
49 H49 -6.3673 -2.2921 0.4806 H
50 H50 -4.9686 -0.2890 0.8257 H
51 H51 -1.3443 2.1730 1.2337 H
52 H52 -2.2328 4.4631 1.4982 H
53 H53 -4.3946 5.0953 0.4404 H
54 H54 -5.6350 3.4218 -0.9231 H
55 H55 -4.7209 1.1501 -1.2275 H
@<TRIPOS>BOND
1 1 5 1
2 1 6 1
3 1 34 1
4 1 35 1
5 2 4 1
6 2 6 1
7 2 32 1
8 2 33 1
9 3 4 1
10 3 5 1
11 3 9 2
12 4 36 1
13 4 37 1
14 5 15 1
15 5 29 1
16 6 30 1
17 6 31 1
18 7 8 Ar
19 7 12 1
20 7 14 1
21 8 9 Ar
22 8 10 Ar
23 9 43 1
24 10 11 Ar
25 11 12 1
26 11 16 Ar
27 12 13 2
28 14 15 1
29 14 44 1
30 14 45 1
31 15 41 1
32 15 42 1
33 16 17 1
34 16 23 1
35 17 19 Ar
36 17 20 Ar
37 18 21 Ar
38 18 22 Ar
39 18 53 1
40 19 22 Ar
41 19 55 1
42 20 21 Ar
43 20 51 1
44 21 52 1
45 22 54 1
46 23 25 Ar
47 23 26 Ar
48 24 27 Ar
49 24 28 Ar
50 24 48 1
51 25 28 Ar
52 25 50 1
53 26 27 Ar
54 26 46 1
55 27 47 1
56 28 49 1
57 29 38 1
58 29 39 1
59 29 40 1

DAIN **1”** (-75 °):
$E(S_0)$ = -1191.15603685 A.U.
$E(S_1)$ = -1191.10581893 A.U.

@<TRIPOS>MOLECULE
Molecule Name
55 59
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 5.4366 0.7253 0.6805 C
2 C2 5.7253 0.9954 -1.8065 C
3 C3 3.6238 -0.0967 -0.8582 C
4 C4 4.6080 -0.0422 -2.0142 C
5 C5 4.2517 -0.2831 0.5254 C
6 C6 6.4413 0.7448 -0.4769 C
7 N7 0.9937 -0.4263 0.9449 N
8 C8 1.1061 -0.0479 -0.3716 C
9 C9 2.3059 0.0151 -1.1639 C
10 N10 -0.0876 0.1933 -0.9299 N
11 C11 -1.0285 -0.0930 0.0118 C
12 C12 -0.3806 -0.5230 1.2686 C
13 O13 -0.8169 -0.7833 2.3854 O
14 C14 2.0414 -0.8318 1.8631 C
15 C15 3.3026 0.0178 1.7122 C
16 C16 -2.4456 0.0799 -0.1621 C
17 C17 -3.0237 1.4123 -0.1215 C
18 C18 -4.1056 4.0194 0.0232 C
19 C19 -4.2358 1.7418 -0.7780 C
20 C20 -2.3652 2.4405 0.5949 C
21 C21 -2.8993 3.7224 0.6626 C
22 C22 -4.7702 3.0214 -0.6983 C
23 C23 -3.2508 -1.1233 -0.2794 C
24 C24 -4.7205 -3.5189 -0.5483 C
25 C25 -4.5999 -1.2066 0.1507 C
26 C26 -2.6634 -2.2846 -0.8387 C
27 C27 -3.3904 -3.4644 -0.9676 C
28 C28 -5.3212 -2.3835 0.0119 C
29 C29 4.7927 -1.7314 0.6500 C
30 H30 7.1934 1.5216 -0.2895 H
31 H31 6.9880 -0.2068 -0.5265 H
32 H32 6.4318 0.9559 -2.6450 H
33 H33 5.2869 2.0031 -1.8050 H
34 H34 5.9523 0.5072 1.6251 H
35 H35 5.0109 1.7334 0.7850 H
36 H36 4.0694 0.1589 -2.9464 H
37 H37 5.0779 -1.0309 -2.1392 H
38 H38 5.5645 -1.9436 -0.0946 H
39 H39 5.2360 -1.8861 1.6417 H
40 H40 3.9983 -2.4716 0.5130 H
41 H41 3.8934 -0.1062 2.6296 H
42 H42 3.0017 1.0728 1.6784 H
43 H43 2.0529 0.1964 -2.2062 H
44 H44 2.2596 -1.9010 1.7412 H
45 H45 1.6154 -0.7108 2.8637 H
46 H46 -1.6457 -2.2255 -1.2089 H
47 H47 -2.9215 -4.3401 -1.4083 H
48 H48 -5.2895 -4.4387 -0.6544 H
49 H49 -6.3497 -2.4303 0.3602 H
50 H50 -5.0557 -0.3485 0.6334 H
51 H51 -1.4510 2.2038 1.1283 H
52 H52 -2.3806 4.4906 1.2300 H
53 H53 -4.5261 5.0193 0.0864 H
54 H54 -5.6977 3.2508 -1.2163 H
55 H55 -4.7312 0.9884 -1.3820 H
@<TRIPOS>BOND
1 1 5 1
2 1 6 1
3 1 34 1
4 1 35 1
5 2 4 1
6 2 6 1
7 2 32 1
8 2 33 1
9 3 4 1
10 3 5 1
11 3 9 2
12 4 36 1
13 4 37 1
14 5 15 1
15 5 29 1
16 6 30 1
17 6 31 1
18 7 8 Ar
19 7 12 1
20 7 14 1
21 8 9 Ar
22 8 10 Ar
23 9 43 1
24 10 11 Ar
25 11 12 1
26 11 16 Ar
27 12 13 2
28 14 15 1

29 14 44 1
30 14 45 1
31 15 41 1
32 15 42 1
33 16 17 1
34 16 23 1
35 17 19 Ar
36 17 20 Ar
37 18 21 Ar
38 18 22 Ar
39 18 53 1
40 19 22 Ar
41 19 55 1
42 20 21 Ar
43 20 51 1
44 21 52 1
45 22 54 1
46 23 25 Ar
47 23 26 Ar
48 24 27 Ar
49 24 28 Ar
50 24 48 1
51 25 28 Ar
52 25 50 1
53 26 27 Ar
54 26 46 1
55 27 47 1
56 28 49 1
57 29 38 1
58 29 39 1
59 29 40 1

DAIN **1"** (-90 °):
$E(S_0)$ = -1191.13967958 A.U.
$E(S_1)$ = -1191.11456501 A.U.

@<TRIPOS>MOLECULE
Molecule Name
55 59
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 5.3851 0.8304 0.5473 C
2 C2 5.6248 0.8945 -1.9563 C
3 C3 3.5876 -0.2009 -0.8770 C
4 C4 4.5482 -0.2011 -2.0539 C
5 C5 4.2469 -0.2403 0.5040 C
6 C6 6.3719 0.7871 -0.6249 C
7 N7 1.0075 -0.5077 1.0035 N
8 C8 1.0820 -0.2854 -0.3455 C
9 C9 2.2581 -0.1884 -1.1623 C
10 N10 -0.1417 -0.0847 -0.8820 N
11 C11 -1.0223 -0.0938 0.1424 C
12 C12 -0.3419 -0.3614 1.4107 C
13 O13 -0.7579 -0.5682 2.5523 O
14 C14 2.0878 -0.7707 1.9335 C
15 C15 3.3070 0.1186 1.6844 C
16 C16 -2.4698 0.0720 -0.0308 C
17 C17 -3.0165 1.4026 0.0102 C
18 C18 -4.0074 4.0498 0.0766 C
19 C19 -4.3844 1.6710 0.2969 C
20 C20 -2.1618 2.5147 -0.2170 C
21 C21 -2.6557 3.8145 -0.1830 C
22 C22 -4.8684 2.9690 0.3176 C
23 C23 -3.2569 -1.1091 -0.3116 C
24 C24 -4.7379 -3.4675 -0.7889 C
25 C25 -2.8541 -2.3527 0.2400 C
26 C26 -4.4248 -1.0927 -1.1199 C
27 C27 -5.1515 -2.2512 -1.3496 C
28 C28 -3.5878 -3.5107 0.0013 C
29 C29 4.8553 -1.6465 0.7471 C
30 H30 7.0960 1.6049 -0.5201 H
31 H31 6.9530 -0.1446 -0.6017 H
32 H32 6.3179 0.8122 -2.8028 H
33 H33 5.1454 1.8807 -2.0296 H
34 H34 5.9224 0.7222 1.4990 H
35 H35 4.9151 1.8238 0.5666 H
36 H36 3.9855 -0.0998 -2.9881 H
37 H37 5.0577 -1.1763 -2.1090 H
38 H38 5.6202 -1.9003 0.0079 H
39 H39 5.3255 -1.6878 1.7379 H
40 H40 4.0912 -2.4287 0.7000 H
41 H41 3.9206 0.0974 2.5951 H
42 H42 2.9576 1.1528 1.5707 H
43 H43 1.9775 -0.1153 -2.2110 H
44 H44 2.3540 -1.8348 1.9006 H
45 H45 1.6701 -0.5808 2.9265 H
46 H46 -4.7184 -0.1672 -1.6041 H
47 H47 -6.0316 -2.2186 -1.9864 H
48 H48 -5.3103 -4.3731 -0.9706 H
49 H49 -3.2686 -4.4490 0.4469 H
50 H50 -2.0009 -2.3793 0.9075 H
51 H51 -1.1255 2.3294 -0.4735 H
52 H52 -1.9855 4.6487 -0.3725 H
53 H53 -4.3912 5.0662 0.0974 H
54 H54 -5.9143 3.1507 0.5499 H
55 H55 -5.0441 0.8475 0.5483 H
@<TRIPOS>BOND
1 1 5 1
2 1 6 1
3 1 34 1
4 1 35 1
5 2 4 1
6 2 6 1
7 2 32 1
8 2 33 1
9 3 4 1
10 3 5 1
11 3 9 2
12 4 36 1
13 4 37 1
14 5 15 1
15 5 29 1
16 6 30 1
17 6 31 1
18 7 8 Ar
19 7 12 1
20 7 14 1
21 8 9 Ar
22 8 10 Ar
23 9 43 1
24 10 11 Ar
25 11 12 1
26 11 16 1
27 12 13 2
28 14 15 1
29 14 44 1
30 14 45 1
31 15 41 1
32 15 42 1
33 16 17 Ar
34 16 23 Ar
35 17 19 Ar
36 17 20 Ar
37 18 21 Ar
38 18 22 Ar
39 18 53 1
40 19 22 2
41 19 55 1
42 20 21 Ar
43 20 51 1
44 21 52 1
45 22 54 1
46 23 25 Ar
47 23 26 Ar
48 24 27 Ar
49 24 28 Ar
50 24 48 1
51 25 28 Ar
52 25 50 1
53 26 27 Ar
54 26 46 1
55 27 47 1
56 28 49 1
57 29 38 1
58 29 39 1
59 29 40 1

DAIN **2a"** (optimized):
$E(S_0)$ = -1192.42253415 A.U.
No imaginary frequencies.

@<TRIPOS>MOLECULE
Molecule Name
57 61
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 5.2680 -0.6300 1.1920 C
2 C2 5.5785 1.8590 0.8863 C
3 C3 4.5305 1.8246 -0.2323 C
4 C4 4.2088 -0.7169 0.0568 C
5 C5 6.2863 0.5070 1.0319 C
6 N6 1.0043 -1.1982 -0.4893 N
7 C7 1.1048 0.1539 -0.7749 C
8 N8 -0.0221 0.7978 -0.6871 N
9 C9 -1.0009 -0.1474 -0.3331 C
10 C10 -0.3385 -1.4891 -0.1948 C
11 O11 -0.7473 -2.5948 0.1225 O
12 C12 2.0615 -2.1954 -0.4562 C
13 C13 3.2173 -1.8335 0.4864 C
14 C14 -2.3163 0.1482 -0.0918 C
15 C15 -2.8226 1.5427 -0.0690 C
16 C16 -3.8568 4.1672 -0.0353 C
17 C17 -2.0502 2.6178 0.4130 C
18 C18 -4.1278 1.8163 -0.5243 C
19 C19 -4.6345 3.1136 -0.5184 C
20 C20 -2.5661 3.9110 0.4331 C
21 C21 -3.3199 -0.9289 0.1386 C
22 C22 -5.2696 -2.9102 0.5639 C
23 C23 -4.1503 -0.8874 1.2713 C
24 C24 -3.4950 -1.9717 -0.7839 C
25 C25 -4.4647 -2.9498 -0.5764 C
26 C26 -5.1069 -1.8777 1.4894 C
27 C27 4.9052 -1.1354 -1.2562 C
28 H28 6.9593 0.5201 1.8986 H
29 H29 6.9223 0.3261 0.1551 H
30 H30 6.3067 2.6572 0.6953 H
31 H31 5.0817 2.1108 1.8348 H
32 H32 5.7896 -1.5938 1.2671 H
33 H33 4.7393 -0.4923 2.1468 H
34 H34 3.9891 2.7789 -0.2619 H
35 H35 5.0295 1.7276 -1.2070 H
36 H36 5.6790 -0.4271 -1.5652 H
37 H37 5.3909 -2.1103 -1.1254 H
38 H38 4.2090 -1.2337 -2.0949 H
39 H39 3.8033 -2.7508 0.6385 H
40 H40 2.7868 -1.5779 1.4640 H
41 H41 2.4203 -2.3944 -1.4740 H
42 H42 1.5721 -3.1083 -0.1045 H
43 H43 -2.8687 -2.0081 -1.6692 H
44 H44 -4.5891 -3.7464 -1.3050 H

45 H45 -6.0220 -3.6770 0.7283 H
46 H46 -5.7291 -1.8387 2.3797 H
47 H47 -4.0334 -0.0786 1.9870 H
48 H48 -4.7397 1.0026 -0.8994 H
49 H49 -5.6392 3.3000 -0.8884 H
50 H50 -4.2534 5.1791 -0.0205 H
51 H51 -1.9567 4.7240 0.8193 H
52 H52 -1.0453 2.4289 0.7672 H
53 C53 2.4065 0.7925 -1.1373 C
54 C54 3.5086 0.6800 -0.0494 C
55 H55 2.7720 0.3823 -2.0888 H
56 H56 2.1789 1.8471 -1.3181 H
57 H57 3.0145 0.8519 0.9201 H
@<TRIPOS>BOND
1 1 4 1
2 1 5 1
3 1 32 1
4 1 33 1
5 2 3 1
6 2 5 1
7 2 30 1
8 2 31 1
9 3 34 1
10 3 35 1
11 3 54 1
12 4 13 1
13 4 27 1
14 4 54 1
15 5 28 1
16 5 29 1
17 6 7 1
18 6 10 1
19 6 12 1
20 7 8 2
21 7 53 1
22 8 9 1
23 9 10 1
24 9 14 2
25 10 11 2
26 12 13 1
27 12 41 1
28 12 42 1
29 13 39 1
30 13 40 1
31 14 15 1
32 14 21 1
33 15 17 Ar
34 15 18 Ar
35 16 19 Ar
36 16 20 Ar
37 16 50 1
38 17 20 Ar
39 17 52 1
40 18 19 Ar
41 18 48 1
42 19 49 1
43 20 51 1
44 21 23 Ar
45 21 24 Ar
46 22 25 Ar
47 22 26 Ar
48 22 45 1
49 23 26 Ar
50 23 47 1
51 24 25 Ar
52 24 43 1
53 25 44 1
54 26 46 1
55 27 36 1
56 27 37 1
57 27 38 1
58 53 54 1
59 53 55 1
60 53 56 1
61 54 57 1

DAIN **2a''** (0 °):
$E(S_0)$ = -1192.42164740 A.U.
$E(S_1)$ = -1192.30206382 A.U.

@<TRIPOS>MOLECULE
Molecule Name
57 61
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 5.2859 -0.7225 1.1360 C
2 C2 5.5770 1.7866 1.1094 C
3 C3 4.5253 1.8723 -0.0044 C
4 C4 4.2274 -0.6907 -0.0041 C
5 C5 6.2950 0.4323 1.0984 C
6 N6 1.0262 -1.1275 -0.6087 N
7 C7 1.1163 0.2485 -0.7409 C
8 N8 -0.0152 0.8699 -0.5844 N
9 C9 -0.9856 -0.1147 -0.3255 C
10 C10 -0.3120 -1.4584 -0.3381 C
11 O11 -0.7133 -2.5968 -0.1561 O
12 C12 2.0917 -2.1132 -0.6896 C
13 C13 3.2439 -1.8564 0.2917 C
14 C14 -2.3099 0.1410 -0.0941 C
15 C15 -2.8728 1.5150 -0.0922 C
16 C16 -4.0323 4.0879 -0.1223 C
17 C17 -2.1497 2.6394 0.3532 C
18 C18 -4.1940 1.7132 -0.5412 C
19 C19 -4.7617 2.9847 -0.5683 C
20 C20 -2.7280 3.9063 0.3424 C
21 C21 -3.2782 -0.9612 0.1867 C
22 C22 -5.1752 -2.9612 0.7385 C
23 C23 -4.0048 -0.9482 1.3886 C
24 C24 -3.5287 -1.9837 -0.7394 C
25 C25 -4.4741 -2.9712 -0.4687 C
26 C26 -4.9341 -1.9486 1.6689 C
27 C27 4.9309 -0.9495 -1.3543 C
28 H28 6.9726 0.3536 1.9580 H
29 H29 6.9263 0.3536 0.2036 H
30 H30 6.2986 2.6078 1.0138 H
31 H31 5.0789 1.9204 2.0810 H
32 H32 5.8133 -1.6857 1.1063 H
33 H33 4.7551 -0.6913 2.0991 H
34 H34 3.9732 2.8173 0.0788 H
35 H35 5.0211 1.8950 -0.9853 H
36 H36 5.6770 -0.1851 -1.5881 H
37 H37 5.4523 -1.9142 -1.3235 H
38 H38 4.2350 -0.9873 -2.1981 H
39 H39 3.8357 -2.7813 0.3375 H
40 H40 2.8096 -1.7197 1.2913 H
41 H41 2.4534 -2.1866 -1.7227 H
42 H42 1.6083 -3.0650 -0.4504 H
43 H43 -2.9794 -2.0012 -1.6749 H
44 H44 -4.6583 -3.7530 -1.2008 H
45 H45 -5.9070 -3.7358 0.9518 H
46 H46 -5.4761 -1.9316 2.6108 H
47 H47 -3.8315 -0.1513 2.1064 H
48 H48 -4.7717 0.8617 -0.8856 H
49 H49 -5.7775 3.1115 -0.9334 H
50 H50 -4.4772 5.0796 -0.1330 H
51 H51 -2.1550 4.7576 0.7012 H
52 H52 -1.1329 2.5098 0.6990 H
53 C53 2.4148 0.9322 -1.0235 C
54 C54 3.5163 0.7039 0.0475 C
55 H55 2.7834 0.6356 -2.0148 H
56 H56 2.1809 1.9992 -1.0837 H
57 H57 3.0207 0.7612 1.0294 H
@<TRIPOS>BOND
1 1 4 1
2 1 5 1
3 1 32 1
4 1 33 1
5 2 3 1
6 2 5 1
7 2 30 1
8 2 31 1
9 3 34 1
10 3 35 1
11 3 54 1
12 4 13 1
13 4 27 1
14 4 54 1
15 5 28 1
16 5 29 1
17 6 7 1
18 6 10 1
19 6 12 1
20 7 8 2
21 7 53 1
22 8 9 1
23 9 10 1
24 9 14 2
25 10 11 2
26 12 13 1
27 12 41 1
28 12 42 1
29 13 39 1
30 13 40 1
31 14 15 1
32 14 21 1
33 15 17 Ar
34 15 18 Ar
35 16 19 Ar
36 16 20 Ar
37 16 50 1
38 17 20 Ar
39 17 52 1
40 18 19 Ar
41 18 48 1
42 19 49 1
43 20 51 1
44 21 23 Ar
45 21 24 Ar
46 22 25 Ar
47 22 26 Ar
48 22 45 1
49 23 26 Ar
50 23 47 1
51 24 25 Ar
52 24 43 1
53 25 44 1
54 26 46 1
55 27 36 1
56 27 37 1
57 27 38 1
58 53 54 1
59 53 55 1
60 53 56 1
61 54 57 1

DAIN **2a''** (15 °):
$E(S_0)$ = -1192.42200716 A.U.
$E(S_1)$ = -1192.30774764 A.U.

@<TRIPOS>MOLECULE
Molecule Name
57 61
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 5.2825 -0.9413 0.8959 C
2 C2 5.5001 1.4445 1.6894 C
3 C3 4.4540 1.8603 0.6484 C
4 C4 4.2218 -0.5735 -0.1806 C
5 C5 6.2592 0.1887 1.2469 C
6 N6 1.0316 -0.8622 -0.9167 N
7 C7 1.0942 0.4934 -0.6328 C
8 N8 -0.0485 1.0160 -0.2950 N
9 C9 -0.9891 -0.0279 -0.3169 C
10 C10 -0.2891 -1.2967 -0.7077 C
11 O11 -0.6735 -2.4425 -0.8803 O
12 C12 2.1176 -1.7540 -1.2916 C
13 C13 3.2656 -1.7946 -0.2753 C
14 C14 -2.3241 0.1218 -0.0444 C
15 C15 -2.9715 1.4537 -0.0143 C
16 C16 -4.2594 3.9622 0.0501 C
17 C17 -2.5480 2.5057 -0.8501 C
18 C18 -4.0591 1.6902 0.8498 C
19 C19 -4.6892 2.9317 0.8880 C
20 C20 -3.1891 3.7409 -0.8201 C
21 C21 -3.1896 -1.0614 0.2084 C
22 C22 -4.8595 -3.2631 0.7321 C
23 C23 -2.8396 -2.0131 1.1793 C
24 C24 -4.4002 -1.2264 -0.4868 C
25 C25 -5.2211 -2.3244 -0.2361 C
26 C26 -3.6687 -3.1003 1.4429 C
27 C27 4.9278 -0.3737 -1.5398 C
28 H28 6.9367 -0.1468 2.0425 H
29 H29 6.8966 0.4245 0.3841 H
30 H30 6.1955 2.2725 1.8764 H
31 H31 4.9918 1.2413 2.6436 H
32 H32 5.8383 -1.8281 0.5613 H
33 H33 4.7543 -1.2392 1.8138 H
34 H34 3.8767 2.7139 1.0259 H
35 H35 4.9556 2.2127 -0.2641 H
36 H36 5.6433 0.4533 -1.5220 H
37 H37 5.4825 -1.2806 -1.8104 H
38 H38 4.2247 -0.1704 -2.3537 H
39 H39 3.8778 -2.6735 -0.5220 H
40 H40 2.8322 -1.9915 0.7145 H
41 H41 2.4788 -1.4957 -2.2946 H
42 H42 1.6537 -2.7421 -1.3630 H
43 H43 -4.6882 -0.4940 -1.2355 H
44 H44 -6.1456 -2.4445 -0.7947 H
45 H45 -5.5042 -4.1143 0.9346 H
46 H46 -3.3831 -3.8233 2.2023 H
47 H47 -1.9147 -1.8894 1.7341 H
48 H48 -4.4000 0.8946 1.5044 H
49 H49 -5.5183 3.0932 1.5720 H
50 H50 -4.7554 4.9290 0.0727 H
51 H51 -2.8531 4.5344 -1.4825 H
52 H52 -1.7149 2.3449 -1.5226 H
53 C53 2.3817 1.2516 -0.6627 C
54 C54 3.4739 0.7169 0.3021 C
55 H55 2.7708 1.2902 -1.6893 H
56 H56 2.1241 2.2787 -0.3876 H
57 H57 2.9644 0.4453 1.2399 H
@<TRIPOS>BOND
1 1 4 1
2 1 5 1
3 1 32 1
4 1 33 1
5 2 3 1
6 2 5 1
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8 2 31 1
9 3 34 1
10 3 35 1
11 3 54 1
12 4 13 1
13 4 27 1
14 4 54 1
15 5 28 1
16 5 29 1
17 6 7 1
18 6 10 1
19 6 12 1
20 7 8 2
21 7 53 1
22 8 9 1
23 9 10 1
24 9 14 2
25 10 11 2
26 12 13 1
27 12 41 1
28 12 42 1
29 13 39 1
30 13 40 1
31 14 15 1
32 14 21 1
33 15 17 Ar
34 15 18 Ar
35 16 19 Ar
36 16 20 Ar
37 16 50 1
38 17 20 Ar
39 17 52 1
40 18 19 Ar
41 18 48 1
42 19 49 1
43 20 51 1
44 21 23 Ar
45 21 24 Ar
46 22 25 Ar
47 22 26 Ar
48 22 45 1
49 23 26 Ar
50 23 47 1
51 24 25 Ar
52 24 43 1
53 25 44 1
54 26 46 1
55 27 36 1
56 27 37 1
57 27 38 1
58 53 54 1
59 53 55 1
60 53 56 1
61 54 57 1

DAIN **2a”** (30 °):
$E(S_0)$ = -1192.41694522 A.U.
$E(S_1)$ = -1192.31185465 A.U.

@<TRIPOS>MOLECULE
Molecule Name
57 61
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 5.3369 -1.0550 0.5641 C
2 C2 5.5738 1.0478 1.9362 C
3 C3 4.4669 1.6919 1.0904 C
4 C4 4.2221 -0.4456 -0.3337 C
5 C5 6.3201 -0.0330 1.1475 C
6 N6 1.0131 -0.5969 -1.0114 N
7 C7 1.0675 0.6454 -0.4002 C
8 N8 -0.0821 1.0595 0.0560 N
9 C9 -1.0075 0.0421 -0.2181 C
10 C10 -0.3024 -1.0863 -0.9023 C
11 O11 -0.6869 -2.1503 -1.3630 O
12 C12 2.0900 -1.3508 -1.6308 C
13 C13 3.2786 -1.6238 -0.7000 C
14 C14 -2.3568 0.1097 0.0488 C
15 C15 -3.0806 1.3964 0.0347 C
16 C16 -4.5032 3.8304 -0.0453 C
17 C17 -4.2376 1.5882 0.8171 C
18 C18 -2.6515 2.4598 -0.7846 C
19 C19 -3.3570 3.6582 -0.8256 C
20 C20 -4.9386 2.7909 0.7789 C
21 C21 -3.1225 -1.1361 0.2875 C
22 C22 -4.5677 -3.4972 0.7928 C
23 C23 -2.6209 -2.1136 1.1648 C
24 C24 -4.3686 -1.3637 -0.3255 C
25 C25 -5.0795 -2.5361 -0.0820 C
26 C26 -3.3380 -3.2799 1.4178 C
27 C27 4.8650 0.1138 -1.6216 C
28 H28 7.0427 -0.5471 1.7937 H
29 H29 6.9067 0.4351 0.3449 H
30 H30 6.2699 1.8176 2.2930 H
31 H31 5.1241 0.5956 2.8326 H
32 H32 5.8815 -1.8159 -0.0117 H
33 H33 4.8558 -1.5889 1.3975 H
34 H34 3.8987 2.4038 1.7032 H
35 H35 4.9174 2.2833 0.2802 H
36 H36 5.5801 0.9142 -1.4135 H
37 H37 5.4106 -0.6820 -2.1436 H
38 H38 4.1284 0.5149 -2.3246 H
39 H39 3.8906 -2.3974 -1.1842 H
40 H40 2.8877 -2.0749 0.2223 H
41 H41 2.4092 -0.8504 -2.5530 H
42 H42 1.6302 -2.2984 -1.9266 H
43 H43 -4.7664 -0.6225 -1.0120 H
44 H44 -6.0321 -2.7018 -0.5781 H
45 H45 -5.1256 -4.4091 0.9888 H
46 H46 -2.9378 -4.0199 2.1058 H
47 H47 -1.6697 -1.9389 1.6583 H
48 H48 -1.7665 2.3317 -1.3963 H
49 H49 -3.0148 4.4598 -1.4750 H
50 H50 -5.0532 4.7672 -0.0811 H
51 H51 -5.8242 2.9176 1.3961 H
52 H52 -4.5772 0.7879 1.4667 H
53 C53 2.3456 1.4055 -0.2465 C
54 C54 3.4839 0.6568 0.4989 C
55 H55 2.6994 1.7369 -1.2329 H
56 H56 2.0851 2.3111 0.3088 H
57 H57 3.0187 0.1406 1.3535 H
@<TRIPOS>BOND
1 1 4 1
2 1 5 1
3 1 32 1
4 1 33 1
5 2 3 1
6 2 5 1
7 2 30 1
8 2 31 1
9 3 34 1
10 3 35 1
11 3 54 1
12 4 13 1
13 4 27 1
14 4 54 1
15 5 28 1
16 5 29 1
17 6 7 1
18 6 10 1
19 6 12 1
20 7 8 2
21 7 53 1
22 8 9 1
23 9 10 1
24 9 14 2
25 10 11 2

26 12 13 1
27 12 41 1
28 12 42 1
29 13 39 1
30 13 40 1
31 14 15 1
32 14 21 1
33 15 17 Ar
34 15 18 Ar
35 16 19 Ar
36 16 20 Ar
37 16 50 1
38 17 20 Ar
39 17 52 1
40 18 19 Ar
41 18 48 1
42 19 49 1
43 20 51 1
44 21 23 Ar
45 21 24 Ar
46 22 25 Ar
47 22 26 Ar
48 22 45 1
49 23 26 Ar
50 23 47 1
51 24 25 Ar
52 24 43 1
53 25 44 1
54 26 46 1
55 27 36 1
56 27 37 1
57 27 38 1
58 53 54 1
59 53 55 1
60 53 56 1
61 54 57 1

DAIN **2a”** (45 °):
$E(S_0)$ = -1192.40594926 A.U.
$E(S_1)$ = -1192.31404564 A.U.

@<TRIPOS>MOLECULE
Molecule Name
57 61
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 5.2029 1.1067 -0.3860 C
2 C2 5.3295 -0.5765 -2.2679 C
3 C3 4.3204 -1.4534 -1.5189 C
4 C4 4.1689 0.2578 0.4092 C
5 C5 6.1346 0.2968 -1.2992 C
6 N6 0.9989 0.1675 1.2999 N
7 C7 1.0315 -0.8567 0.3711 C
8 N8 -0.1219 -1.0920 -0.1987 N
9 C9 -1.0120 -0.1461 0.3135 C
10 C10 -0.3008 0.7219 1.2960 C
11 O11 -0.6733 1.6314 2.0227 O
12 C12 2.1140 0.7458 2.0340 C
13 C13 3.2401 1.2739 1.1321 C
14 C14 -2.3580 -0.0608 -0.0219 C
15 C15 -3.1954 -1.2684 -0.0806 C
16 C16 -4.7811 -3.5997 -0.1739 C
17 C17 -4.3194 -1.3513 -0.9299 C
18 C18 -2.8834 -2.3905 0.7144 C
19 C19 -3.6675 -3.5386 0.6683 C
20 C20 -5.1030 -2.5008 -0.9737 C
21 C21 -2.9447 1.2663 -0.2783 C
22 C22 -4.0075 3.8168 -0.8278 C
23 C23 -2.1862 2.2347 -0.9649 C
24 C24 -4.2526 1.6083 0.1245 C
25 C25 -4.7757 2.8687 -0.1458 C
26 C26 -2.7117 3.4947 -1.2359 C
27 C27 4.9151 -0.5878 1.4628 C
28 H28 6.7854 0.9840 -1.8549 H
29 H29 6.8035 -0.3361 -0.6992 H
30 H30 5.9993 -1.1989 -2.8747 H
31 H31 4.7846 0.0723 -2.9699 H
32 H32 5.7937 1.7026 0.3233 H
33 H33 4.6521 1.8280 -1.0082 H
34 H34 3.7136 -2.0146 -2.2407 H
35 H35 4.8546 -2.2056 -0.9200 H
36 H36 5.6171 -1.2870 1.0024 H
37 H37 5.4897 0.0665 2.1295 H
38 H38 4.2362 -1.1732 2.0898 H
39 H39 3.8783 1.9138 1.7583 H
40 H40 2.7798 1.9369 0.3864 H
41 H41 2.4854 0.0243 2.7729 H
42 H42 1.6753 1.5771 2.5941 H
43 H43 -4.8438 0.8842 0.6763 H
44 H44 -5.7803 3.1181 0.1855 H
45 H45 -4.4185 4.7999 -1.0414 H
46 H46 -2.1124 4.2243 -1.7739 H
47 H47 -1.1892 1.9738 -1.3054 H
48 H48 -2.0271 -2.3426 1.3779 H
49 H49 -3.4134 -4.3882 1.2964 H
50 H50 -5.3926 -4.4975 -0.2066 H
51 H51 -5.9587 -2.5443 -1.6423 H
52 H52 -4.5594 -0.5116 -1.5740 H
53 C53 2.2988 -1.5507 -0.0052 C
54 C54 3.3799 -0.6227 -0.6185 C
55 H55 2.7092 -2.0860 0.8616 H
56 H56 2.0100 -2.3122 -0.7359 H
57 H57 2.8543 0.0805 -1.2829 H
@<TRIPOS>BOND
1 1 4 1
2 1 5 1
3 1 32 1
4 1 33 1
5 2 3 1
6 2 5 1
7 2 30 1
8 2 31 1
9 3 34 1
10 3 35 1
11 3 54 1
12 4 13 1
13 4 27 1
14 4 54 1
15 5 28 1
16 5 29 1
17 6 7 1
18 6 10 1
19 6 12 1
20 7 8 2
21 7 53 1
22 8 9 1
23 9 10 1
24 9 14 Ar
25 10 11 2
26 12 13 1
27 12 41 1
28 12 42 1
29 13 39 1
30 13 40 1
31 14 15 1
32 14 21 1
33 15 17 Ar
34 15 18 Ar
35 16 19 Ar
36 16 20 Ar
37 16 50 1
38 17 20 Ar
39 17 52 1
40 18 19 Ar
41 18 48 1
42 19 49 1
43 20 51 1
44 21 23 Ar
45 21 24 Ar
46 22 25 Ar
47 22 26 Ar
48 22 45 1
49 23 26 Ar
50 23 47 1
51 24 25 Ar
52 24 43 1
53 25 44 1
54 26 46 1
55 27 36 1
56 27 37 1
57 27 38 1
58 53 54 1
59 53 55 1
60 53 56 1
61 54 57 1

DAIN **2a”** (60 °):
$E(S_0)$ = -1192.39101366 A.U.
$E(S_1)$ = -1192.31586830 A.U.

@<TRIPOS>MOLECULE
Molecule Name
57 61
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 5.2790 1.0637 0.1220 C
2 C2 5.4940 0.1186 -2.2089 C
3 C3 4.3958 -0.8976 -1.8725 C
4 C4 4.1740 0.0444 0.5210 C
5 C5 6.2522 0.5603 -0.9520 C
6 N6 0.9716 -0.2324 1.2066 N
7 C7 1.0188 -0.8825 -0.0067 C
8 N8 -0.1375 -0.9096 -0.6320 N
9 C9 -1.0229 -0.1848 0.1543 C
10 C10 -0.3275 0.3119 1.3661 C
11 O11 -0.7089 0.9277 2.3532 O
12 C12 2.0622 0.0313 2.1310 C
13 C13 3.2377 0.7960 1.5068 C
14 C14 -2.3937 -0.0146 -0.1191 C
15 C15 -3.2828 -1.1740 -0.2103 C
16 C16 -4.9800 -3.4271 -0.3185 C
17 C17 -2.9699 -2.3566 0.4950 C
18 C18 -4.4654 -1.1608 -0.9844 C
19 C19 -5.3039 -2.2694 -1.0317 C
20 C20 -3.8075 -3.4657 0.4406 C
21 C21 -2.9111 1.3517 -0.2191 C
22 C22 -3.8258 4.0069 -0.4769 C
23 C23 -2.0819 2.3585 -0.7600 C
24 C24 -4.2130 1.7166 0.1952 C
25 C25 -4.6628 3.0247 0.0648 C
26 C26 -2.5342 3.6693 -0.8846 C
27 C27 4.8295 -1.1481 1.2517 C
28 H28 6.9703 1.3530 -1.1985 H
29 H29 6.8435 -0.2790 -0.5629 H
30 H30 6.1849 -0.3053 -2.9486 H
31 H31 5.0348 0.9999 -2.6810 H
32 H32 5.8336 1.3598 1.0232 H
33 H33 4.7897 1.9759 -0.2515 H
34 H34 3.8185 -1.1308 -2.7765 H
35 H35 4.8508 -1.8458 -1.5520 H
36 H36 5.5426 -1.6847 0.6195 H

37 H37 5.3784 -0.7891 2.1310 H
38 H38 4.1003 -1.8831 1.6060 H
39 H39 3.8591 1.1580 2.3381 H
40 H40 2.8340 1.6907 1.0135 H
41 H41 2.3955 -0.9095 2.5855 H
42 H42 1.6134 0.6315 2.9280 H
43 H43 -4.8534 0.9688 0.6514 H
44 H44 -5.6622 3.2876 0.4010 H
45 H45 -4.1814 5.0286 -0.5800 H
46 H46 -1.8822 4.4261 -1.3122 H
47 H47 -1.0940 2.0846 -1.1149 H
48 H48 -4.7053 -0.2797 -1.5708 H
49 H49 -6.2052 -2.2377 -1.6382 H
50 H50 -5.6370 -4.2920 -0.3534 H
51 H51 -3.5517 -4.3602 1.0024 H
52 H52 -2.0755 -2.3790 1.1085 H
53 C53 2.2855 -1.4241 -0.5855 C
54 C54 3.4237 -0.3871 -0.7858 C
55 H55 2.6482 -2.2597 0.0291 H
56 H56 2.0072 -1.8507 -1.5538 H
57 H57 2.9547 0.5255 -1.1870 H
@<TRIPOS>BOND
1 1 4 1
2 1 5 1
3 1 32 1
4 1 33 1
5 2 3 1
6 2 5 1
7 2 30 1
8 2 31 1
9 3 34 1
10 3 35 1
11 3 54 1
12 4 13 1
13 4 27 1
14 4 54 1
15 5 28 1
16 5 29 1
17 6 7 Ar
18 6 10 1
19 6 12 1
20 7 8 2
21 7 53 1
22 8 9 1
23 9 10 1
24 9 14 Ar
25 10 11 2
26 12 13 1
27 12 41 1
28 12 42 1
29 13 39 1
30 13 40 1
31 14 15 1
32 14 21 1
33 15 17 Ar
34 15 18 Ar
35 16 19 Ar
36 16 20 Ar
37 16 50 1
38 17 20 Ar
39 17 52 1
40 18 19 Ar
41 18 48 1
42 19 49 1
43 20 51 1
44 21 23 Ar
45 21 24 Ar
46 22 25 Ar
47 22 26 Ar
48 22 45 1
49 23 26 Ar
50 23 47 1
51 24 25 Ar
52 24 43 1
53 25 44 1
54 26 46 1
55 27 36 1
56 27 37 1
57 27 38 1
58 53 54 1
59 53 55 1
60 53 56 1
61 54 57 1

DAIN **2a''** (75 °):
$E(S_0)$ = -1192.37333383 A.U.
$E(S_1)$ = -1192.31878580 A.U.

@<TRIPOS>MOLECULE
Molecule Name
57 61
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 5.2329 0.8931 0.5311 C
2 C2 5.4562 0.8564 -1.9845 C
3 C3 4.3819 -0.2368 -2.0365 C
4 C4 4.1443 -0.2173 0.5308 C
5 C5 6.2106 0.8352 -0.6505 C
6 N6 0.9433 -0.7410 1.0528 N
7 C7 1.0017 -0.9097 -0.3060 C
8 N8 -0.1537 -0.6745 -0.9077 N
9 C9 -1.0236 -0.2492 0.0736 C
10 C10 -0.3508 -0.2493 1.3828 C
11 O11 -0.7434 -0.0371 2.5267 O
12 C12 2.0275 -0.8296 2.0172 C
13 C13 3.1997 0.1152 1.7198 C
14 C14 -2.4064 0.0605 -0.1431 C
15 C15 -3.3716 -1.0131 -0.3307 C
16 C16 -5.2150 -3.1338 -0.6180 C
17 C17 -4.5670 -0.8495 -1.0727 C
18 C18 -3.1238 -2.2805 0.2466 C
19 C19 -4.0330 -3.3233 0.1019 C
20 C20 -5.4765 -1.8911 -1.2060 C
21 C21 -2.8001 1.4574 -0.0672 C
22 C22 -3.4581 4.2005 0.0336 C
23 C23 -1.8510 2.4512 -0.4086 C
24 C24 -4.0902 1.8859 0.3379 C
25 C25 -4.4126 3.2346 0.3794 C
26 C26 -2.1775 3.8031 -0.3541 C
27 C27 4.8130 -1.5865 0.7837 C
28 H28 6.9062 1.6820 -0.5919 H
29 H29 6.8270 -0.0717 -0.5897 H
30 H30 6.1533 0.7392 -2.8238 H
31 H31 4.9760 1.8376 -2.1133 H
32 H32 5.7862 0.8500 1.4793 H
33 H33 4.7272 1.8702 0.5160 H
34 H34 3.8116 -0.1503 -2.9704 H
35 H35 4.8605 -1.2260 -2.0638 H
36 H36 5.5514 -1.8414 0.0180 H
37 H37 5.3347 -1.5772 1.7486 H
38 H38 4.0906 -2.4080 0.8134 H
39 H39 3.8172 0.1544 2.6284 H
40 H40 2.7904 1.1255 1.5842 H
41 H41 2.3609 -1.8713 2.0996 H
42 H42 1.5719 -0.5622 2.9751 H
43 H43 -4.8175 1.1469 0.6574 H
44 H44 -5.4027 3.5431 0.7045 H
45 H45 -3.7157 5.2557 0.0677 H
46 H46 -1.4360 4.5480 -0.6303 H
47 H47 -0.8747 2.1363 -0.7604 H
48 H48 -2.2287 -2.4158 0.8439 H
49 H49 -3.8271 -4.2836 0.5670 H
50 H50 -5.9284 -3.9470 -0.7208 H
51 H51 -6.3835 -1.7439 -1.7863 H
52 H52 -4.7529 0.0954 -1.5732 H
53 C53 2.2682 -1.2060 -1.0386 C
54 C54 3.3997 -0.1596 -0.8462 C
55 H55 2.6348 -2.2074 -0.7710 H
56 H56 1.9939 -1.2507 -2.0969 H
57 H57 2.9224 0.8319 -0.8972 H
@<TRIPOS>BOND
1 1 4 1
2 1 5 1
3 1 32 1
4 1 33 1
5 2 3 1
6 2 5 1
7 2 30 1
8 2 31 1
9 3 34 1
10 3 35 1
11 3 54 1
12 4 13 1
13 4 27 1
14 4 54 1
15 5 28 1
16 5 29 1
17 6 7 Ar
18 6 10 1
19 6 12 1
20 7 8 Ar
21 7 53 1
22 8 9 Ar
23 9 10 1
24 9 14 Ar
25 10 11 2
26 12 13 1
27 12 41 1
28 12 42 1
29 13 39 1
30 13 40 1
31 14 15 1
32 14 21 1
33 15 17 Ar
34 15 18 Ar
35 16 19 Ar
36 16 20 Ar
37 16 50 1
38 17 20 Ar
39 17 52 1
40 18 19 Ar
41 18 48 1
42 19 49 1
43 20 51 1
44 21 23 Ar
45 21 24 Ar
46 22 25 Ar
47 22 26 Ar
48 22 45 1
49 23 26 Ar
50 23 47 1
51 24 25 Ar
52 24 43 1
53 25 44 1
54 26 46 1
55 27 36 1
56 27 37 1
57 27 38 1
58 53 54 1
59 53 55 1
60 53 56 1
61 54 57 1

DAIN **2a''** (90 °):

$E(S_0)$ = -1192.35552554 A.U.
$E(S_1)$ = -1192.32790086 A.U.

@<TRIPOS>MOLECULE
Molecule Name
57 61
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 5.4422 0.7040 0.5820 C
2 C2 5.6400 0.8951 -1.9272 C
3 C3 4.4230 -0.0275 -2.0670 C
4 C4 4.2081 -0.2396 0.4981 C
5 C5 6.3930 0.6247 -0.6201 C
6 N6 0.9825 -0.4904 1.0441 N
7 C7 1.0147 -0.5080 -0.3195 C
8 N8 -0.1859 -0.2950 -0.8598 N
9 C9 -1.0712 -0.2142 0.1807 C
10 C10 -0.3763 -0.3317 1.4536 C
11 O11 -0.7365 -0.1862 2.6254 O
12 C12 2.0618 -0.7273 1.9905 C
13 C13 3.3175 0.1103 1.7223 C
14 C14 -2.5002 0.0438 -0.0064 C
15 C15 -3.3848 -1.0797 -0.1793 C
16 C16 -5.0403 -3.3426 -0.5385 C
17 C17 -2.8444 -2.3314 -0.5769 C
18 C18 -4.7869 -1.0111 0.0537 C
19 C19 -5.5964 -2.1196 -0.1350 C
20 C20 -3.6641 -3.4418 -0.7508 C
21 C21 -2.9352 1.4217 -0.1016 C
22 C22 -3.7136 4.1344 -0.2069 C
23 C23 -4.0270 1.8416 -0.9069 C
24 C24 -2.2431 2.4115 0.6415 C
25 C25 -2.6324 3.7469 0.5864 C
26 C26 -4.4085 3.1738 -0.9548 C
27 C27 4.6858 -1.7036 0.6108 C
28 H28 7.2063 1.3501 -0.4918 H
29 H29 6.8694 -0.3643 -0.6668 H
30 H30 6.3065 0.7747 -2.7907 H
31 H31 5.3000 1.9413 -1.9378 H
32 H32 5.9908 0.4911 1.5100 H
33 H33 5.0823 1.7401 0.6703 H
34 H34 3.8587 0.2359 -2.9710 H
35 H35 4.7589 -1.0640 -2.2116 H
36 H36 5.3603 -1.9825 -0.2034 H
37 H37 5.2323 -1.8482 1.5511 H
38 H38 3.8573 -2.4173 0.6037 H
39 H39 3.9461 0.0276 2.6200 H
40 H40 3.0141 1.1637 1.6553 H
41 H41 2.2976 -1.7989 2.0306 H
42 H42 1.6406 -0.4589 2.9641 H
43 H43 -1.4450 2.1044 1.3070 H
44 H44 -2.0986 4.4860 1.1775 H
45 H45 -4.0160 5.1775 -0.2468 H
46 H46 -5.2349 3.4761 -1.5927 H
47 H47 -4.5344 1.1128 -1.5307 H
48 H48 -5.2171 -0.0880 0.4276 H
49 H49 -6.6634 -2.0475 0.0589 H
50 H50 -5.6796 -4.2099 -0.6801 H
51 H51 -3.2292 -4.3858 -1.0682 H
52 H52 -1.7855 -2.3918 -0.7971 H
53 C53 2.2266 -0.8342 -1.1279 C
54 C54 3.4718 0.0507 -0.8521 C
55 H55 2.4970 -1.8940 -1.0074 H
56 H56 1.9230 -0.7116 -2.1722 H
57 H57 3.1170 1.0915 -0.7939 H
@<TRIPOS>BOND
1 1 4 1
2 1 5 1
3 1 32 1
4 1 33 1
5 2 3 1
6 2 5 1
7 2 30 1
8 2 31 1
9 3 34 1
10 3 35 1
11 3 54 1
12 4 13 1
13 4 27 1
14 4 54 1
15 5 28 1
16 5 29 1
17 6 7 Ar
18 6 10 1
19 6 12 1
20 7 8 Ar
21 7 53 1
22 8 9 Ar
23 9 10 1
24 9 14 1
25 10 11 2
26 12 13 1
27 12 41 1
28 12 42 1
29 13 39 1
30 13 40 1
31 14 15 Ar
32 14 21 1
33 15 17 Ar
34 15 18 Ar
35 16 19 Ar
36 16 20 Ar
37 16 50 1
38 17 20 Ar
39 17 52 1
40 18 19 2
41 18 48 1
42 19 49 1
43 20 51 1
44 21 23 Ar
45 21 24 Ar
46 22 25 Ar
47 22 26 Ar
48 22 45 1
49 23 26 Ar
50 23 47 1
51 24 25 Ar
52 24 43 1
53 25 44 1
54 26 46 1
55 27 36 1
56 27 37 1
57 27 38 1
58 53 54 1
59 53 55 1
60 53 56 1
61 54 57 1

DAIN **2a''** (-15 °):
$E(S_0)$ = -1192.42197063 A.U.
$E(S_1)$ = -1192.30793760 A.U.

@<TRIPOS>MOLECULE
Molecule Name
57 61
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 5.2497 -0.5369 1.2301 C
2 C2 5.5591 1.9115 0.6948 C
3 C3 4.5198 1.7704 -0.4241 C
4 C4 4.1938 -0.7331 0.1048 C
5 C5 6.2679 0.5809 0.9702 C
6 N6 0.9855 -1.2429 -0.3850 N
7 C7 1.0937 0.0730 -0.8072 C
8 N8 -0.0262 0.7343 -0.7709 N
9 C9 -1.0065 -0.1630 -0.3127 C
10 C10 -0.3569 -1.4907 -0.0510 C
11 O11 -0.7734 -2.5502 0.3904 O
12 C12 2.0369 -2.2390 -0.2661 C
13 C13 3.1990 -1.8036 0.6349 C
14 C14 -2.3254 0.1570 -0.1189 C
15 C15 -2.7900 1.5627 -0.0635 C
16 C16 -3.7341 4.2171 0.0609 C
17 C17 -1.9834 2.5927 0.4587 C
18 C18 -4.0813 1.8968 -0.5176 C
19 C19 -4.5446 3.2092 -0.4643 C
20 C20 -2.4543 3.9011 0.5236 C
21 C21 -3.3467 -0.9064 0.0781 C
22 C22 -5.3130 -2.8874 0.4235 C
23 C23 -4.2442 -0.8472 1.1583 C
24 C24 -3.4634 -1.9685 -0.8326 C
25 C25 -4.4401 -2.9465 -0.6649 C
26 C26 -5.2101 -1.8360 1.3365 C
27 C27 4.8955 -1.2737 -1.1611 C
28 H28 6.9345 0.6770 1.8368 H
29 H29 6.9116 0.3225 0.1184 H
30 H30 6.2867 2.6914 0.4371 H
31 H31 5.0528 2.2477 1.6117 H
32 H32 5.7710 -1.4893 1.3989 H
33 H33 4.7173 -0.3103 2.1660 H
34 H34 3.9785 2.7176 -0.5458 H
35 H35 5.0262 1.5861 -1.3821 H
36 H36 5.6356 -0.5745 -1.5600 H
37 H37 5.4210 -2.2080 -0.9288 H
38 H38 4.1919 -1.4902 -1.9712 H
39 H39 3.7819 -2.7068 0.8635 H
40 H40 2.7756 -1.4620 1.5891 H
41 H41 2.3901 -2.5307 -1.2631 H
42 H42 1.5440 -3.1138 0.1681 H
43 H43 -2.7861 -2.0168 -1.6794 H
44 H44 -4.5182 -3.7579 -1.3836 H
45 H45 -6.0718 -3.6539 0.5572 H
46 H46 -5.8843 -1.7833 2.1872 H
47 H47 -4.1696 -0.0273 1.8667 H
48 H48 -4.7168 1.1186 -0.9277 H
49 H49 -5.5401 3.4438 -0.8319 H
50 H50 -4.0967 5.2405 0.1120 H
51 H51 -1.8196 4.6787 0.9407 H
52 H52 -0.9882 2.3563 0.8134 H
53 C53 2.3993 0.6555 -1.2413 C
54 C54 3.4961 0.6479 -0.1416 C
55 H55 2.7620 0.1421 -2.1419 H
56 H56 2.1838 1.6876 -1.5326 H
57 H57 2.9981 0.9139 0.8040 H
@<TRIPOS>BOND
1 1 4 1
2 1 5 1
3 1 32 1
4 1 33 1
5 2 3 1
6 2 5 1
7 2 30 1
8 2 31 1
9 3 34 1
10 3 35 1
11 3 54 1
12 4 13 1
13 4 27 1
14 4 54 1
15 5 28 1
16 5 29 1
17 6 7 1

18 6 10 1
19 6 12 1
20 7 8 2
21 7 53 1
22 8 9 1
23 9 10 1
24 9 14 2
25 10 11 2
26 12 13 1
27 12 41 1
28 12 42 1
29 13 39 1
30 13 40 1
31 14 15 1
32 14 21 1
33 15 17 Ar
34 15 18 Ar
35 16 19 Ar
36 16 20 Ar
37 16 50 1
38 17 20 Ar
39 17 52 1
40 18 19 Ar
41 18 48 1
42 19 49 1
43 20 51 1
44 21 23 Ar
45 21 24 Ar
46 22 25 Ar
47 22 26 Ar
48 22 45 1
49 23 26 Ar
50 23 47 1
51 24 25 Ar
52 24 43 1
53 25 44 1
54 26 46 1
55 27 36 1
56 27 37 1
57 27 38 1
58 53 54 1
59 53 55 1
60 53 56 1
61 54 57 1

DAIN **2a”** (-30 °):
$E(S_0)$ = -1192.41683577 A.U.
$E(S_1)$ = -1192.31174113 A.U.

@<TRIPOS>MOLECULE
Molecule Name
57 61
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 -5.3167 -0.3347 -1.1999 C
2 C2 -5.6756 1.9113 -0.1025 C
3 C3 -4.5491 1.5810 0.8848 C
4 C4 -4.1846 -0.7273 -0.2076 C
5 C5 -6.3539 0.6407 -0.6272 C
6 N6 -0.9469 -1.2602 0.0469 N
7 C7 -1.0658 -0.0604 0.7304 C
8 N8 0.0527 0.6013 0.8342 N
9 C9 1.0399 -0.1909 0.2306 C
10 C10 0.4067 -1.4409 -0.2956 C
11 O11 0.8386 -2.3834 -0.9417 O
12 C12 -1.9885 -2.2193 -0.2845 C
13 C13 -3.1885 -1.6041 -1.0165 C
14 C14 2.3652 0.1666 0.1165 C
15 C15 2.7636 1.5846 0.0059 C
16 C16 3.5453 4.2813 -0.2580 C
17 C17 1.9204 2.5253 -0.6183 C
18 C18 4.0053 2.0326 0.4994 C
19 C19 4.3900 3.3649 0.3717 C
20 C20 2.3099 3.8544 -0.7517 C
21 C21 3.4131 -0.8765 0.0546 C
22 C22 5.4136 -2.8567 -0.0007 C
23 C23 4.4890 -0.7909 -0.8497 C
24 C24 3.3680 -1.9729 0.9346 C
25 C25 4.3581 -2.9509 0.9087 C
26 C26 5.4745 -1.7743 -0.8811 C
27 C27 -4.7882 -1.5692 0.9372 C
28 H28 -7.0870 0.8937 -1.4036 H
29 H29 -6.9191 0.1607 0.1826 H
30 H30 -6.4105 2.5732 0.3731 H
31 H31 -5.2557 2.4717 -0.9508 H
32 H32 -5.8132 -1.2483 -1.5545 H
33 H33 -4.8549 0.1289 -2.0848 H
34 H34 -4.0305 2.5039 1.1742 H
35 H35 -4.9744 1.1691 1.8111 H
36 H36 -5.5470 -1.0244 1.5060 H
37 H37 -5.2721 -2.4631 0.5250 H
38 H38 -4.0370 -1.9122 1.6552 H
39 H39 -3.7595 -2.4401 -1.4445 H
40 H40 -2.8071 -1.0258 -1.8689 H
41 H41 -2.3077 -2.7546 0.6188 H
42 H42 -1.4966 -2.9513 -0.9320 H
43 H43 2.5567 -2.0394 1.6530 H
44 H44 4.3087 -3.7859 1.6024 H
45 H45 6.1868 -3.6204 -0.0204 H
46 H46 6.2894 -1.6980 -1.5962 H
47 H47 4.5376 0.0438 -1.5425 H
48 H48 4.6628 1.3283 0.9990 H
49 H49 5.3490 3.6887 0.7678 H
50 H50 3.8472 5.3199 -0.3644 H
51 H51 1.6489 4.5597 -1.2485 H
52 H52 0.9628 2.1997 -1.0071 H
53 C53 -2.3594 0.4043 1.3174 C
54 C54 -3.5151 0.5949 0.3001 C
55 H55 -2.6750 -0.2788 2.1177 H
56 H56 -2.1340 1.3622 1.7955 H
57 H57 -3.0820 1.0810 -0.5888 H
@<TRIPOS>BOND
1 1 4 1
2 1 5 1
3 1 32 1
4 1 33 1
5 2 3 1
6 2 5 1
7 2 30 1
8 2 31 1
9 3 34 1
10 3 35 1
11 3 54 1
12 4 13 1
13 4 27 1
14 4 54 1
15 5 28 1
16 5 29 1
17 6 7 1
18 6 10 1
19 6 12 1
20 7 8 2
21 7 53 1
22 8 9 1
23 9 10 1
24 9 14 2
25 10 11 2
26 12 13 1
27 12 41 1
28 12 42 1
29 13 39 1
30 13 40 1
31 14 15 1
32 14 21 1
33 15 17 Ar
34 15 18 Ar
35 16 19 Ar
36 16 20 Ar
37 16 50 1
38 17 20 Ar
39 17 52 1
40 18 19 Ar
41 18 48 1
42 19 49 1
43 20 51 1
44 21 23 Ar
45 21 24 Ar
46 22 25 Ar
47 22 26 Ar
48 22 45 1
49 23 26 Ar
50 23 47 1
51 24 25 Ar
52 24 43 1
53 25 44 1
54 26 46 1
55 27 36 1
56 27 37 1
57 27 38 1
58 53 54 1
59 53 55 1
60 53 56 1
61 54 57 1

DAIN **2a”** (-45 °):
$E(S_0)$ = -1192.40596285 A.U.
$E(S_1)$ = -1192.31420955 A.U.

@<TRIPOS>MOLECULE
Molecule Name
57 61
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 -5.2857 -0.1124 -1.2047 C
2 C2 -5.6273 1.8908 0.2917 C
3 C3 -4.5306 1.3546 1.2203 C
4 C4 -4.1618 -0.6988 -0.3034 C
5 C5 -6.3161 0.7528 -0.4695 C
6 N6 -0.9240 -1.2270 -0.1657 N
7 C7 -1.0489 -0.2189 0.7715 C
8 N8 0.0699 0.4129 1.0186 N
9 C9 1.0531 -0.2174 0.2526 C
10 C10 0.4348 -1.3220 -0.5346 C
11 O11 0.8749 -2.0890 -1.3790 O
12 C12 -1.9485 -2.1227 -0.6766 C
13 C13 -3.1642 -1.3985 -1.2667 C
14 C14 2.3823 0.1802 0.1740 C
15 C15 2.7428 1.5956 0.0036 C
16 C16 3.4304 4.3037 -0.3923 C
17 C17 1.8468 2.4895 -0.6188 C
18 C18 3.9870 2.1020 0.4362 C
19 C19 4.3271 3.4368 0.2364 C
20 C20 2.1879 3.8235 -0.8151 C
21 C21 3.4284 -0.8573 0.1670 C
22 C22 5.3904 -2.8789 0.1985 C
23 C23 4.5725 -0.7703 -0.6538 C
24 C24 3.2951 -1.9828 1.0037 C
25 C25 4.2654 -2.9812 1.0189 C
26 C26 5.5398 -1.7697 -0.6390 C
27 C27 -4.7770 -1.7455 0.6509 C
28 H28 -7.0365 1.1574 -1.1920 H

29 H29 -6.8997 0.1410 0.2324 H
30 H30 -6.3595 2.4717 0.8667 H
31 H31 -5.1744 2.5857 -0.4310 H
32 H32 -5.7901 -0.9384 -1.7244 H
33 H33 -4.8159 0.4992 -1.9895 H
34 H34 -4.0064 2.1921 1.6988 H
35 H35 -4.9855 0.7767 2.0379 H
36 H36 -5.5226 -1.3027 1.3166 H
37 H37 -5.2781 -2.5339 0.0756 H
38 H38 -4.0287 -2.2327 1.2836 H
39 H39 -3.7302 -2.1461 -1.8404 H
40 H40 -2.7953 -0.6672 -1.9992 H
41 H41 -2.2431 -2.8413 0.0997 H
42 H42 -1.4467 -2.6939 -1.4634 H
43 H43 2.4313 -2.0498 1.6577 H
44 H44 4.1464 -3.8384 1.6762 H
45 H45 6.1482 -3.6580 0.2118 H
46 H46 6.4063 -1.6915 -1.2902 H
47 H47 4.6806 0.0736 -1.3279 H
48 H48 4.6801 1.4415 0.9471 H
49 H49 5.2904 3.8042 0.5807 H
50 H50 3.6973 5.3451 -0.5514 H
51 H51 1.4854 4.4903 -1.3081 H
52 H52 0.8873 2.1188 -0.9617 H
53 C53 -2.3488 0.0904 1.4408 C
54 C54 -3.4932 0.4894 0.4693 C
55 H55 -2.6626 -0.7559 2.0679 H
56 H56 -2.1435 0.9236 2.1192 H
57 H57 -3.0439 1.1414 -0.2961 H
@<TRIPOS>BOND
1 1 4 1
2 1 5 1
3 1 32 1
4 1 33 1
5 2 3 1
6 2 5 1
7 2 30 1
8 2 31 1
9 3 34 1
10 3 35 1
11 3 54 1
12 4 13 1
13 4 27 1
14 4 54 1
15 5 28 1
16 5 29 1
17 6 7 1
18 6 10 1
19 6 12 1
20 7 8 2
21 7 53 1
22 8 9 1
23 9 10 1
24 9 14 Ar
25 10 11 2
26 12 13 1
27 12 41 1
28 12 42 1
29 13 39 1
30 13 40 1
31 14 15 1
32 14 21 1
33 15 17 Ar
34 15 18 Ar
35 16 19 Ar
36 16 20 Ar
37 16 50 1
38 17 20 Ar
39 17 52 1
40 18 19 Ar
41 18 48 1
42 19 49 1
43 20 51 1
44 21 23 Ar
45 21 24 Ar
46 22 25 Ar
47 22 26 Ar
48 22 45 1
49 23 26 Ar
50 23 47 1
51 24 25 Ar
52 24 43 1
53 25 44 1
54 26 46 1
55 27 36 1
56 27 37 1
57 27 38 1
58 53 54 1
59 53 55 1
60 53 56 1
61 54 57 1

DAIN **2a''** (-60 °):
$E(S_0)$ = -1192.39086015 A.U.
$E(S_1)$ = -1192.31577549 A.U.

@<TRIPOS>MOLECULE
Molecule Name
57 61
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 5.2720 0.2507 1.1044 C
2 C2 5.6242 1.6961 -0.9409 C
3 C3 4.5140 0.9123 -1.6511 C
4 C4 4.1517 -0.5805 0.4164 C
5 C5 6.3052 0.8498 0.1419 C
6 N6 0.9172 -1.1633 0.4632 N
7 C7 1.0334 -0.4206 -0.6908 C
8 N8 -0.0910 0.1486 -1.0634 N
9 C9 -1.0588 -0.2743 -0.1612 C
10 C10 -0.4437 -1.1642 0.8544 C
11 O11 -0.8760 -1.6947 1.8700 O
12 C12 1.9620 -1.8688 1.1868 C
13 C13 3.1584 -0.9781 1.5442 C
14 C14 -2.4000 0.1540 -0.1631 C
15 C15 -2.7260 1.5717 0.0041 C
16 C16 -3.3314 4.2982 0.4195 C
17 C17 -1.8346 2.4196 0.6975 C
18 C18 -3.9221 2.1382 -0.4920 C
19 C19 -4.2229 3.4794 -0.2794 C
20 C20 -2.1340 3.7624 0.9010 C
21 C21 -3.4492 -0.8648 -0.2334 C
22 C22 -5.4255 -2.8632 -0.4688 C
23 C23 -4.7002 -0.7314 0.4123 C
24 C24 -3.2176 -2.0324 -0.9932 C
25 C25 -4.1938 -3.0187 -1.1067 C
26 C26 -5.6735 -1.7155 0.2926 C
27 C27 4.7677 -1.8608 -0.1917 C
28 H28 7.0221 1.4591 0.7073 H
29 H29 6.8910 0.0486 -0.3277 H
30 H30 6.3618 2.0532 -1.6711 H
31 H31 5.1869 2.5923 -0.4767 H
32 H32 5.7738 -0.3782 1.8526 H
33 H33 4.7950 1.0711 1.6616 H
34 H34 3.9988 1.5691 -2.3634 H
35 H35 4.9531 0.1001 -2.2466 H
36 H36 5.5345 -1.6483 -0.9435 H
37 H37 5.2464 -2.4545 0.5969 H
38 H38 4.0232 -2.5047 -0.6722 H
39 H39 3.7342 -1.5090 2.3154 H
40 H40 2.7743 -0.0664 2.0215 H
41 H41 2.2825 -2.7528 0.6214 H
42 H42 1.4774 -2.2276 2.0998 H
43 H43 -2.2755 -2.1306 -1.5224 H
44 H44 -3.9976 -3.9038 -1.7059 H
45 H45 -6.1905 -3.6291 -0.5645 H
46 H46 -6.6240 -1.5988 0.8064 H
47 H47 -4.8858 0.1374 1.0354 H
48 H48 -4.6037 1.5186 -1.0659 H
49 H49 -5.1483 3.8928 -0.6717 H
50 H50 -3.5687 5.3452 0.5885 H
51 H51 -1.4378 4.3909 1.4499 H
52 H52 -0.9188 1.9995 1.0996 H
53 C53 2.3120 -0.3133 -1.4549 C
54 C54 3.4783 0.3359 -0.6642 C
55 H55 2.6176 -1.2982 -1.8357 H
56 H56 2.0798 0.3019 -2.3296 H
57 H57 3.0510 1.1920 -0.1185 H
@<TRIPOS>BOND
1 1 4 1
2 1 5 1
3 1 32 1
4 1 33 1
5 2 3 1
6 2 5 1
7 2 30 1
8 2 31 1
9 3 34 1
10 3 35 1
11 3 54 1
12 4 13 1
13 4 27 1
14 4 54 1
15 5 28 1
16 5 29 1
17 6 7 Ar
18 6 10 1
19 6 12 1
20 7 8 2
21 7 53 1
22 8 9 1
23 9 10 1
24 9 14 Ar
25 10 11 2
26 12 13 1
27 12 41 1
28 12 42 1
29 13 39 1
30 13 40 1
31 14 15 1
32 14 21 1
33 15 17 Ar
34 15 18 Ar
35 16 19 Ar
36 16 20 Ar
37 16 50 1
38 17 20 Ar
39 17 52 1
40 18 19 Ar
41 18 48 1
42 19 49 1
43 20 51 1
44 21 23 Ar
45 21 24 Ar
46 22 25 Ar
47 22 26 Ar
48 22 45 1
49 23 26 Ar
50 23 47 1
51 24 25 Ar
52 24 43 1
53 25 44 1
54 26 46 1
55 27 36 1
56 27 37 1

57 27 38 1
58 53 54 1
59 53 55 1
60 53 56 1
61 54 57 1

DAIN **2a''** (-75 °):
$E(S_0)$ = -1192.36497223 A.U.
$E(S_1)$ = -1192.32007275 A.U

@<TRIPOS>MOLECULE
Molecule Name
57 61
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 5.3816 0.3714 0.9350 C
2 C2 5.6937 1.4372 -1.3303 C
3 C3 4.5121 0.6091 -1.8529 C
4 C4 4.1894 -0.5047 0.4541 C
5 C5 6.3918 0.7341 -0.1613 C
6 N6 0.9467 -0.9080 0.7183 N
7 C7 1.0364 -0.4511 -0.5682 C
8 N8 -0.1304 -0.0402 -1.0483 N
9 C9 -1.0650 -0.2921 -0.0705 C
10 C10 -0.4223 -0.8970 1.0997 C
11 O11 -0.8386 -1.2572 2.2010 O
12 C12 1.9836 -1.5080 1.5443 C
13 C13 3.2399 -0.6392 1.6770 C
14 C14 -2.4376 0.1102 -0.1706 C
15 C15 -2.7839 1.5185 0.0236 C
16 C16 -3.3785 4.2166 0.6247 C
17 C17 -1.8803 2.5592 -0.3067 C
18 C18 -3.9959 1.8756 0.6593 C
19 C19 -4.2753 3.2049 0.9679 C
20 C20 -2.1804 3.8825 -0.0198 C
21 C21 -3.4783 -0.9083 -0.3264 C
22 C22 -5.4304 -2.8818 -0.8562 C
23 C23 -3.3244 -2.2332 0.1490 C
24 C24 -4.6391 -0.6065 -1.0751 C
25 C25 -5.5911 -1.5867 -1.3476 C
26 C26 -4.2941 -3.1937 -0.0985 C
27 C27 4.7177 -1.9002 0.0579 C
28 H28 7.1743 1.3780 0.2596 H
29 H29 6.9001 -0.1693 -0.5245 H
30 H30 6.4029 1.6370 -2.1436 H
31 H31 5.3241 2.4165 -0.9918 H
32 H32 5.8904 -0.1447 1.7607 H
33 H33 4.9761 1.3028 1.3574 H
34 H34 3.9815 1.1717 -2.6322 H
35 H35 4.8857 -0.3028 -2.3405 H
36 H36 5.4064 -1.8534 -0.7893 H
37 H37 5.2622 -2.3477 0.8986 H
38 H38 3.9180 -2.5949 -0.2150 H
39 H39 3.8292 -1.0600 2.5038 H
40 H40 2.9244 0.3620 2.0013 H
41 H41 2.2264 -2.5121 1.1731 H
42 H42 1.5192 -1.6371 2.5262 H
43 H43 -4.7665 0.3921 -1.4786 H
44 H44 -6.4616 -1.3330 -1.9467 H
45 H45 -6.1776 -3.6434 -1.0618 H
46 H46 -4.1650 -4.1974 0.2979 H
47 H47 -2.4587 -2.4836 0.7520 H
48 H48 -4.6932 1.1006 0.9563 H
49 H49 -5.2014 3.4474 1.4826 H
50 H50 -3.6041 5.2531 0.8600 H
51 H51 -1.4763 4.6632 -0.2959 H
52 H52 -0.9499 2.3029 -0.8027 H
53 C53 2.2920 -0.4991 -1.3737 C
54 C54 3.5039 0.2384 -0.7415 C
55 H55 2.5650 -1.5416 -1.5939 H
56 H56 2.0482 -0.0350 -2.3341 H
57 H57 3.1217 1.1879 -0.3352 H
@<TRIPOS>BOND
1 1 4 1
2 1 5 1
3 1 32 1
4 1 33 1
5 2 3 1
6 2 5 1
7 2 30 1
8 2 31 1
9 3 34 1
10 3 35 1
11 3 54 1
12 4 13 1
13 4 27 1
14 4 54 1
15 5 28 1
16 5 29 1
17 6 7 Ar
18 6 10 1
19 6 12 1
20 7 8 Ar
21 7 53 1
22 8 9 Ar
23 9 10 1
24 9 14 Ar
25 10 11 2
26 12 13 1
27 12 41 1
28 12 42 1
29 13 39 1
30 13 40 1
31 14 15 1
32 14 21 1
33 15 17 Ar
34 15 18 Ar
35 16 19 Ar
36 16 20 Ar
37 16 50 1
38 17 20 Ar
39 17 52 1
40 18 19 Ar
41 18 48 1
42 19 49 1
43 20 51 1
44 21 23 Ar
45 21 24 Ar
46 22 25 Ar
47 22 26 Ar
48 22 45 1
49 23 26 Ar
50 23 47 1
51 24 25 Ar
52 24 43 1
53 25 44 1
54 26 46 1
55 27 36 1
56 27 37 1
57 27 38 1
58 53 54 1
59 53 55 1
60 53 56 1
61 54 57 1

DAIN **2a''** (-90 °):
$E(S_0)$ = -1192.34787565 A.U.
$E(S_1)$ = -1192.33611499 A.U.

@<TRIPOS>MOLECULE
Molecule Name
57 61
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 5.3117 0.7195 0.7042 C
2 C2 5.6085 0.9188 -1.7988 C
3 C3 4.4711 -0.0919 -1.9873 C
4 C4 4.1536 -0.3092 0.5640 C
5 C5 6.3180 0.7153 -0.4547 C
6 N6 0.9174 -0.6916 0.9578 N
7 C7 1.0157 -0.6837 -0.3968 C
8 N8 -0.1593 -0.4364 -0.9902 N
9 C9 -1.0818 -0.3370 0.0073 C
10 C10 -0.4586 -0.5097 1.3136 C
11 O11 -0.8633 -0.4149 2.4732 O
12 C12 1.9619 -0.9325 1.9413 C
13 C13 3.1907 -0.0331 1.7527 C
14 C14 -2.4726 0.0547 -0.2207 C
15 C15 -2.7773 1.4851 -0.1488 C
16 C16 -3.2453 4.2573 0.1597 C
17 C17 -1.8981 2.4440 -0.7097 C
18 C18 -3.8878 1.9603 0.5846 C
19 C19 -4.1053 3.3283 0.7434 C
20 C20 -2.1394 3.8027 -0.5707 C
21 C21 -3.4725 -0.9707 -0.3257 C
22 C22 -5.3690 -3.0537 -0.6386 C
23 C23 -3.1084 -2.3389 -0.1688 C
24 C24 -4.8196 -0.6977 -0.7034 C
25 C25 -5.7388 -1.7222 -0.8668 C
26 C26 -4.0481 -3.3519 -0.2863 C
27 C27 4.7268 -1.7371 0.6922 C
28 H28 7.0645 1.5032 -0.2924 H
29 H29 6.8738 -0.2317 -0.4712 H
30 H30 6.3238 0.8446 -2.6277 H
31 H31 5.1912 1.9358 -1.8361 H
32 H32 5.8325 0.5410 1.6548 H
33 H33 4.8716 1.7249 0.7807 H
34 H34 3.9373 0.1246 -2.9214 H
35 H35 4.8864 -1.1035 -2.1010 H
36 H36 5.4743 -1.9543 -0.0757 H
37 H37 5.2170 -1.8578 1.6661 H
38 H38 3.9571 -2.5118 0.6210 H
39 H39 3.7822 -0.1118 2.6761 H
40 H40 2.8412 1.0069 1.6991 H
41 H41 2.2381 -1.9948 1.9485 H
42 H42 1.4908 -0.7177 2.9051 H
43 H43 -5.1197 0.3235 -0.9054 H
44 H44 -6.7533 -1.4865 -1.1771 H
45 H45 -6.0946 -3.8519 -0.7679 H
46 H46 -3.7452 -4.3849 -0.1385 H
47 H47 -2.0720 -2.5826 0.0343 H
48 H48 -4.5422 1.2556 1.0852 H
49 H49 -4.9519 3.6648 1.3362 H
50 H50 -3.4233 5.3222 0.2803 H
51 H51 -1.4601 4.5171 -1.0289 H
52 H52 -1.0329 2.0951 -1.2655 H
53 C53 2.2673 -0.9988 -1.1437 C
54 C54 3.4613 -0.0618 -0.8197 C
55 H55 2.5623 -2.0465 -0.9852 H
56 H56 2.0116 -0.9053 -2.2037 H
57 H57 3.0558 0.9616 -0.7828 H
@<TRIPOS>BOND
1 1 4 1
2 1 5 1
3 1 32 1
4 1 33 1
5 2 3 1
6 2 5 1
7 2 30 1
8 2 31 1
9 3 34 1

10 3 35 1
11 3 54 1
12 4 13 1
13 4 27 1
14 4 54 1
15 5 28 1
16 5 29 1
17 6 7 Ar
18 6 10 1
19 6 12 1
20 7 8 Ar
21 7 53 1
22 8 9 Ar
23 9 10 1
24 9 14 1
25 10 11 2
26 12 13 1
27 12 41 1
28 12 42 1
29 13 39 1
30 13 40 1
31 14 15 1
32 14 21 Ar
33 15 17 Ar
34 15 18 Ar
35 16 19 Ar
36 16 20 Ar
37 16 50 1
38 17 20 Ar
39 17 52 1
40 18 19 Ar
41 18 48 1
42 19 49 1
43 20 51 1
44 21 23 Ar
45 21 24 Ar
46 22 25 Ar
47 22 26 Ar
48 22 45 1
49 23 26 Ar
50 23 47 1
51 24 25 Ar
52 24 43 1
53 25 44 1
54 26 46 1
55 27 36 1
56 27 37 1
57 27 38 1
58 53 54 1
59 53 55 1
60 53 56 1
61 54 57 1

DAIN **2b"** (optimized):
$E(S_0)$ = -1192.41737889 A.U.
No imaginary frequencies.

@<TRIPOS>MOLECULE
Molecule Name
57 61
SMALL
NO_CHARGES

@<TRIPOS>ATOM

1	C1	-5.2736	-0.0868	-1.1613 C
2	C2	-5.5087	1.9893	0.2511 C
3	C3	-4.6220	1.3370	1.3218 C
4	C4	-4.3325	-0.7714	-0.1337 C
5	C5	-6.2591	0.9188	-0.5520 C
6	N6	-1.0378	-1.1005	-0.1065 N
7	C7	-1.1412	0.2785	0.0276 C
8	N8	0.0068	0.8823	0.1270 N
9	C9	0.9994	-0.1090	0.0532 C
10	C10	0.3247	-1.4418	-0.0859 C
11	O11	0.7405	-2.5851	-0.1944 O
12	C12	-2.0784	-2.1175	-0.2083 C
13	C13	-3.3234	-1.6276	-0.9509 C
14	C14	2.3454	0.1431	0.0282 C
15	C15	2.8856	1.5257	0.0041 C
16	C16	3.9838	4.1235	-0.0064 C
17	C17	2.2593	2.5717	-0.7007 C
18	C18	4.0805	1.8124	0.6934 C
19	C19	4.6164	3.0979	0.6984 C
20	C20	2.8078	3.8519	-0.7089 C
21	C21	3.3501	-0.9568	0.0237 C
22	C22	5.3101	-2.9749	-0.0104 C
23	C23	4.3609	-0.9631	-0.9535 C
24	C24	3.3497	-1.9722	0.9922 C
25	C25	4.3244	-2.9676	0.9785 C
26	C26	5.3234	-1.9702	-0.9794 C
27	C27	-5.1436	-1.7227	0.7740 C
28	H28	-6.8528	1.3823	-1.3500 H
29	H29	-6.9720	0.4017	0.1038 H
30	H30	-6.2157	2.6800	0.7277 H
31	H31	-4.8965	2.5969	-0.4310 H
32	H32	-5.8147	-0.8647	-1.7176 H
33	H33	-4.6613	0.4419	-1.9064 H
34	H34	-4.0668	2.1023	1.8792 H
35	H35	-5.2696	0.8389	2.0546 H
36	H36	-5.8685	-1.1952	1.4016 H
37	H37	-5.7007	-2.4499	0.1707 H
38	H38	-4.4864	-2.2844	1.4486 H
39	H39	-3.8590	-2.5077	-1.3286 H
40	H40	-2.9931	-1.0750	-1.8395 H
41	H41	-2.3342	-2.4890	0.7930 H
42	H42	-1.6134	-2.9535	-0.7390 H
43	H43	2.5840	-1.9761	1.7608 H
44	H44	4.3106	-3.7426	1.7403 H
45	H45	6.0650	-3.7568	-0.0233 H
46	H46	6.0864	-1.9665	-1.7535 H
47	H47	4.3809	-0.1768	-1.7027 H
48	H48	4.5809	1.0199	1.2405 H
49	H49	5.5314	3.2968	1.2503 H
50	H50	4.4059	5.1251	-0.0114 H
51	H51	2.3134	4.6418	-1.2684 H
52	H52	1.3402	2.3714	-1.2361 H
53	C53	-2.4483	1.0167	0.0263 C
54	C54	-3.6166	0.3045	0.7532 C
55	H55	-3.1831	-0.2154	1.6202 H
56	H56	-2.2379	1.9830	0.4953 H
57	H57	-2.7240	1.2432	-1.0130 H

@<TRIPOS>BOND
1 1 4 1
2 1 5 1
3 1 32 1
4 1 33 1
5 2 3 1
6 2 5 1
7 2 30 1
8 2 31 1
9 3 34 1
10 3 35 1
11 3 54 1
12 4 13 1
13 4 27 1
14 4 54 1
15 5 28 1
16 5 29 1
17 6 7 1
18 6 10 1
19 6 12 1
20 7 8 2
21 7 53 1
22 8 9 1
23 9 10 1
24 9 14 2
25 10 11 2
26 12 13 1
27 12 41 1
28 12 42 1
29 13 39 1
30 13 40 1
31 14 15 1
32 14 21 1
33 15 17 Ar
34 15 18 Ar
35 16 19 Ar
36 16 20 Ar
37 16 50 1
38 17 20 Ar
39 17 52 1
40 18 19 Ar
41 18 48 1
42 19 49 1
43 20 51 1
44 21 23 Ar
45 21 24 Ar
46 22 25 Ar
47 22 26 Ar
48 22 45 1
49 23 26 Ar
50 23 47 1
51 24 25 Ar
52 24 43 1
53 25 44 1
54 26 46 1
55 27 36 1
56 27 37 1
57 27 38 1
58 53 54 1
59 53 56 1
60 53 57 1
61 54 55 1

DAIN **2b"** (0 °):
$E(S_0)$ = -1192.41687050 A.U.
$E(S_1)$ = -1192.29821072 A.U.

@<TRIPOS>MOLECULE
Molecule Name
57 61
SMALL
NO_CHARGES

@<TRIPOS>ATOM

1	C1	5.2782	-0.1485	1.1663 C
2	C2	5.5008	2.0084	-0.1298 C
3	C3	4.6192	1.4094	-1.2354 C
4	C4	4.3407	-0.7770	0.1008 C
5	C5	6.2558	0.9005	0.6175 C
6	N6	1.0473	-1.1022	0.0407 N
7	C7	1.1496	0.2826	0.0148 C
8	N8	0.0013	0.8916	-0.0329 N
9	C9	-0.9919	-0.1023	-0.0264 C
10	C10	-0.3148	-1.4416	0.0017 C
11	O11	-0.7281	-2.5910	0.0109 O
12	C12	2.0895	-2.1220	0.0704 C
13	C13	3.3283	-1.6855	0.8563 C
14	C14	-2.3384	0.1462	-0.0213 C
15	C15	-2.8925	1.5241	-0.0223 C
16	C16	-4.0303	4.1054	-0.0682 C
17	C17	-2.2756	2.5979	0.6493 C
18	C18	-4.0986	1.7756	-0.7067 C
19	C19	-4.6533	3.0525	-0.7403 C

20 C20 -2.8439 3.8693 0.6296 C
21 C21 -3.3408 -0.9592 0.0149 C
22 C22 -5.3009 -2.9743 0.1129 C
23 C23 -4.3000 -0.9801 1.0416 C
24 C24 -3.3923 -1.9561 -0.9705 C
25 C25 -4.3676 -2.9504 -0.9248 C
26 C26 -5.2617 -1.9871 1.0992 C
27 C27 5.1594 -1.6690 -0.8592 C
28 H28 6.8402 1.3240 1.4440 H
29 H29 6.9791 0.4296 -0.0616 H
30 H30 6.2048 2.7291 -0.5644 H
31 H31 4.8815 2.5727 0.5821 H
32 H32 5.8273 -0.9536 1.6733 H
33 H33 4.6645 0.3303 1.9427 H
34 H34 4.0611 2.2008 -1.7520 H
35 H35 5.2679 0.9518 -1.9930 H
36 H36 5.9167 -1.1096 -1.4164 H
37 H37 5.6801 -2.4570 -0.3013 H
38 H38 4.5120 -2.1568 -1.5978 H
39 H39 3.8609 -2.5892 1.1787 H
40 H40 2.9908 -1.1937 1.7774 H
41 H41 2.3537 -2.4146 -0.9543 H
42 H42 1.6240 -2.9971 0.5330 H
43 H43 -2.6653 -1.9503 -1.7755 H
44 H44 -4.3940 -3.7117 -1.7001 H
45 H45 -6.0560 -3.7553 0.1509 H
46 H46 -5.9841 -1.9959 1.9113 H
47 H47 -4.2817 -0.2060 1.8037 H
48 H48 -4.5940 0.9619 -1.2265 H
49 H49 -5.5763 3.2233 -1.2883 H
50 H50 -4.4678 5.1004 -0.0845 H
51 H51 -2.3566 4.6805 1.1645 H
52 H52 -1.3481 2.4257 1.1792 H
53 C53 2.4581 1.0171 0.0602 C
54 C54 3.6195 0.3470 -0.7180 C
55 H55 3.1766 -0.1217 -1.6091 H
56 H56 2.2491 2.0125 -0.3442 H
57 H57 2.7389 1.1754 1.1107 H
@<TRIPOS>BOND
1 1 4 1
2 1 5 1
3 1 32 1
4 1 33 1
5 2 3 1
6 2 5 1
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9 3 34 1
10 3 35 1
11 3 54 1
12 4 13 1
13 4 27 1
14 4 54 1
15 5 28 1
16 5 29 1
17 6 7 1
18 6 10 1
19 6 12 1
20 7 8 2
21 7 53 1
22 8 9 1
23 9 10 1
24 9 14 2
25 10 11 2
26 12 13 1
27 12 41 1
28 12 42 1
29 13 39 1
30 13 40 1
31 14 15 1
32 14 21 1
33 15 17 Ar
34 15 18 Ar
35 16 19 Ar
36 16 20 Ar
37 16 50 1
38 17 20 Ar
39 17 52 1
40 18 19 Ar
41 18 48 1
42 19 49 1
43 20 51 1
44 21 23 Ar
45 21 24 Ar
46 22 25 Ar
47 22 26 Ar
48 22 45 1
49 23 26 Ar
50 23 47 1
51 24 25 Ar
52 24 43 1
53 25 44 1
54 26 46 1
55 27 36 1
56 27 37 1
57 27 38 1
58 53 54 1
59 53 56 1
60 53 57 1
61 54 55 1

DAIN **2b”** (15 °):
$E(S_0)$ = -1192.41702092 A.U.
$E(S_1)$ = -1192.30399100 A.U.

@<TRIPOS>MOLECULE
Molecule Name
57 61
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 -5.3274 -0.5023 -1.0333 C
2 C2 -5.4880 1.9520 -0.4643 C
3 C3 -4.5384 1.7205 0.7183 C
4 C4 -4.3205 -0.7806 0.1164 C
5 C5 -6.2775 0.6756 -0.7803 C
6 N6 -1.0237 -1.1063 0.1436 N
7 C7 -1.1288 0.2317 -0.2202 C
8 N8 0.0174 0.8352 -0.3388 N
9 C9 1.0098 -0.1215 -0.0696 C
10 C10 0.3411 -1.4261 0.2438 C
11 O11 0.7641 -2.5257 0.5664 O
12 C12 -2.0631 -2.0914 0.4284 C
13 C13 -3.3431 -1.8802 -0.3859 C
14 C14 2.3554 0.1402 -0.0693 C
15 C15 2.8716 1.5293 -0.0339 C
16 C16 3.9059 4.1507 0.0372 C
17 C17 2.2149 2.5451 0.6868 C
18 C18 4.0611 1.8585 -0.7123 C
19 C19 4.5673 3.1559 -0.6852 C
20 C20 2.7315 3.8375 0.7255 C
21 C21 3.3580 -0.9564 -0.0643 C
22 C22 5.3011 -2.9914 -0.0769 C
23 C23 3.2859 -2.0128 -0.9870 C
24 C24 4.4311 -0.9335 0.8442 C
25 C25 5.3865 -1.9475 0.8462 C
26 C26 4.2506 -3.0169 -0.9966 C
27 C27 -5.0716 -1.3236 1.3519 C
28 H28 -6.9155 0.8265 -1.6603 H
29 H29 -6.9556 0.4479 0.0539 H
30 H30 -6.1700 2.7804 -0.2349 H
31 H31 -4.9181 2.2599 -1.3530 H
32 H32 -5.9002 -1.4187 -1.2317 H
33 H33 -4.7639 -0.2954 -1.9552 H
34 H34 -3.9562 2.6270 0.9269 H
35 H35 -5.1393 1.5352 1.6187 H
36 H36 -5.7672 -0.5919 1.7720 H
37 H37 -5.6523 -2.2164 1.0900 H
38 H38 -4.3756 -1.6039 2.1518 H
39 H39 -3.8903 -2.8316 -0.4048 H
40 H40 -3.0534 -1.6838 -1.4260 H
41 H41 -2.2744 -2.1002 1.5060 H
42 H42 -1.6153 -3.0615 0.1945 H
43 H43 4.5048 -0.1202 1.5603 H
44 H44 6.1996 -1.9205 1.5670 H
45 H45 6.0510 -3.7782 -0.0826 H
46 H46 4.1811 -3.8222 -1.7231 H
47 H47 2.4725 -2.0358 -1.7053 H
48 H48 4.5802 1.0894 -1.2755 H
49 H49 5.4801 3.3889 -1.2271 H
50 H50 4.3040 5.1617 0.0669 H
51 H51 2.2153 4.6037 1.2981 H
52 H52 1.3001 2.3100 1.2165 H
53 C53 -2.4402 0.9062 -0.4936 C
54 C54 -3.5648 0.5362 0.5078 C
55 H55 -3.0801 0.3591 1.4784 H
56 H56 -2.2312 1.9799 -0.4657 H
57 H57 -2.7493 0.6843 -1.5241 H
@<TRIPOS>BOND
1 1 4 1
2 1 5 1
3 1 32 1
4 1 33 1
5 2 3 1
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9 3 34 1
10 3 35 1
11 3 54 1
12 4 13 1
13 4 27 1
14 4 54 1
15 5 28 1
16 5 29 1
17 6 7 1
18 6 10 1
19 6 12 1
20 7 8 2
21 7 53 1
22 8 9 1
23 9 10 1
24 9 14 2
25 10 11 2
26 12 13 1
27 12 41 1
28 12 42 1
29 13 39 1
30 13 40 1
31 14 15 1
32 14 21 1
33 15 17 Ar
34 15 18 Ar
35 16 19 Ar
36 16 20 Ar
37 16 50 1
38 17 20 Ar
39 17 52 1
40 18 19 Ar
41 18 48 1
42 19 49 1
43 20 51 1
44 21 23 Ar
45 21 24 Ar
46 22 25 Ar
47 22 26 Ar

48 22 45 1
49 23 26 Ar
50 23 47 1
51 24 25 Ar
52 24 43 1
53 25 44 1
54 26 46 1
55 27 36 1
56 27 37 1
57 27 38 1
58 53 54 1
59 53 56 1
60 53 57 1
61 54 55 1

DAIN **2b”** (30 °):
$E(S_0)$ = -1192.41190845 A.U.
$E(S_1)$ = -1192.30765366 A.U.

@<TRIPOS>MOLECULE
Molecule Name
57 61
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 -5.2544 -0.7051 -1.0075 C
2 C2 -5.4590 1.8110 -0.9509 C
3 C3 -4.5678 1.8370 0.2992 C
4 C4 -4.3075 -0.7279 0.2223 C
5 C5 -6.2248 0.4846 -1.0403 C
6 N6 -1.0062 -0.9921 0.4293 N
7 C7 -1.1111 0.2377 -0.2077 C
8 N8 0.0386 0.8009 -0.4545 N
9 C9 1.0248 -0.0915 -0.0134 C
10 C10 0.3606 -1.2987 0.5681 C
11 O11 0.7892 -2.3020 1.1183 O
12 C12 -2.0528 -1.8916 0.9040 C
13 C13 -3.2967 -1.8912 0.0093 C
14 C14 2.3804 0.1446 -0.0756 C
15 C15 2.9223 1.5157 0.0111 C
16 C16 3.9764 4.1239 0.2083 C
17 C17 4.1298 1.8615 -0.6281 C
18 C18 2.2546 2.5125 0.7502 C
19 C19 2.7789 3.7976 0.8500 C
20 C20 4.6487 3.1504 -0.5332 C
21 C21 3.3246 -0.9912 -0.1816 C
22 C22 5.1189 -3.1441 -0.4475 C
23 C23 3.0673 -2.0371 -1.0854 C
24 C24 4.5065 -1.0437 0.5813 C
25 C25 5.3901 -2.1125 0.4545 C
26 C26 3.9554 -3.1006 -1.2188 C
27 C27 -5.1195 -1.0228 1.5032 C
28 H28 -6.8215 0.4458 -1.9603 H
29 H29 -6.9370 0.4162 -0.2069 H
30 H30 -6.1561 2.6581 -0.9290 H
31 H31 -4.8463 1.9393 -1.8552 H
32 H32 -5.8104 -1.6520 -1.0426 H
33 H33 -4.6485 -0.6800 -1.9249 H
34 H34 -4.0005 2.7755 0.3454 H
35 H35 -5.2104 1.8291 1.1892 H
36 H36 -5.8524 -0.2412 1.7229 H
37 H37 -5.6670 -1.9682 1.4044 H
38 H38 -4.4659 -1.1075 2.3794 H
39 H39 -3.8319 -2.8358 0.1719 H
40 H40 -2.9612 -1.9158 -1.0353 H
41 H41 -2.3113 -1.6418 1.9418 H
42 H42 -1.5917 -2.8830 0.9292 H
43 H43 4.7165 -0.2482 1.2897 H
44 H44 6.2897 -2.1429 1.0636 H
45 H45 5.8121 -3.9746 -0.5513 H
46 H46 3.7412 -3.8950 -1.9287 H
47 H47 2.1701 -1.9958 -1.6951 H
48 H48 1.3258 2.2650 1.2505 H
49 H49 2.2529 4.5473 1.4351 H
50 H50 4.3830 5.1287 0.2879 H
51 H51 5.5768 3.3959 -1.0428 H
52 H52 4.6526 1.1127 -1.2146 H
53 C53 -2.4182 0.8348 -0.6377 C
54 C54 -3.5791 0.6502 0.3743 C
55 H55 -3.1318 0.6774 1.3783 H
56 H56 -2.2150 1.8975 -0.8029 H
57 H57 -2.6940 0.4265 -1.6198 H
@<TRIPOS>BOND
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2 1 5 1
3 1 32 1
4 1 33 1
5 2 3 1
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8 2 31 1
9 3 34 1
10 3 35 1
11 3 54 1
12 4 13 1
13 4 27 1
14 4 54 1
15 5 28 1
16 5 29 1
17 6 7 1
18 6 10 1
19 6 12 1
20 7 8 2
21 7 53 1
22 8 9 1
23 9 10 1
24 9 14 2
25 10 11 2
26 12 13 1
27 12 41 1
28 12 42 1
29 13 39 1
30 13 40 1
31 14 15 1
32 14 21 1
33 15 17 Ar
34 15 18 Ar
35 16 19 Ar
36 16 20 Ar
37 16 50 1
38 17 20 Ar
39 17 52 1
40 18 19 Ar
41 18 48 1
42 19 49 1
43 20 51 1
44 21 23 Ar
45 21 24 Ar
46 22 25 Ar
47 22 26 Ar
48 22 45 1
49 23 26 Ar
50 23 47 1
51 24 25 Ar
52 24 43 1
53 25 44 1
54 26 46 1
55 27 36 1
56 27 37 1
57 27 38 1
58 53 54 1
59 53 56 1
60 53 57 1
61 54 55 1

DAIN **2b”** (45 °):
$E(S_0)$ = -1192.40127043 A.U.
$E(S_1)$ = -1192.31022986 A.U.

@<TRIPOS>MOLECULE
Molecule Name
57 61
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 -5.2418 -0.8826 -0.8464 C
2 C2 -5.4532 1.5862 -1.3370 C
3 C3 -4.5535 1.8813 -0.1291 C
4 C4 -4.2860 -0.6372 0.3528 C
5 C5 -6.2138 0.2697 -1.1332 C
6 N6 -0.9939 -0.8382 0.6135 N
7 C7 -1.0966 0.2120 -0.2858 C
8 N8 0.0593 0.7035 -0.6519 N
9 C9 1.0359 -0.0725 -0.0263 C
10 C10 0.3763 -1.1130 0.8101 C
11 O11 0.8088 -1.9619 1.5769 O
12 C12 -2.0340 -1.6294 1.2625 C
13 C13 -3.2810 -1.8218 0.3937 C
14 C14 2.4065 0.1377 -0.1192 C
15 C15 2.9769 1.4865 0.0126 C
16 C16 4.0592 4.0751 0.3075 C
17 C17 4.2018 1.8370 -0.5939 C
18 C18 2.3045 2.4734 0.7627 C
19 C19 2.8406 3.7486 0.9086 C
20 C20 4.7370 3.1134 -0.4453 C
21 C21 3.2892 -1.0313 -0.2778 C
22 C22 4.9225 -3.2992 -0.6312 C
23 C23 2.8865 -2.0909 -1.1142 C
24 C24 4.5352 -1.1353 0.3753 C
25 C25 5.3396 -2.2570 0.2019 C
26 C26 3.6940 -3.2115 -1.2887 C
27 C27 -5.0897 -0.6421 1.6724 C
28 H28 -6.8133 0.0312 -2.0211 H
29 H29 -6.9259 0.3840 -0.3045 H
30 H30 -6.1551 2.4159 -1.4883 H
31 H31 -4.8493 1.5227 -2.2538 H
32 H32 -5.7963 -1.8152 -0.6729 H
33 H33 -4.6397 -1.0547 -1.7504 H
34 H34 -3.9922 2.8114 -0.2854 H
35 H35 -5.1921 2.0575 0.7465 H
36 H36 -5.8226 0.1681 1.7236 H
37 H37 -5.6365 -1.5862 1.7851 H
38 H38 -4.4296 -0.5355 2.5414 H
39 H39 -3.8162 -2.7067 0.7615 H
40 H40 -2.9499 -2.0747 -0.6218 H
41 H41 -2.2898 -1.1786 2.2308 H
42 H42 -1.5663 -2.5926 1.4859 H
43 H43 4.8517 -0.3420 1.0454 H
44 H44 6.2887 -2.3263 0.7268 H
45 H45 5.5536 -4.1734 -0.7677 H
46 H46 3.3676 -4.0143 -1.9443 H
47 H47 1.9428 -2.0094 -1.6441 H
48 H48 1.3651 2.2209 1.2419 H
49 H49 2.3096 4.4897 1.5002 H
50 H50 4.4773 5.0712 0.4260 H
51 H51 5.6790 3.3616 -0.9272 H
52 H52 4.7213 1.1027 -1.2012 H
53 C53 -2.4023 0.7005 -0.8409 C
54 C54 -3.5578 0.7405 0.1924 C
55 H55 -3.1053 0.9890 1.1631 H
56 H56 -2.2005 1.7022 -1.2328 H
57 H57 -2.6816 0.0888 -1.7098 H
@<TRIPOS>BOND

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8 2 31 1
9 3 34 1
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11 3 54 1
12 4 13 1
13 4 27 1
14 4 54 1
15 5 28 1
16 5 29 1
17 6 7 1
18 6 10 1
19 6 12 1
20 7 8 2
21 7 53 1
22 8 9 1
23 9 10 1
24 9 14 Ar
25 10 11 2
26 12 13 1
27 12 41 1
28 12 42 1
29 13 39 1
30 13 40 1
31 14 15 1
32 14 21 1
33 15 17 Ar
34 15 18 Ar
35 16 19 Ar
36 16 20 Ar
37 16 50 1
38 17 20 Ar
39 17 52 1
40 18 19 Ar
41 18 48 1
42 19 49 1
43 20 51 1
44 21 23 Ar
45 21 24 Ar
46 22 25 Ar
47 22 26 Ar
48 22 45 1
49 23 26 Ar
50 23 47 1
51 24 25 Ar
52 24 43 1
53 25 44 1
54 26 46 1
55 27 36 1
56 27 37 1
57 27 38 1
58 53 54 1
59 53 56 1
60 53 57 1
61 54 55 1

DAIN **2b”** (60 °):
$E(S_0)$ = -1192.38606534 A.U.
$E(S_1)$ = -1192.31128005 A.U.

@<TRIPOS>MOLECULE
Molecule Name
57 61
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 -5.2024 -1.0637 -0.6268 C
2 C2 -5.4044 1.1621 -1.8067 C
3 C3 -4.5543 1.8056 -0.7032 C
4 C4 -4.2935 -0.4711 0.4852 C
5 C5 -6.1660 -0.0551 -1.2661 C
6 N6 -0.9991 -0.5660 0.8623 N
7 C7 -1.0913 0.1947 -0.2857 C
8 N8 0.0774 0.5469 -0.7734 N
9 C9 1.0360 -0.0605 0.0253 C
10 C10 0.3725 -0.8239 1.1084 C
11 O11 0.7986 -1.4443 2.0745 O
12 C12 -2.0564 -1.1234 1.6992 C
13 C13 -3.2802 -1.5781 0.8963 C
14 C14 2.4270 0.0908 -0.1315 C
15 C15 3.0457 1.4141 -0.0308 C
16 C16 4.2149 3.9696 0.2361 C
17 C17 2.4388 2.4141 0.7599 C
18 C18 4.2493 1.7393 -0.6962 C
19 C19 4.8274 2.9970 -0.5594 C
20 C20 3.0168 3.6724 0.8908 C
21 C21 3.2357 -1.1160 -0.3126 C
22 C22 4.7273 -3.4718 -0.7374 C
23 C23 2.6852 -2.2101 -1.0155 C
24 C24 4.5566 -1.2397 0.1770 C
25 C25 5.2906 -2.4001 -0.0355 C
26 C26 3.4222 -3.3731 -1.2225 C
27 C27 -5.1465 -0.1104 1.7218 C
28 H28 -6.7270 -0.5456 -2.0715 H
29 H29 -6.9116 0.2765 -0.5302 H
30 H30 -6.1030 1.9011 -2.2192 H
31 H31 -4.7595 0.8488 -2.6407 H
32 H32 -5.7604 -1.9135 -0.2104 H
33 H33 -4.5674 -1.4854 -1.4204 H
34 H34 -3.9865 2.6549 -1.1043 H
35 H35 -5.2231 2.2256 0.0603 H
36 H36 -5.8788 0.6725 1.5063 H
37 H37 -5.6979 -0.9877 2.0817 H
38 H38 -4.5208 0.2496 2.5474 H
39 H39 -3.8231 -2.3231 1.4924 H
40 H40 -2.9200 -2.1136 0.0086 H
41 H41 -2.3407 -0.3937 2.4693 H
42 H42 -1.5957 -1.9663 2.2220 H
43 H43 4.9872 -0.4281 0.7545 H
44 H44 6.2995 -2.4802 0.3605 H
45 H45 5.3052 -4.3768 -0.9051 H
46 H46 2.9822 -4.1984 -1.7758 H
47 H47 1.6856 -2.1149 -1.4267 H
48 H48 4.7130 1.0009 -1.3425 H
49 H49 5.7502 3.2258 -1.0860 H
50 H50 4.6684 4.9510 0.3453 H
51 H51 2.5380 4.4209 1.5167 H
52 H52 1.5232 2.1771 1.2913 H
53 C53 -2.3837 0.4974 -0.9826 C
54 C54 -3.5687 0.8175 -0.0361 C
55 H55 -3.1498 1.3381 0.8367 H
56 H56 -2.1744 1.3462 -1.6412 H
57 H57 -2.6414 -0.3406 -1.6459 H
@<TRIPOS>BOND
1 1 4 1
2 1 5 1
3 1 32 1
4 1 33 1
5 2 3 1
6 2 5 1
7 2 30 1
8 2 31 1
9 3 34 1
10 3 35 1
11 3 54 1
12 4 13 1
13 4 27 1
14 4 54 1
15 5 28 1
16 5 29 1
17 6 7 Ar
18 6 10 1
19 6 12 1
20 7 8 2
21 7 53 1
22 8 9 1
23 9 10 1
24 9 14 Ar
25 10 11 2
26 12 13 1
27 12 41 1
28 12 42 1
29 13 39 1
30 13 40 1
31 14 15 1
32 14 21 1
33 15 17 Ar
34 15 18 Ar
35 16 19 Ar
36 16 20 Ar
37 16 50 1
38 17 20 Ar
39 17 52 1
40 18 19 Ar
41 18 48 1
42 19 49 1
43 20 51 1
44 21 23 Ar
45 21 24 Ar
46 22 25 Ar
47 22 26 Ar
48 22 45 1
49 23 26 Ar
50 23 47 1
51 24 25 Ar
52 24 43 1
53 25 44 1
54 26 46 1
55 27 36 1
56 27 37 1
57 27 38 1
58 53 54 1
59 53 56 1
60 53 57 1
61 54 55 1

DAIN **2b”** (75 °):
$E(S_0)$ = -1192.36820362 A.U.
$E(S_1)$ = -1192.31394684 A.U.

@<TRIPOS>MOLECULE
Molecule Name
57 61
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 -5.2458 -1.1510 -0.2124 C
2 C2 -5.4138 0.5099 -2.1061 C
3 C3 -4.5245 1.4789 -1.3152 C
4 C4 -4.2934 -0.2353 0.6031 C
5 C5 -6.1978 -0.4051 -1.1579 C
6 N6 -0.9974 -0.2917 0.9706 N
7 C7 -1.0887 0.0566 -0.3546 C
8 N8 0.0926 0.2363 -0.9227 N
9 C9 1.0373 -0.0825 0.0285 C
10 C10 0.3785 -0.4558 1.2899 C
11 O11 0.8028 -0.7125 2.4137 O

12 C12 -2.0542 -0.5108 1.9513 C
13 C13 -3.3032 -1.1692 1.3576 C
14 C14 2.4526 0.0336 -0.1659 C
15 C15 3.0811 1.3475 -0.1482 C
16 C16 4.2713 3.9055 -0.0141 C
17 C17 2.4953 2.3882 0.6099 C
18 C18 4.2749 1.6376 -0.8527 C
19 C19 4.8628 2.8943 -0.7794 C
20 C20 3.0837 3.6471 0.6740 C
21 C21 3.2225 -1.1942 -0.2659 C
22 C22 4.6324 -3.6257 -0.5363 C
23 C23 2.5933 -2.3517 -0.7852 C
24 C24 4.5815 -1.3003 0.1258 C
25 C25 5.2741 -2.4942 -0.0157 C
26 C26 3.2904 -3.5497 -0.9128 C
27 C27 -5.1026 0.5622 1.6491 C
28 H28 -6.7907 -1.1313 -1.7286 H
29 H29 -6.9176 0.1936 -0.5822 H
30 H30 -6.0985 1.0756 -2.7503 H
31 H31 -4.7960 -0.1044 -2.7774 H
32 H32 -5.8168 -1.7799 0.4847 H
33 H33 -4.6433 -1.8465 -0.8153 H
34 H34 -3.9457 2.1132 -1.9987 H
35 H35 -5.1682 2.1634 -0.7458 H
36 H36 -5.8299 1.2348 1.1860 H
37 H37 -5.6539 -0.1155 2.3121 H
38 H38 -4.4446 1.1763 2.2754 H
39 H39 -3.8528 -1.6522 2.1762 H
40 H40 -2.9752 -1.9844 0.6998 H
41 H41 -2.3053 0.4408 2.4391 H
42 H42 -1.6069 -1.1457 2.7213 H
43 H43 5.0702 -0.4442 0.5789 H
44 H44 6.3118 -2.5563 0.3010 H
45 H45 5.1783 -4.5588 -0.6466 H
46 H46 2.7902 -4.4221 -1.3248 H
47 H47 1.5681 -2.2748 -1.1301 H
48 H48 4.7159 0.8730 -1.4846 H
49 H49 5.7756 3.0959 -1.3340 H
50 H50 4.7346 4.8869 0.0446 H
51 H51 2.6232 4.4250 1.2773 H
52 H52 1.5982 2.1770 1.1817 H
53 C53 -2.3749 0.1147 -1.1211 C
54 C54 -3.5491 0.7676 -0.3458 C
55 H55 -3.1089 1.5530 0.2851 H
56 H56 -2.1498 0.6813 -2.0303 H
57 H57 -2.6538 -0.8944 -1.4578 H
@<TRIPOS>BOND
1 1 4 1
2 1 5 1
3 1 32 1
4 1 33 1
5 2 3 1
6 2 5 1
7 2 30 1
8 2 31 1
9 3 34 1
10 3 35 1
11 3 54 1
12 4 13 1
13 4 27 1
14 4 54 1
15 5 28 1
16 5 29 1
17 6 7 Ar
18 6 10 1
19 6 12 1
20 7 8 Ar
21 7 53 1
22 8 9 Ar
23 9 10 1
24 9 14 Ar
25 10 11 2
26 12 13 1
27 12 41 1
28 12 42 1
29 13 39 1
30 13 40 1
31 14 15 1
32 14 21 1
33 15 17 Ar
34 15 18 Ar
35 16 19 Ar
36 16 20 Ar
37 16 50 1
38 17 20 Ar
39 17 52 1
40 18 19 Ar
41 18 48 1
42 19 49 1
43 20 51 1
44 21 23 Ar
45 21 24 Ar
46 22 25 Ar
47 22 26 Ar
48 22 45 1
49 23 26 Ar
50 23 47 1
51 24 25 Ar
52 24 43 1
53 25 44 1
54 26 46 1
55 27 36 1
56 27 37 1
57 27 38 1
58 53 54 1
59 53 56 1
60 53 57 1
61 54 55 1

DAIN **2b”** (90 °):
$E(S_0)$ = -1192.35093358 A.U.
$E(S_1)$ = -1192.32262986 A.U.

@<TRIPOS>MOLECULE
Molecule Name
57 61
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 -5.2594 -1.0943 -0.3174 C
2 C2 -5.3096 0.6412 -2.1559 C
3 C3 -4.3907 1.5313 -1.3077 C
4 C4 -4.2871 -0.2514 0.5509 C
5 C5 -6.1541 -0.2710 -1.2561 C
6 N6 -1.0240 -0.3947 1.0074 N
7 C7 -1.0689 -0.1457 -0.3346 C
8 N8 0.1453 0.0220 -0.8608 N
9 C9 1.0345 -0.0455 0.1772 C
10 C10 0.3367 -0.3074 1.4278 C
11 O11 0.7233 -0.5743 2.5694 O
12 C12 -2.1045 -0.6323 1.9597 C
13 C13 -3.3499 -1.2376 1.3041 C
14 C14 2.4834 0.0409 -0.0015 C
15 C15 3.1118 1.3364 0.0457 C
16 C16 4.2628 3.9173 0.0881 C
17 C17 2.3214 2.4978 -0.1627 C
18 C18 4.4986 1.5200 0.3042 C
19 C19 5.0614 2.7862 0.3117 C
20 C20 2.8937 3.7655 -0.1399 C
21 C21 3.1976 -1.1782 -0.3221 C
22 C22 4.5364 -3.6099 -0.8476 C
23 C23 4.3511 -1.2174 -1.1491 C
24 C24 2.7351 -2.4030 0.2235 C
25 C25 3.3990 -3.5979 -0.0389 C
26 C26 5.0080 -2.4122 -1.4028 C
27 C27 -5.0873 0.5502 1.6026 C
28 H28 -6.7668 -0.9493 -1.8632 H
29 H29 -6.8580 0.3410 -0.6748 H
30 H30 -5.9563 1.2652 -2.7858 H
31 H31 -4.7115 0.0258 -2.8434 H
32 H32 -5.8762 -1.7176 0.3444 H
33 H33 -4.6733 -1.7938 -0.9307 H
34 H34 -3.7700 2.1664 -1.9528 H
35 H35 -5.0142 2.2147 -0.7173 H
36 H36 -5.7761 1.2697 1.1510 H
37 H37 -5.6849 -0.1256 2.2265 H
38 H38 -4.4202 1.1132 2.2663 H
39 H39 -3.9375 -1.7317 2.0884 H
40 H40 -3.0193 -2.0369 0.6289 H
41 H41 -2.3427 0.3004 2.4879 H
42 H42 -1.6908 -1.3134 2.7096 H
43 H43 1.8944 -2.3887 0.9071 H
44 H44 3.0361 -4.5213 0.4046 H
45 H45 5.0554 -4.5436 -1.0471 H
46 H46 5.8787 -2.4216 -2.0534 H
47 H47 4.6898 -0.3037 -1.6263 H
48 H48 5.1122 0.6571 0.5402 H
49 H49 6.1216 2.9042 0.5197 H
50 H50 4.7091 4.9082 0.0963 H
51 H51 2.2718 4.6389 -0.3172 H
52 H52 1.2711 2.3736 -0.3980 H
53 C53 -2.3263 0.0354 -1.1274 C
54 C54 -3.4737 0.7345 -0.3529 C
55 H55 -2.9982 1.4714 0.3098 H
56 H56 -2.0425 0.6214 -2.0081 H
57 H57 -2.6579 -0.9386 -1.5182 H
@<TRIPOS>BOND
1 1 4 1
2 1 5 1
3 1 32 1
4 1 33 1
5 2 3 1
6 2 5 1
7 2 30 1
8 2 31 1
9 3 34 1
10 3 35 1
11 3 54 1
12 4 13 1
13 4 27 1
14 4 54 1
15 5 28 1
16 5 29 1
17 6 7 Ar
18 6 10 1
19 6 12 1
20 7 8 Ar
21 7 53 1
22 8 9 Ar
23 9 10 1
24 9 14 1
25 10 11 2
26 12 13 1
27 12 41 1
28 12 42 1
29 13 39 1
30 13 40 1
31 14 15 Ar
32 14 21 1
33 15 17 Ar
34 15 18 Ar
35 16 19 Ar
36 16 20 Ar
37 16 50 1
38 17 20 Ar
39 17 52 1

40 18 19 2
41 18 48 1
42 19 49 1
43 20 51 1
44 21 23 Ar
45 21 24 Ar
46 22 25 Ar
47 22 26 Ar
48 22 45 1
49 23 26 Ar
50 23 47 1
51 24 25 Ar
52 24 43 1
53 25 44 1
54 26 46 1
55 27 36 1
56 27 37 1
57 27 38 1
58 53 54 1
59 53 56 1
60 53 57 1
61 54 55 1

DAIN **2b”** (-15 °):
$E(S_0)$ = -1192.41700021 A.U.
$E(S_1)$ = -1192.30278801 A.U.

@<TRIPOS>MOLECULE
Molecule Name
57 61
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 -5.3555 0.1205 -1.0126 C
2 C2 -5.4224 1.9235 0.7665 C
3 C3 -4.4539 1.0926 1.6176 C
4 C4 -4.3312 -0.7271 -0.2100 C
5 C5 -6.2571 1.0168 -0.1485 C
6 N6 -1.0412 -1.0457 -0.4105 N
7 C7 -1.1334 0.3069 -0.1015 C
8 N8 0.0173 0.8871 0.0717 N
9 C9 1.0004 -0.1004 -0.0983 C
10 C10 0.3191 -1.4024 -0.4015 C
11 O11 0.7329 -2.5241 -0.6508 O
12 C12 -2.0938 -2.0307 -0.6535 C
13 C13 -3.3800 -1.4225 -1.2265 C
14 C14 2.3483 0.1343 -0.0109 C
15 C15 2.8943 1.5121 -0.0514 C
16 C16 3.9824 4.1130 -0.1247 C
17 C17 2.3034 2.5213 -0.8363 C
18 C18 4.0467 1.8382 0.6902 C
19 C19 4.5786 3.1253 0.6614 C
20 C20 2.8459 3.8028 -0.8754 C
21 C21 3.3246 -0.9801 0.1071 C
22 C22 5.2271 -3.0336 0.3897 C
23 C23 4.4694 -1.0178 -0.7083 C
24 C24 3.1574 -1.9866 1.0721 C
25 C25 4.1015 -2.9999 1.2157 C
26 C26 5.4059 -2.0410 -0.5759 C
27 C27 -5.0690 -1.8201 0.5924 C
28 H28 -6.9009 1.6199 -0.8013 H
29 H29 -6.9334 0.4031 0.4630 H
30 H30 -6.0770 2.5174 1.4166 H
31 H31 -4.8626 2.6451 0.1536 H
32 H32 -5.9673 -0.5510 -1.6305 H
33 H33 -4.8114 0.7648 -1.7190 H
34 H34 -3.8357 1.7474 2.2450 H
35 H35 -5.0376 0.4725 2.3117 H
36 H36 -5.7469 -1.3951 1.3364 H
37 H37 -5.6647 -2.4553 -0.0745 H
38 H38 -4.3630 -2.4671 1.1260 H
39 H39 -3.9399 -2.2276 -1.7193 H
40 H40 -3.0960 -0.7262 -2.0262 H
41 H41 -2.2974 -2.5866 0.2717 H
42 H42 -1.6640 -2.7508 -1.3563 H
43 H43 2.2873 -1.9587 1.7200 H
44 H44 3.9586 -3.7642 1.9749 H
45 H45 5.9626 -3.8259 0.5013 H
46 H46 6.2780 -2.0601 -1.2241 H
47 H47 4.6149 -0.2426 -1.4547 H
48 H48 4.5167 1.0761 1.3036 H
49 H49 5.4612 3.3561 1.2522 H
50 H50 4.4012 5.1155 -0.1545 H
51 H51 2.3797 4.5628 -1.4970 H
52 H52 1.4174 2.2903 -1.4145 H
53 C53 -2.4408 1.0219 0.0517 C
54 C54 -3.5284 0.1876 0.7739 C
55 H55 -3.0064 -0.4701 1.4829 H
56 H56 -2.2149 1.9364 0.6088 H
57 H57 -2.7933 1.3485 -0.9355 H
@<TRIPOS>BOND
1 1 4 1
2 1 5 1
3 1 32 1
4 1 33 1
5 2 3 1
6 2 5 1
7 2 30 1
8 2 31 1
9 3 34 1
10 3 35 1
11 3 54 1
12 4 13 1
13 4 27 1
14 4 54 1
15 5 28 1
16 5 29 1
17 6 7 1
18 6 10 1
19 6 12 1
20 7 8 2
21 7 53 1
22 8 9 1
23 9 10 1
24 9 14 2
25 10 11 2
26 12 13 1
27 12 41 1
28 12 42 1
29 13 39 1
30 13 40 1
31 14 15 1
32 14 21 1
33 15 17 Ar
34 15 18 Ar
35 16 19 Ar
36 16 20 Ar
37 16 50 1
38 17 20 Ar
39 17 52 1
40 18 19 Ar
41 18 48 1
42 19 49 1
43 20 51 1
44 21 23 Ar
45 21 24 Ar
46 22 25 Ar
47 22 26 Ar
48 22 45 1
49 23 26 Ar
50 23 47 1
51 24 25 Ar
52 24 43 1
53 25 44 1
54 26 46 1
55 27 36 1
56 27 37 1
57 27 38 1
58 53 54 1
59 53 56 1
60 53 57 1
61 54 55 1

DAIN **2b”** (-30 °):
$E(S_0)$ = -1192.41183076 A.U.
$E(S_1)$ = -1192.30673680 A.U.

@<TRIPOS>MOLECULE
Molecule Name
57 61
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 -5.3240 0.3387 -0.9765 C
2 C2 -5.4606 1.7648 1.0974 C
3 C3 -4.5029 0.7970 1.8060 C
4 C4 -4.3042 -0.6366 -0.3279 C
5 C5 -6.2649 1.0306 0.0186 C
6 N6 -1.0175 -0.8849 -0.5672 N
7 C7 -1.1143 0.3637 0.0319 C
8 N8 0.0406 0.8957 0.3250 N
9 C9 1.0185 -0.0331 -0.0547 C
10 C10 0.3440 -1.2338 -0.6358 C
11 O11 0.7638 -2.2610 -1.1475 O
12 C12 -2.0576 -1.8061 -1.0123 C
13 C13 -3.3406 -1.1009 -1.4557 C
14 C14 2.3787 0.1558 0.0516 C
15 C15 2.9830 1.4986 -0.0456 C
16 C16 4.1643 4.0504 -0.2635 C
17 C17 2.3719 2.5172 -0.8042 C
18 C18 4.1985 1.7949 0.6042 C
19 C19 4.7803 3.0556 0.4983 C
20 C20 2.9588 3.7740 -0.9138 C
21 C21 3.2674 -1.0184 0.2164 C
22 C22 4.9385 -3.2533 0.5829 C
23 C23 4.4546 -1.1601 -0.5265 C
24 C24 2.9434 -2.0152 1.1534 C
25 C25 3.7710 -3.1194 1.3370 C
26 C26 5.2766 -2.2705 -0.3504 C
27 C27 -5.0449 -1.8789 0.2176 C
28 H28 -6.9188 1.7297 -0.5179 H
29 H29 -6.9250 0.2927 0.4935 H
30 H30 -6.1315 2.2281 1.8316 H
31 H31 -4.8938 2.5856 0.6344 H
32 H32 -5.9036 -0.2075 -1.7335 H
33 H33 -4.7737 1.1168 -1.5264 H
34 H34 -3.9165 1.3262 2.5683 H
35 H35 -5.0953 0.0485 2.3475 H
36 H36 -5.7643 -1.6357 1.0064 H
37 H37 -5.5989 -2.3784 -0.5864 H
38 H38 -4.3437 -2.6090 0.6398 H
39 H39 -3.8918 -1.7898 -2.1088 H
40 H40 -3.0653 -0.2482 -2.0892 H
41 H41 -2.2646 -2.5407 -0.2228 H
42 H42 -1.6158 -2.3637 -1.8434 H
43 H43 2.0412 -1.9058 1.7475 H
44 H44 3.5053 -3.8757 2.0708 H
45 H45 5.5834 -4.1167 0.7236 H
46 H46 6.1802 -2.3720 -0.9458 H
47 H47 4.7169 -0.4024 -1.2587 H
48 H48 4.6782 1.0303 1.2066 H
49 H49 5.7138 3.2626 1.0150 H

50 H50 4.6203 5.0330 -0.3515 H
51 H51 2.4756 4.5409 -1.5136 H
52 H52 1.4371 2.3086 -1.3108 H
53 C53 -2.4223 1.0303 0.3447 C
54 C54 -3.5353 0.0703 0.8402 C
55 H55 -3.0358 -0.7133 1.4280 H
56 H56 -2.1914 1.7810 1.1073 H
57 H57 -2.7611 1.5930 -0.5364 H
@<TRIPOS>BOND
1 1 4 1
2 1 5 1
3 1 32 1
4 1 33 1
5 2 3 1
6 2 5 1
7 2 30 1
8 2 31 1
9 3 34 1
10 3 35 1
11 3 54 1
12 4 13 1
13 4 27 1
14 4 54 1
15 5 28 1
16 5 29 1
17 6 7 1
18 6 10 1
19 6 12 1
20 7 8 2
21 7 53 1
22 8 9 1
23 9 10 1
24 9 14 2
25 10 11 2
26 12 13 1
27 12 41 1
28 12 42 1
29 13 39 1
30 13 40 1
31 14 15 1
32 14 21 1
33 15 17 Ar
34 15 18 Ar
35 16 19 Ar
36 16 20 Ar
37 16 50 1
38 17 20 Ar
39 17 52 1
40 18 19 Ar
41 18 48 1
42 19 49 1
43 20 51 1
44 21 23 Ar
45 21 24 Ar
46 22 25 Ar
47 22 26 Ar
48 22 45 1
49 23 26 Ar
50 23 47 1
51 24 25 Ar
52 24 43 1
53 25 44 1
54 26 46 1
55 27 36 1
56 27 37 1
57 27 38 1
58 53 54 1
59 53 56 1
60 53 57 1
61 54 55 1

DAIN **2b”** (-45 °):

$E(S_0)$ = -1192.40125484 A.U.
$E(S_1)$ = -1192.30970097 A.U.

@<TRIPOS>MOLECULE
Molecule Name
57 61
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 -5.2718 0.6207 -0.8596 C
2 C2 -5.4186 1.4783 1.5124 C
3 C3 -4.5013 0.3336 1.9645 C
4 C4 -4.2954 -0.5196 -0.4624 C
5 C5 -6.2138 1.0765 0.2636 C
6 N6 -1.0019 -0.7566 -0.7287 N
7 C7 -1.0995 0.3039 0.1579 C
8 N8 0.0592 0.7545 0.5656 N
9 C9 1.0307 -0.0498 -0.0302 C
10 C10 0.3647 -1.0781 -0.8780 C
11 O11 0.7926 -1.9431 -1.6289 O
12 C12 -2.0525 -1.5422 -1.3680 C
13 C13 -3.3153 -0.7236 -1.6527 C
14 C14 2.4024 0.1323 0.0982 C
15 C15 2.9991 1.4709 -0.0290 C
16 C16 4.1297 4.0408 -0.3075 C
17 C17 2.3714 2.4591 -0.8151 C
18 C18 4.2046 1.8103 0.6210 C
19 C19 4.7632 3.0776 0.4813 C
20 C20 2.9315 3.7249 -0.9534 C
21 C21 3.2625 -1.0487 0.2849 C
22 C22 4.8616 -3.3306 0.6990 C
23 C23 4.5296 -1.1656 -0.3241 C
24 C24 2.8202 -2.1037 1.1071 C
25 C25 3.6111 -3.2309 1.3119 C
26 C26 5.3173 -2.2940 -0.1208 C
27 C27 -5.0814 -1.8321 -0.2474 C
28 H28 -6.8238 1.9174 -0.0899 H
29 H29 -6.9183 0.2730 0.5198 H
30 H30 -6.0971 1.7567 2.3287 H
31 H31 -4.8191 2.3735 1.2913 H
32 H32 -5.8513 0.3015 -1.7367 H
33 H33 -4.6864 1.4912 -1.1908 H
34 H34 -3.9128 0.6374 2.8397 H
35 H35 -5.1235 -0.5077 2.2980 H
36 H36 -5.7887 -1.7587 0.5828 H
37 H37 -5.6536 -2.0941 -1.1458 H
38 H38 -4.4085 -2.6693 -0.0262 H
39 H39 -3.8681 -1.2198 -2.4607 H
40 H40 -3.0020 0.2461 -2.0600 H
41 H41 -2.2834 -2.4243 -0.7556 H
42 H42 -1.6128 -1.9148 -2.2980 H
43 H43 1.8589 -2.0126 1.6028 H
44 H44 3.2548 -4.0298 1.9567 H
45 H45 5.4800 -4.2098 0.8599 H
46 H46 6.2842 -2.3725 -0.6108 H
47 H47 4.8779 -0.3758 -0.9823 H
48 H48 4.6901 1.0749 1.2544 H
49 H49 5.6889 3.3181 0.9977 H
50 H50 4.5664 5.0298 -0.4186 H
51 H51 2.4351 4.4669 -1.5732 H
52 H52 1.4475 2.2147 -1.3277 H
53 C53 -2.4020 0.8808 0.6259 C
54 C54 -3.5353 -0.1496 0.8575 C
55 H55 -3.0610 -1.0671 1.2343 H
56 H56 -2.1690 1.4171 1.5513 H
57 H57 -2.7253 1.6506 -0.0894 H
@<TRIPOS>BOND
1 1 4 1
2 1 5 1
3 1 32 1
4 1 33 1
5 2 3 1
6 2 5 1
7 2 30 1
8 2 31 1
9 3 34 1
10 3 35 1
11 3 54 1
12 4 13 1
13 4 27 1
14 4 54 1
15 5 28 1
16 5 29 1
17 6 7 1
18 6 10 1
19 6 12 1
20 7 8 2
21 7 53 1
22 8 9 1
23 9 10 1
24 9 14 Ar
25 10 11 2
26 12 13 1
27 12 41 1
28 12 42 1
29 13 39 1
30 13 40 1
31 14 15 1
32 14 21 1
33 15 17 Ar
34 15 18 Ar
35 16 19 Ar
36 16 20 Ar
37 16 50 1
38 17 20 Ar
39 17 52 1
40 18 19 Ar
41 18 48 1
42 19 49 1
43 20 51 1
44 21 23 Ar
45 21 24 Ar
46 22 25 Ar
47 22 26 Ar
48 22 45 1
49 23 26 Ar
50 23 47 1
51 24 25 Ar
52 24 43 1
53 25 44 1
54 26 46 1
55 27 36 1
56 27 37 1
57 27 38 1
58 53 54 1
59 53 56 1
60 53 57 1
61 54 55 1

DAIN **2b”** (-60 °):
$E(S_0)$ = -1192.38611605 A.U.
$E(S_1)$ = -1192.31095073 A.U.

@<TRIPOS>MOLECULE
Molecule Name
57 61
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 5.2827 0.8999 0.5909 C
2 C2 5.4148 0.9512 -1.9328 C

3 C3 4.4729 -0.2594 -1.9868 C
4 C4 4.2884 -0.2930 0.5847 C
5 C5 6.2172 0.9543 -0.6251 C
6 N6 1.0039 -0.4165 0.9245 N
7 C7 1.0941 0.3217 -0.2381 C
8 N8 -0.0762 0.6077 -0.7660 N
9 C9 -1.0302 -0.0092 0.0305 C
10 C10 -0.3617 -0.7174 1.1477 C
11 O11 -0.7836 -1.3192 2.1275 O
12 C12 2.0508 -0.9521 1.7895 C
13 C13 3.3228 -0.1003 1.7882 C
14 C14 -2.4236 0.0932 -0.1441 C
15 C15 -3.0890 1.3955 -0.0797 C
16 C16 -4.3534 3.9114 0.1207 C
17 C17 -2.5215 2.4376 0.6856 C
18 C18 -4.3018 1.6588 -0.7557 C
19 C19 -4.9272 2.8968 -0.6508 C
20 C20 -3.1462 3.6764 0.7840 C
21 C21 -3.1883 -1.1465 -0.2918 C
22 C22 -4.5894 -3.5706 -0.6348 C
23 C23 -4.5022 -1.3053 0.2062 C
24 C24 -2.5984 -2.2399 -0.9628 C
25 C25 -3.2907 -3.4367 -1.1286 C
26 C26 -5.1919 -2.4991 0.0340 C
27 C27 5.0581 -1.6168 0.7880 C
28 H28 6.8472 1.8507 -0.5626 H
29 H29 6.9030 0.0960 -0.6163 H
30 H30 6.0910 0.9360 -2.7971 H
31 H31 4.8377 1.8841 -2.0114 H
32 H32 5.8668 0.8700 1.5210 H
33 H33 4.7109 1.8386 0.6265 H
34 H34 3.8819 -0.2441 -2.9114 H
35 H35 5.0798 -1.1735 -2.0325 H
36 H36 5.7656 -1.8195 -0.0210 H
37 H37 5.6292 -1.5897 1.7240 H
38 H38 4.3746 -2.4724 0.8415 H
39 H39 3.8803 -0.3236 2.7072 H
40 H40 3.0259 0.9534 1.8704 H
41 H41 2.2684 -1.9912 1.5080 H
42 H42 1.6110 -0.9901 2.7906 H
43 H43 -1.6047 -2.1194 -1.3817 H
44 H44 -2.8201 -4.2623 -1.6558 H
45 H45 -5.1314 -4.5027 -0.7701 H
46 H46 -6.1955 -2.6051 0.4374 H
47 H47 -4.9608 -0.4935 0.7614 H
48 H48 -4.7358 0.8883 -1.3850 H
49 H49 -5.8571 3.0777 -1.1836 H
50 H50 -4.8441 4.8775 0.2045 H
51 H51 -2.6969 4.4582 1.3907 H
52 H52 -1.5996 2.2482 1.2254 H
53 C53 2.3916 0.7187 -0.8763 C
54 C54 3.5132 -0.3453 -0.7766 C
55 H55 3.0226 -1.3270 -0.8375 H
56 H56 2.1530 0.9340 -1.9228 H
57 H57 2.7253 1.6732 -0.4452 H
@<TRIPOS>BOND
1 1 4 1
2 1 5 1
3 1 32 1
4 1 33 1
5 2 3 1
6 2 5 1
7 2 30 1
8 2 31 1
9 3 34 1
10 3 35 1
11 3 54 1
12 4 13 1
13 4 27 1
14 4 54 1
15 5 28 1
16 5 29 1
17 6 7 Ar
18 6 10 1
19 6 12 1
20 7 8 2
21 7 53 1
22 8 9 1
23 9 10 1
24 9 14 Ar
25 10 11 2
26 12 13 1
27 12 41 1
28 12 42 1
29 13 39 1
30 13 40 1
31 14 15 1
32 14 21 1
33 15 17 Ar
34 15 18 Ar
35 16 19 Ar
36 16 20 Ar
37 16 50 1
38 17 20 Ar
39 17 52 1
40 18 19 Ar
41 18 48 1
42 19 49 1
43 20 51 1
44 21 23 Ar
45 21 24 Ar
46 22 25 Ar
47 22 26 Ar
48 22 45 1
49 23 26 Ar
50 23 47 1
51 24 25 Ar
52 24 43 1
53 25 44 1
54 26 46 1
55 27 36 1
56 27 37 1
57 27 38 1
58 53 54 1
59 53 56 1
60 53 57 1
61 54 55 1

DAIN **2b”** (-75 °):
$E(S_0)$ = -1192.36857075 A.U.
$E(S_1)$ = -1192.31430689 A.U.

@<TRIPOS>MOLECULE
Molecule Name
57 61
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 5.2605 1.1048 0.2065 C
2 C2 5.3898 0.2373 -2.1634 C
3 C3 4.4724 -0.9274 -1.7658 C
4 C4 4.2814 -0.0213 0.6402 C
5 C5 6.1932 0.7306 -0.9534 C
6 N6 1.0026 -0.0525 1.0106 N
7 C7 1.0901 0.2301 -0.3300 C
8 N8 -0.0934 0.3110 -0.9181 N
9 C9 -1.0323 0.0032 0.0419 C
10 C10 -0.3677 -0.2626 1.3275 C
11 O11 -0.7874 -0.4664 2.4638 O
12 C12 2.0527 -0.2293 2.0086 C
13 C13 3.3112 0.5837 1.6938 C
14 C14 -2.4505 0.0317 -0.1631 C
15 C15 -3.1530 1.3044 -0.2289 C
16 C16 -4.4797 3.7989 -0.2788 C
17 C17 -2.6125 2.4349 0.4283 C
18 C18 -4.3743 1.4717 -0.9272 C
19 C19 -5.0294 2.6967 -0.9429 C
20 C20 -3.2666 3.6619 0.4001 C
21 C21 -3.1447 -1.2454 -0.1938 C
22 C22 -4.3921 -3.7754 -0.3083 C
23 C23 -4.4890 -1.4178 0.2233 C
24 C24 -2.4465 -2.3859 -0.6592 C
25 C25 -3.0639 -3.6326 -0.7116 C
26 C26 -5.1013 -2.6612 0.1601 C
27 C27 5.0717 -1.1664 1.3126 C
28 H28 6.8008 1.6024 -1.2272 H
29 H29 6.9009 -0.0496 -0.6409 H
30 H30 6.0638 -0.0766 -2.9706 H
31 H31 4.7912 1.0669 -2.5663 H
32 H32 5.8482 1.4186 1.0804 H
33 H33 4.6786 1.9879 -0.0946 H
34 H34 3.8806 -1.2613 -2.6282 H
35 H35 5.0955 -1.7843 -1.4778 H
36 H36 5.7761 -1.6466 0.6277 H
37 H37 5.6492 -0.7870 2.1646 H
38 H38 4.3990 -1.9475 1.6863 H
39 H39 3.8703 0.7181 2.6287 H
40 H40 2.9962 1.5895 1.3878 H
41 H41 2.2861 -1.2967 2.1187 H
42 H42 1.6109 0.0896 2.9574 H
43 H43 -1.4318 -2.2612 -1.0212 H
44 H44 -2.5115 -4.4918 -1.0828 H
45 H45 -4.8764 -4.7471 -0.3569 H
46 H46 -6.1284 -2.7747 0.4968 H
47 H47 -5.0287 -0.5715 0.6353 H
48 H48 -4.7835 0.6361 -1.4860 H
49 H49 -5.9626 2.8016 -1.4902 H
50 H50 -4.9948 4.7557 -0.2906 H
51 H51 -2.8369 4.5114 0.9243 H
52 H52 -1.6936 2.3208 0.9931 H
53 C53 2.3791 0.3607 -1.0846 C
54 C54 3.5120 -0.5802 -0.6043 C
55 H55 3.0333 -1.5224 -0.3020 H
56 H56 2.1295 0.1607 -2.1320 H
57 H57 2.7094 1.4093 -1.0579 H
@<TRIPOS>BOND
1 1 4 1
2 1 5 1
3 1 32 1
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5 2 3 1
6 2 5 1
7 2 30 1
8 2 31 1
9 3 34 1
10 3 35 1
11 3 54 1
12 4 13 1
13 4 27 1
14 4 54 1
15 5 28 1
16 5 29 1
17 6 7 Ar
18 6 10 1
19 6 12 1
20 7 8 Ar
21 7 53 1
22 8 9 Ar
23 9 10 1
24 9 14 Ar
25 10 11 2
26 12 13 1
27 12 41 1
28 12 42 1
29 13 39 1
30 13 40 1

31 14 15 1
32 14 21 1
33 15 17 Ar
34 15 18 Ar
35 16 19 Ar
36 16 20 Ar
37 16 50 1
38 17 20 Ar
39 17 52 1
40 18 19 Ar
41 18 48 1
42 19 49 1
43 20 51 1
44 21 23 Ar
45 21 24 Ar
46 22 25 Ar
47 22 26 Ar
48 22 45 1
49 23 26 Ar
50 23 47 1
51 24 25 Ar
52 24 43 1
53 25 44 1
54 26 46 1
55 27 36 1
56 27 37 1
57 27 38 1
58 53 54 1
59 53 56 1
60 53 57 1
61 54 55 1

DAIN **2b''** (-90 °):
$E(S_0)$ = -1192.34316399 A.U.
$E(S_1)$ = -1192.32939072 A.U.

@<TRIPOS>MOLECULE
Molecule Name
57 61
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 -5.2862 -1.0886 -0.0889 C
2 C2 -5.4174 0.4724 -2.0690 C
3 C3 -4.4422 1.4221 -1.3597 C
4 C4 -4.2587 -0.1878 0.6496 C
5 C5 -6.2227 -0.3360 -1.0445 C
6 N6 -0.9763 -0.3377 0.9588 N
7 C7 -1.0875 -0.1784 -0.3880 C
8 N8 0.1042 -0.0046 -0.9765 N
9 C9 1.0332 0.0130 0.0184 C
10 C10 0.4015 -0.1826 1.3177 C
11 O11 0.8287 -0.3290 2.4637 O
12 C12 -2.0092 -0.4968 1.9792 C
13 C13 -3.2953 -1.1252 1.4324 C
14 C14 2.4744 0.0699 -0.2165 C
15 C15 3.1780 -1.2089 -0.3451 C
16 C16 4.4312 -3.7404 -0.4425 C
17 C17 4.3738 -1.4571 0.3647 C
18 C18 2.6177 -2.2743 -1.0906 C
19 C19 3.2438 -3.5110 -1.1499 C
20 C20 4.9805 -2.7117 0.3213 C
21 C21 3.1346 1.3430 -0.1497 C
22 C22 4.3436 3.9081 -0.1221 C
23 C23 4.5083 1.5211 -0.4892 C
24 C24 2.3858 2.5175 0.1507 C
25 C25 2.9889 3.7654 0.1967 C
26 C26 5.0895 2.7791 -0.4847 C
27 C27 -4.9921 0.7129 1.6685 C
28 H28 -6.8793 -1.0539 -1.5519 H
29 H29 -6.8834 0.3391 -0.4825 H
30 H30 -6.0884 1.0453 -2.7215 H
31 H31 -4.8647 -0.2164 -2.7243 H
32 H32 -5.8692 -1.6463 0.6565 H
33 H33 -4.7416 -1.8457 -0.6720 H
34 H34 -3.8467 1.9792 -2.0944 H
35 H35 -5.0224 2.1739 -0.8091 H
36 H36 -5.6829 1.4129 1.1902 H
37 H37 -5.5766 0.1048 2.3696 H
38 H38 -4.2827 1.3075 2.2561 H
39 H39 -3.8495 -1.5450 2.2819 H
40 H40 -3.0128 -1.9831 0.8091 H
41 H41 -2.2067 0.4729 2.4548 H
42 H42 -1.5661 -1.1329 2.7512 H
43 H43 1.3211 2.4255 0.3308 H
44 H44 2.3946 4.6398 0.4478 H
45 H45 4.8056 4.8914 -0.1219 H
46 H46 6.1333 2.8870 -0.7673 H
47 H47 5.0984 0.6644 -0.7913 H
48 H48 1.6912 -2.1013 -1.6301 H
49 H49 2.8046 -4.3065 -1.7464 H
50 H50 4.9121 -4.7140 -0.4788 H
51 H51 5.8861 -2.8832 0.8975 H
52 H52 4.7895 -0.6836 1.0005 H
53 C53 -2.3784 -0.0723 -1.1366 C
54 C54 -3.4861 0.7054 -0.3784 C
55 H55 -2.9768 1.4951 0.1916 H
56 H56 -2.1348 0.4251 -2.0813 H
57 H57 -2.7304 -1.0775 -1.4134 H
@<TRIPOS>BOND
1 1 4 1
2 1 5 1
3 1 32 1
4 1 33 1
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10 3 35 1
11 3 54 1
12 4 13 1
13 4 27 1
14 4 54 1
15 5 28 1
16 5 29 1
17 6 7 Ar
18 6 10 1
19 6 12 1
20 7 8 Ar
21 7 53 1
22 8 9 Ar
23 9 10 1
24 9 14 1
25 10 11 2
26 12 13 1
27 12 41 1
28 12 42 1
29 13 39 1
30 13 40 1
31 14 15 1
32 14 21 Ar
33 15 17 Ar
34 15 18 Ar
35 16 19 Ar
36 16 20 Ar
37 16 50 1
38 17 20 Ar
39 17 52 1
40 18 19 Ar
41 18 48 1
42 19 49 1
43 20 51 1
44 21 23 Ar
45 21 24 Ar
46 22 25 Ar
47 22 26 Ar
48 22 45 1
49 23 26 2
50 23 47 1
51 24 25 Ar
52 24 43 1
53 25 44 1
54 26 46 1
55 27 36 1
56 27 37 1
57 27 38 1
58 53 54 1
59 53 56 1
60 53 57 1
61 54 55 1