

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 CH₂Cl₂ and was washed with a saturated solution of NH₄Cl, water, and brine; dried over MgSO₄; 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 CH₂Cl₂ (120 mL) and stirred overnight.¹⁾ After filtration of the mixture, the filtrate was washed with water and then brine, dried over MgSO₄, and concentrated under reduced pressure. The residue was recrystallized from ether and hexane to yield **8** (4.16 g, 80%). ¹H-NMR (CDCl₃) 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). ¹³C-NMR (CDCl₃) 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 C₂₅H₂₂NO₂ 368.1651; Found 368.1648. Di(naphthalen-2-yl)methanimine: ¹H-NMR (CDCl₃) δ: 9.95 (1H, br s), 8.04 (2H, br s), 7.94-7.84 (8H, m), 7.59-7.51 (4H, m). ¹³C-NMR (CDCl₃) 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 C₂₁H₁₆N 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 CH₂Cl₂ (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),

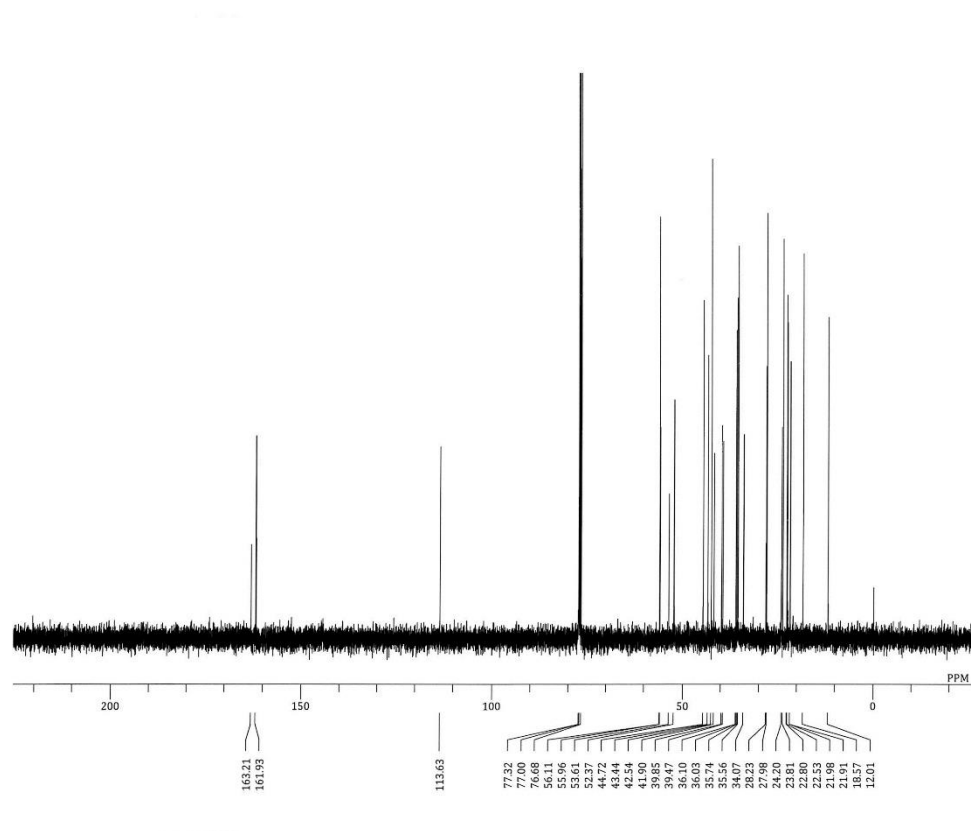
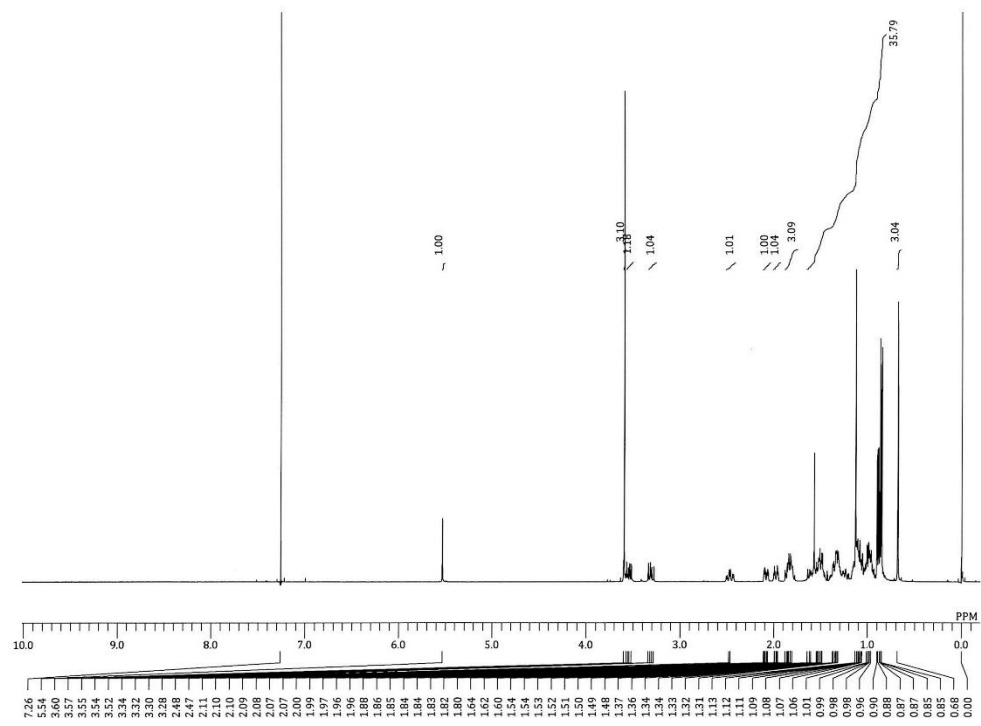
and acetic acid (27 μ L, 0.48 mmol) in toluene (1.2 mL) was stirred at room temperature for 2.5 days. The mixture was diluted with ethyl acetate and was washed with 5% aqueous HCl. The acidic aqueous layer was re-extracted with ethyl acetate after neutralization with a saturated solution of NaHCO₃. The combined organic layers were washed with a saturated solution of NaHCO₃ and brine, dried over Na₂SO₄, 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. ¹H-NMR (CDCl₃) 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). ¹³C-NMR (CDCl₃) 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 C₂₁H₁₉N₂O 315.1498; Found 315.1495.

2. References

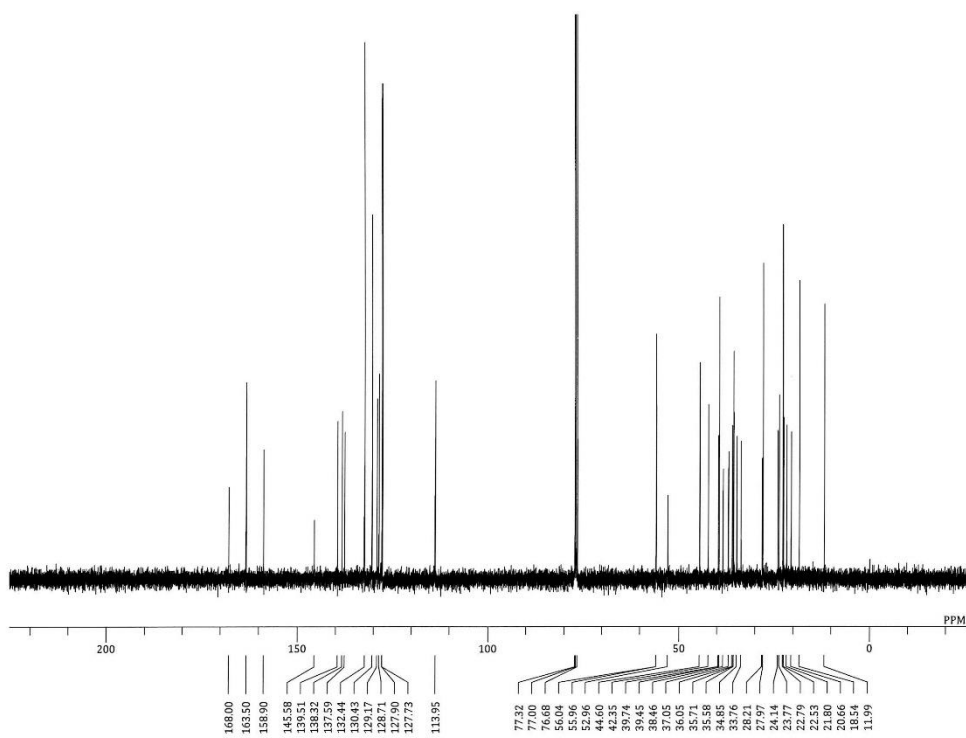
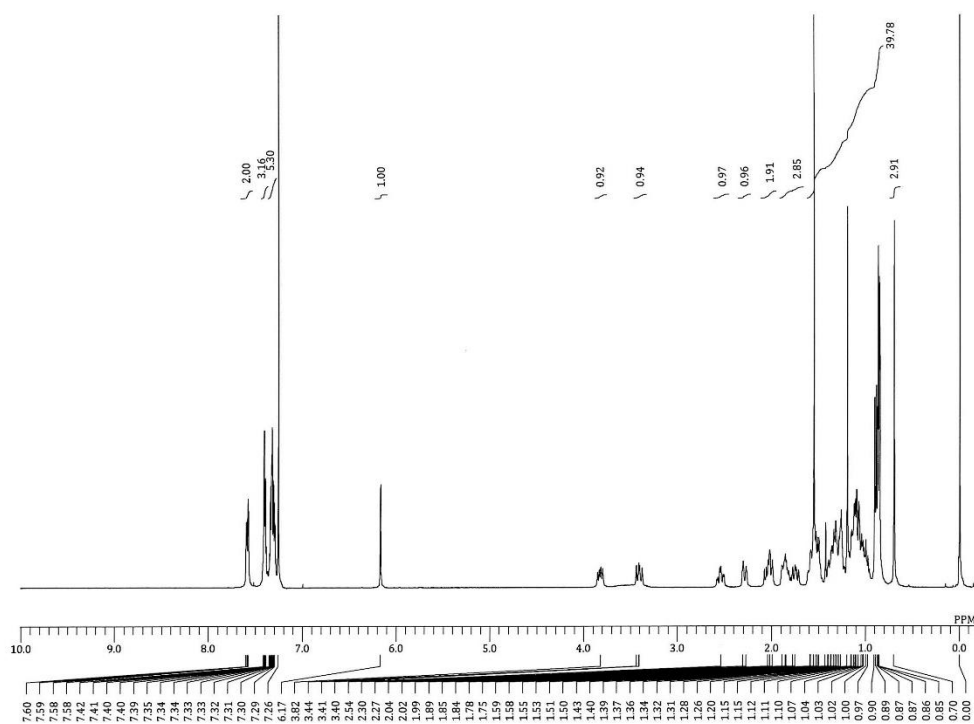
- 1) M. J. O'Donnell and R. L. Polt, *J. Org. Chem.* 1982, **47**, 2663–2666.
- 2) S. Álvarez, G. Domínguez, A. Gradillas and J. Pérez-Castells, *Eur. J. Org. Chem.* 2013, 3094–3102.

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

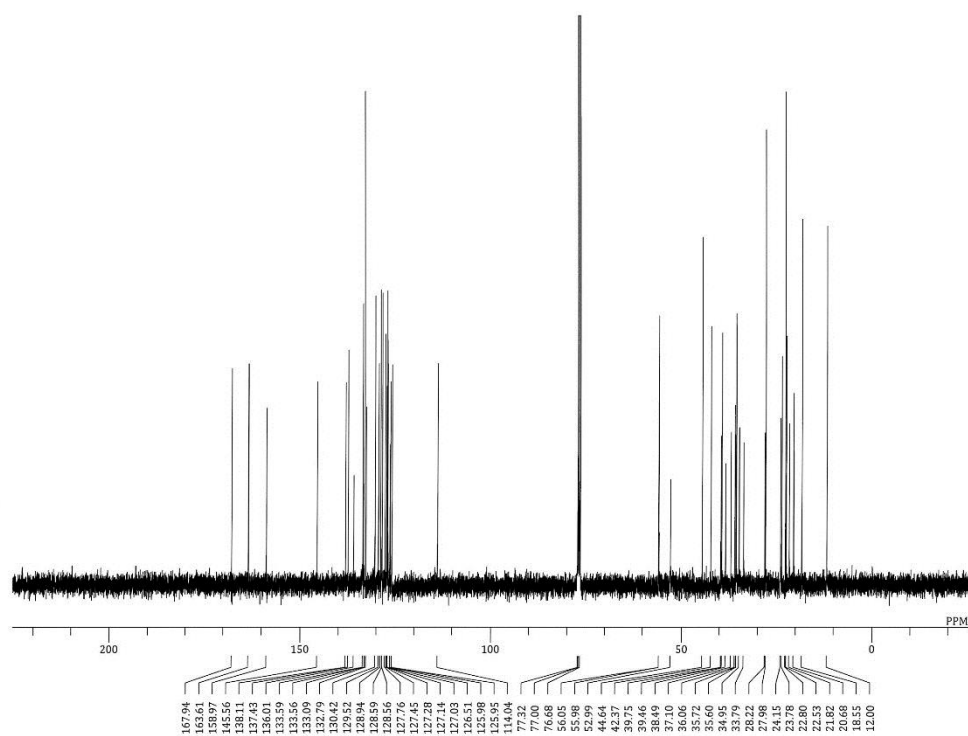
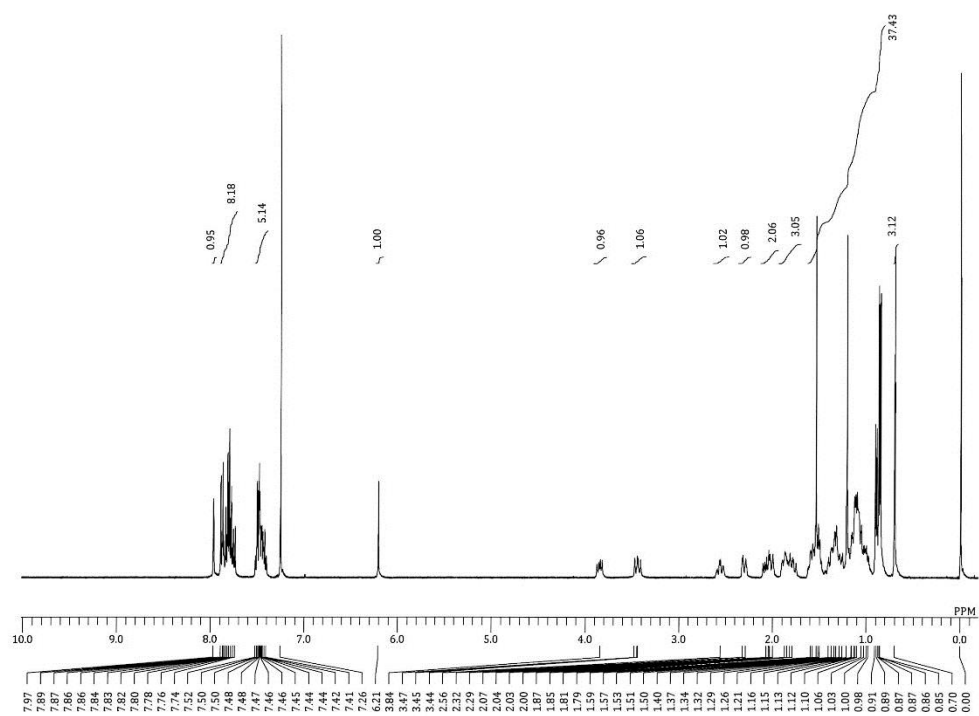
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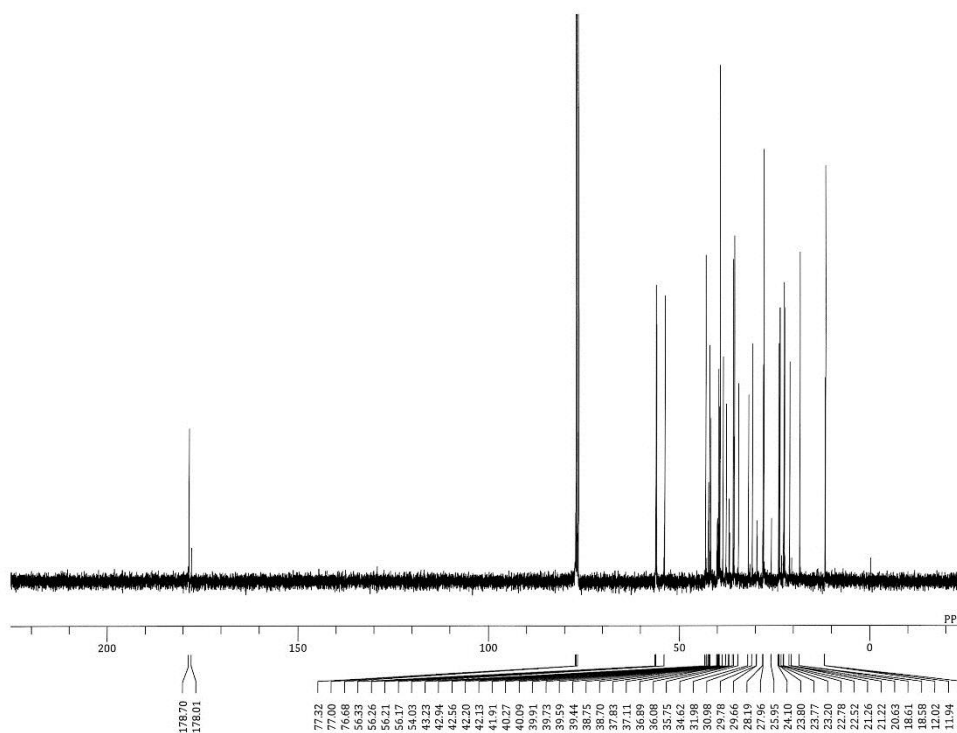
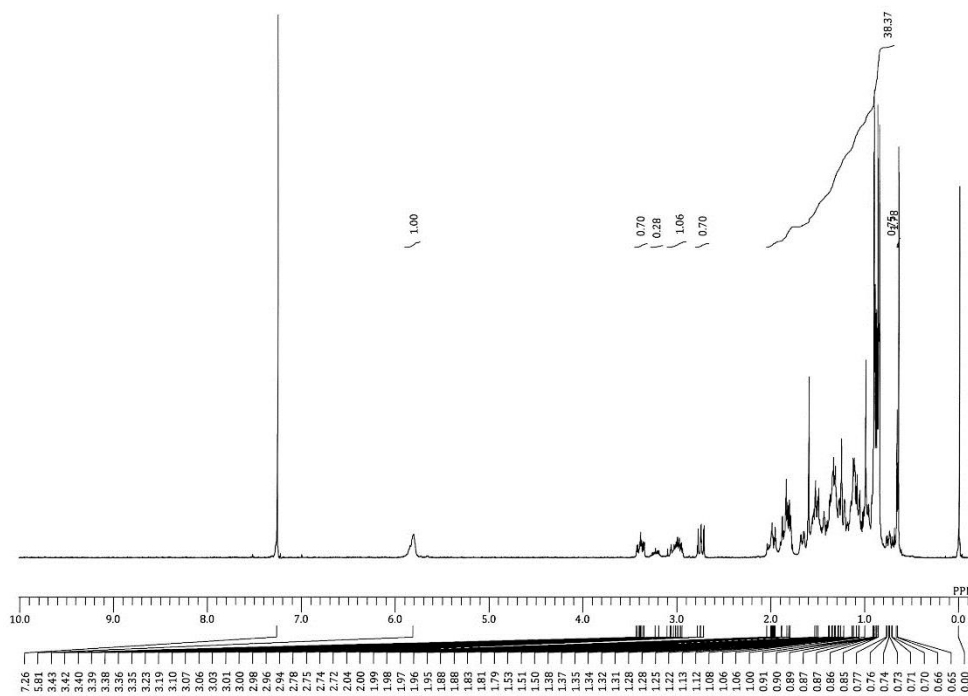
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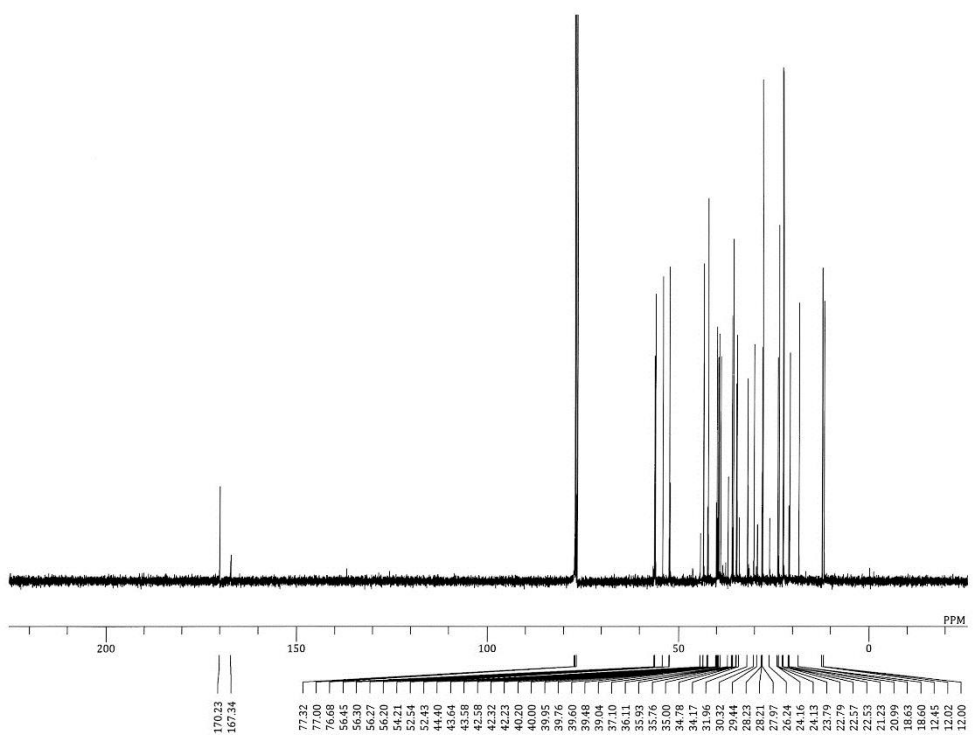
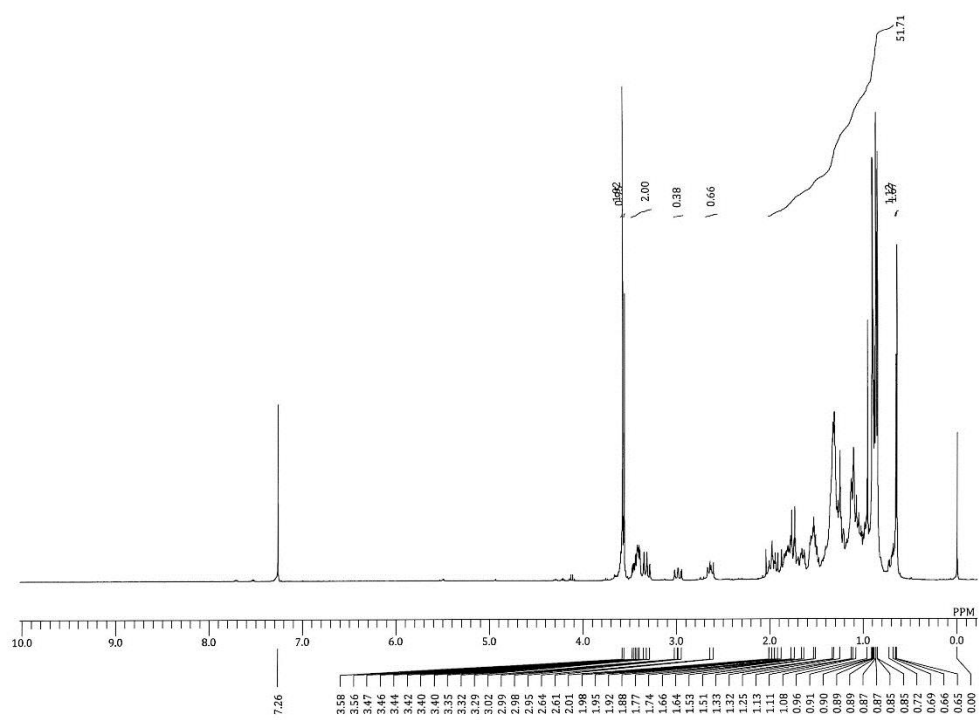
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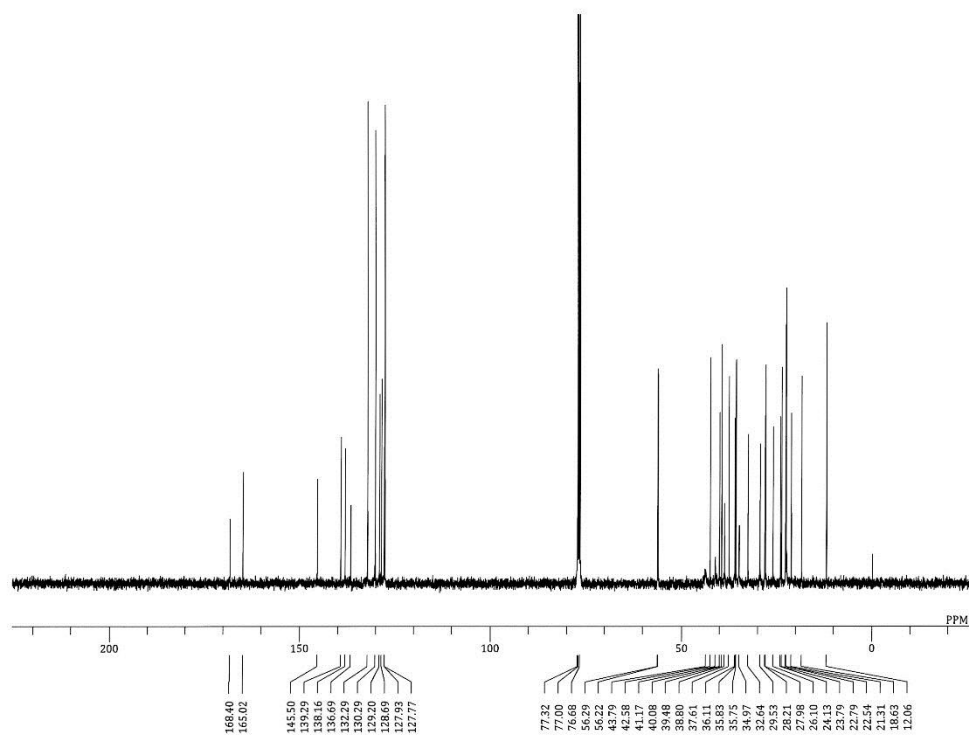
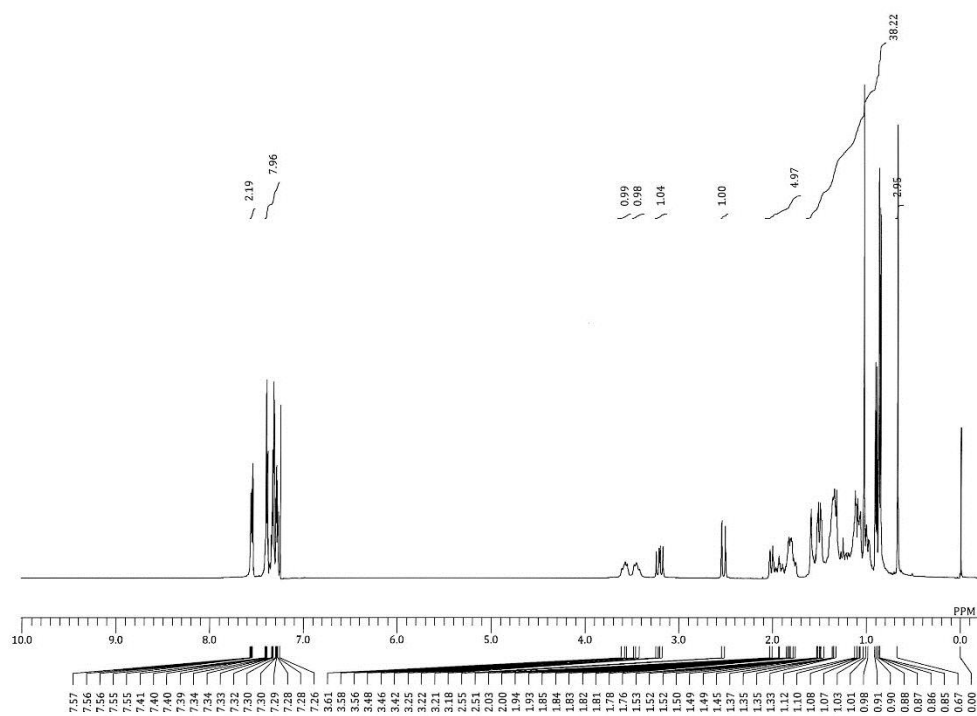
Compound 9 (from 5)



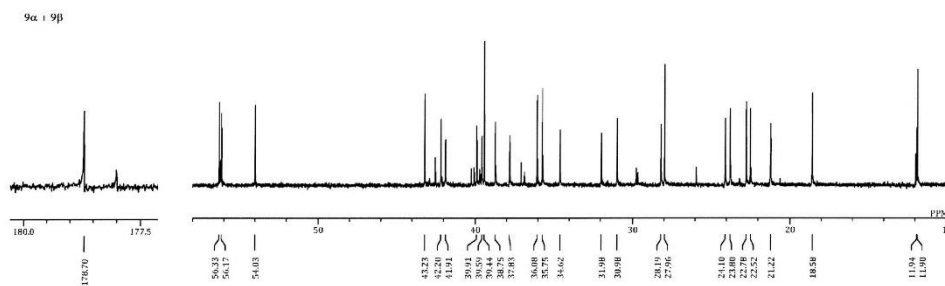
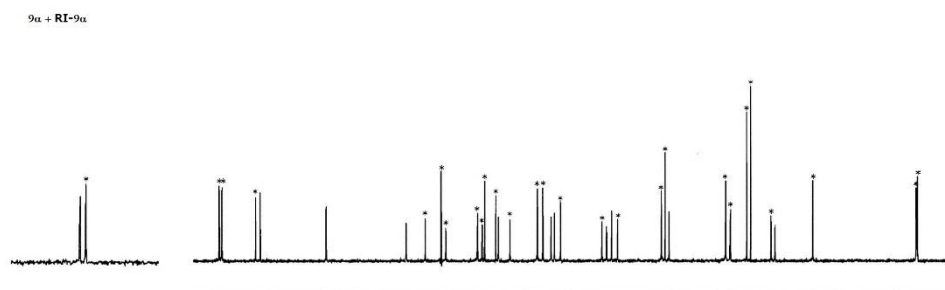
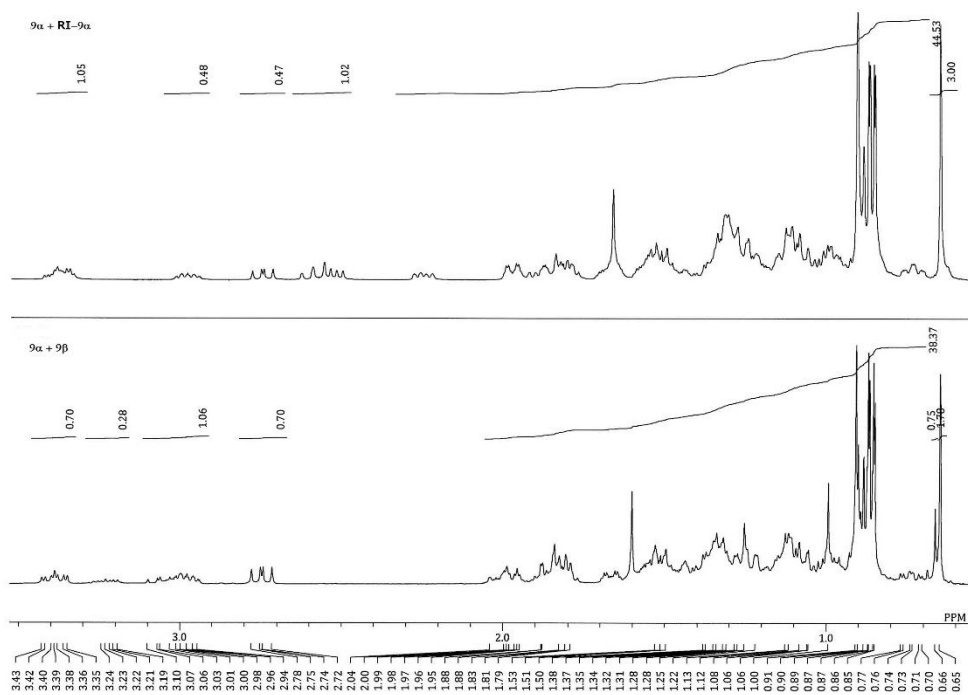
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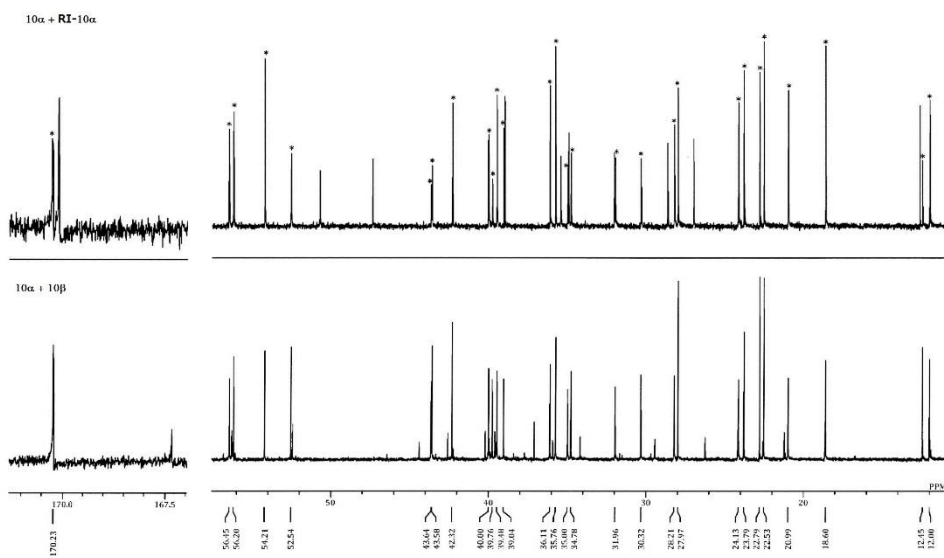
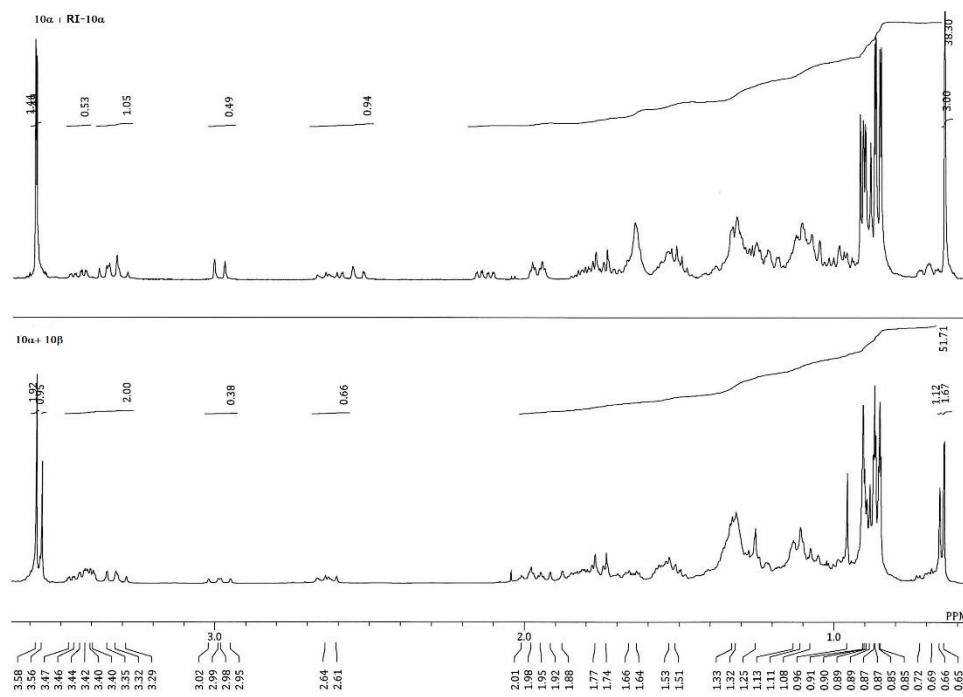
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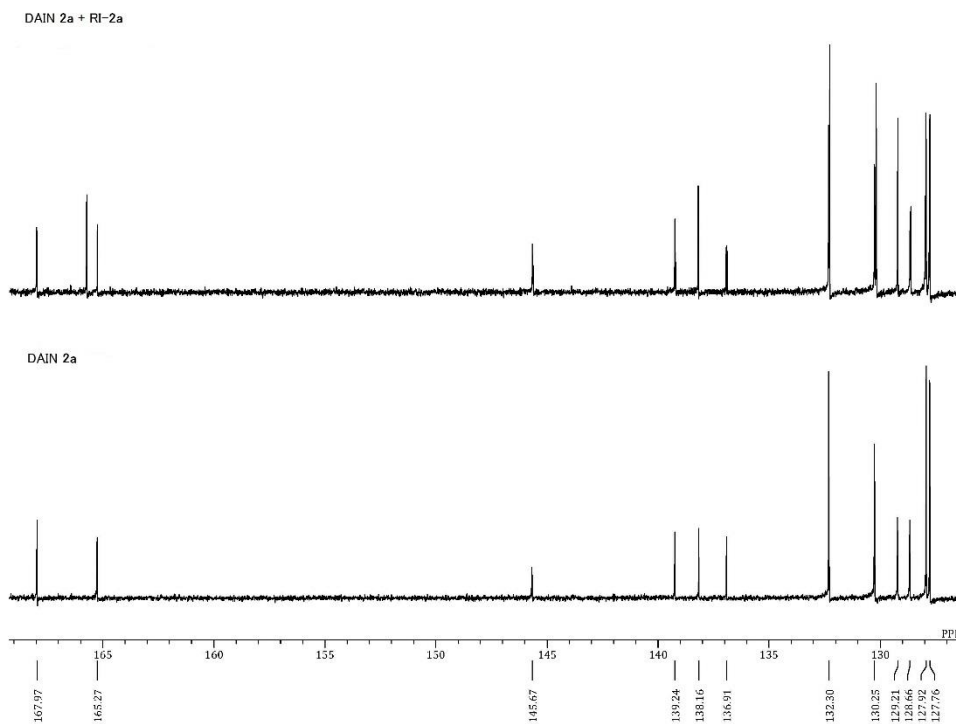
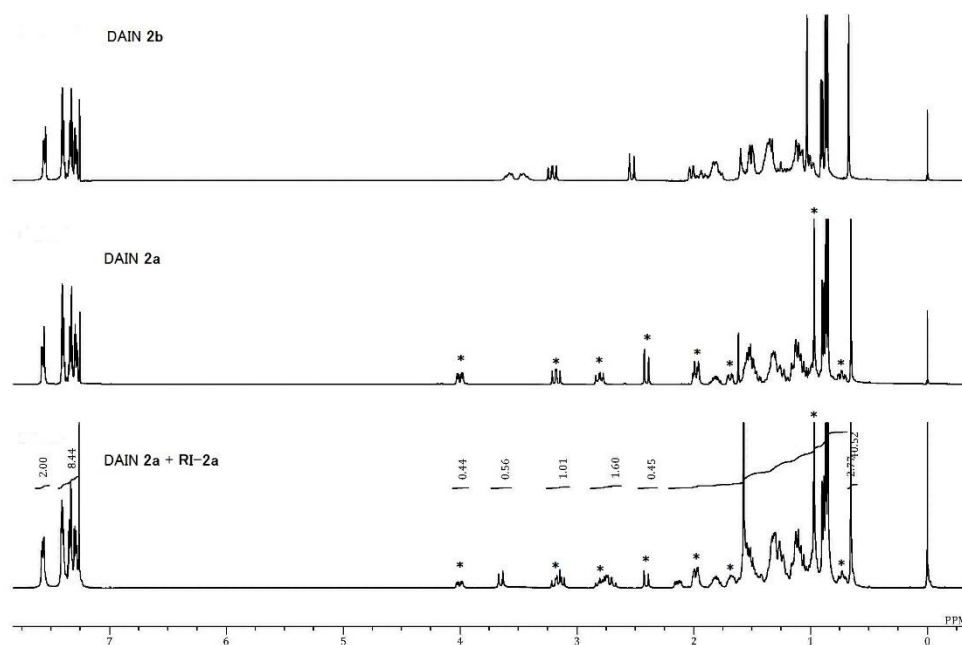
Compound **9a** + RI-**9a** (comparison with **9**)

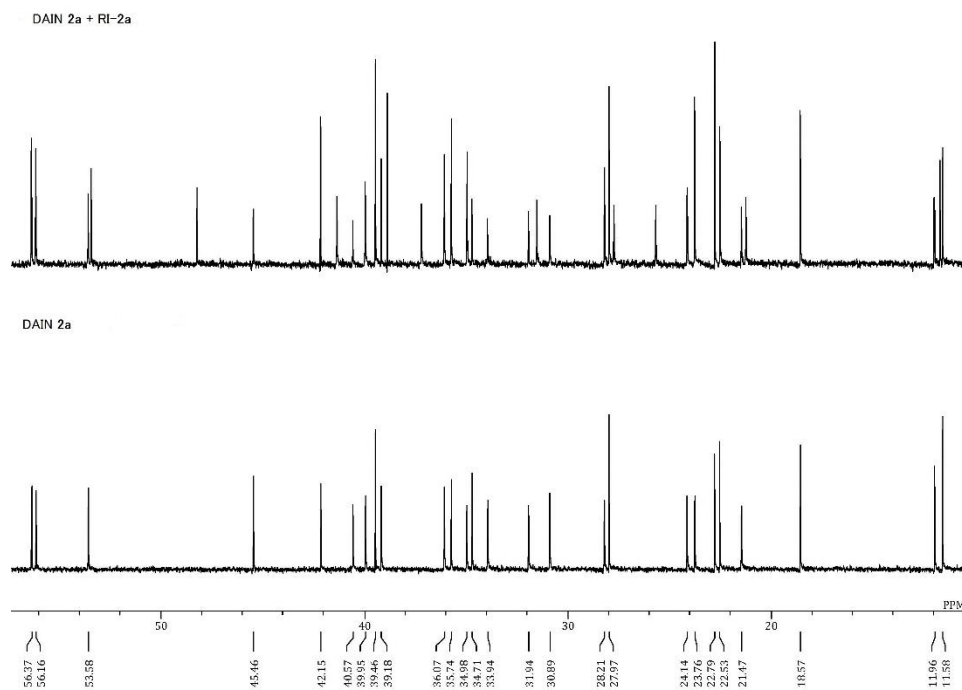


Compound **10 α** + RI-**10 α** (comparison with **10**)

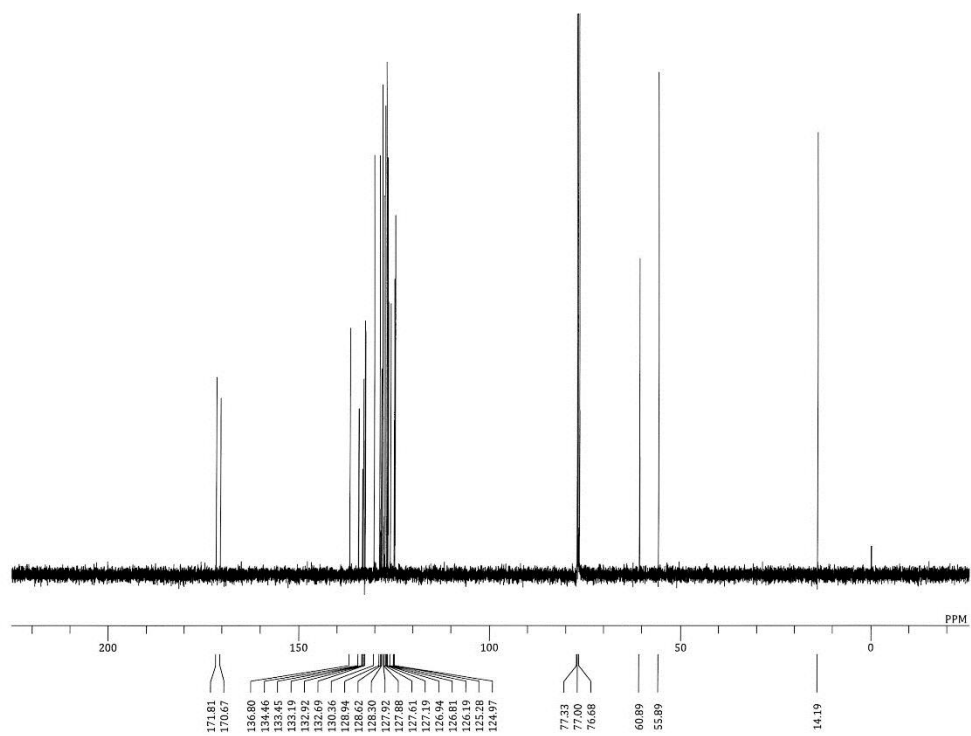
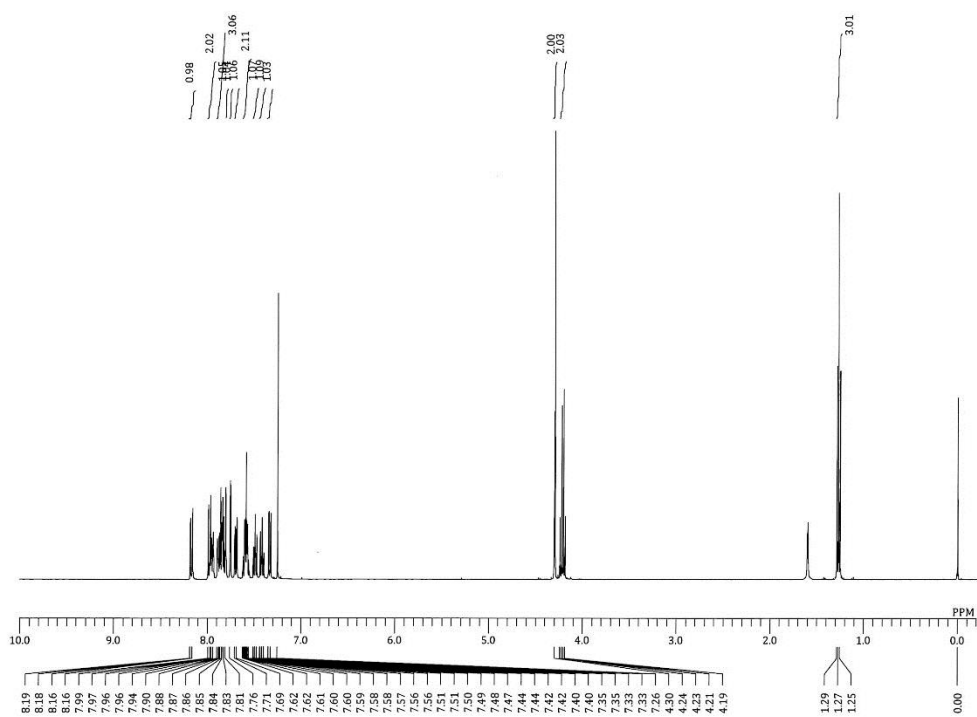


Compound 2a + RI-2a (comparison with 2a)

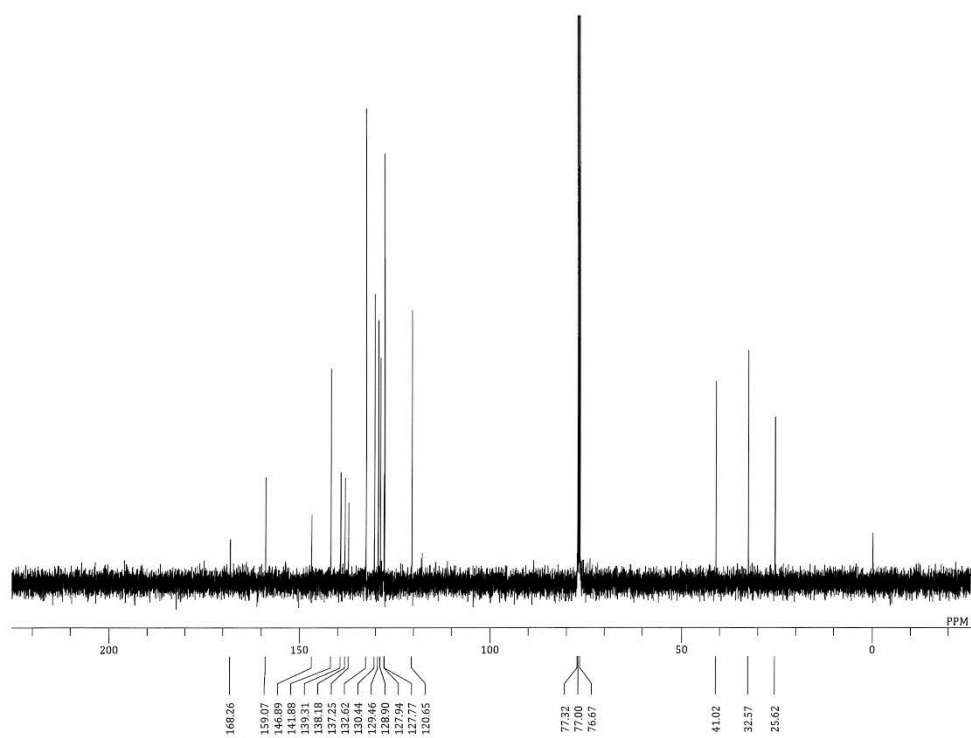
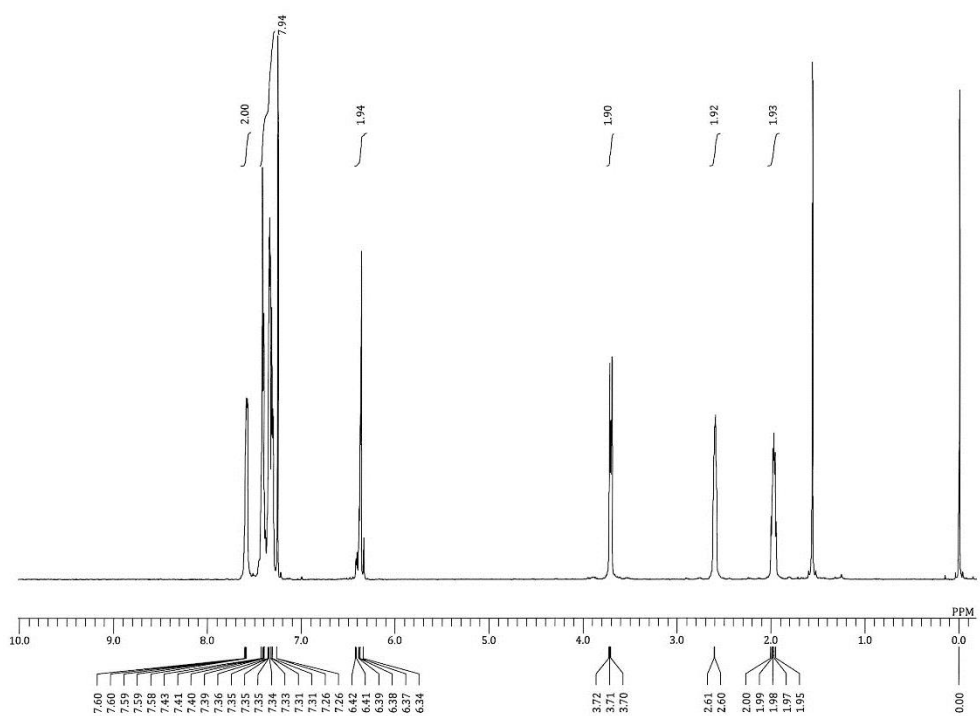




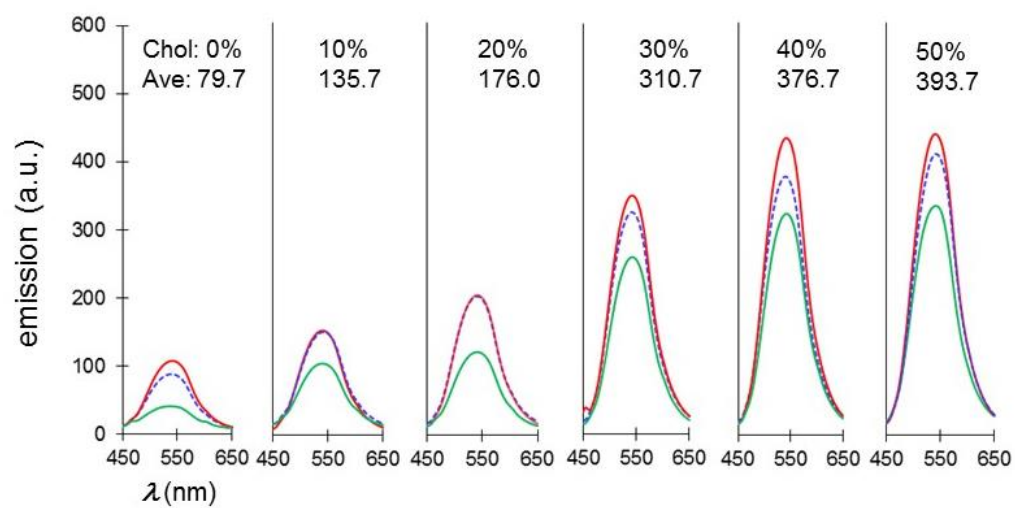
Compound 8



Compound 13



4. Figures S1—S3.



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

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

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

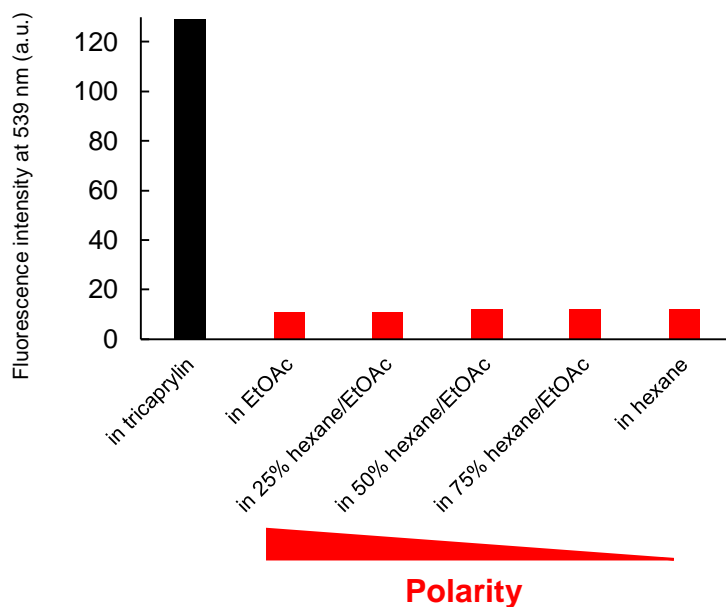


Fig. S2. Fluorescence of Ch-DAIN 1 in EtOAc/hexane and tricaprylin.

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.

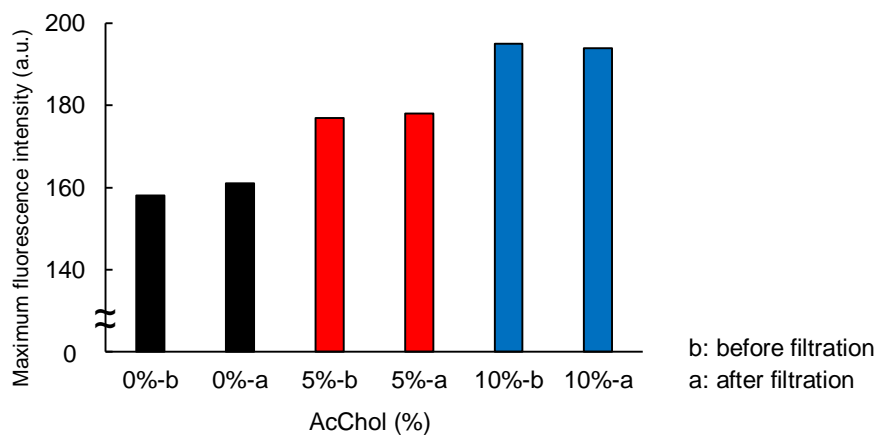


Fig. S3. Fluorescence of Ch-DAIN 1 in tricaprylin containing 0, 5, 10% cholesterol acetate (AcChol) before and after filtration (0.2 μm , PTFE filter).

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

78 84

SMALL

NO_CHARGES

@<TRIPOS>ATOM

1 C1	-3.3147	-0.3806	0.1966 C
2 C2	-3.4809	2.1448	0.4007 C
3 C3	-1.3897	0.9376	1.1593 C
4 C4	-2.3135	2.1185	1.3956 C
5 C5	-2.0809	-0.4347	1.2000 C
6 C6	-4.2663	0.8296	0.4316 C
7 N7	1.1943	-0.9316	0.9435 N
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
11 C11	3.1517	-0.0688	0.1965 C
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
27 H27	-2.8658	-0.2164	-0.7970 H
28 H28	-4.7255	0.7388	1.4270 H
29 H29	-4.8657	0.8169	-1.6034 H
30 H30	-4.1420	2.9894	0.6303 H
31 H31	-3.0891	2.3139	-0.6129 H
32 H32	-2.7231	2.0682	2.4152 H
33 H33	-1.7443	3.0520	1.3393 H
34 H34	0.1721	2.2892	0.8739 H
35 H35	0.0669	-1.6770	2.5436 H
36 H36	0.5385	-2.8220	1.2915 H
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
53 H53	-1.7118	-0.6335	3.3564 H
54 H54	-9.1068	-1.0315	-1.0622 H
55 H55	-8.1469	-2.1144	-2.0863 H
56 H56	-9.0368	-0.7678	-2.8065 H
57 C57	5.3701	-1.0527	-0.3979 C

58 C58	7.1377	-3.1866	-0.8898 C
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.

@<TRIPOS>MOLECULE

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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Ch(an)-DAIN 2b*:

E = -1543.82114804 A.U.

No imaginary frequencies.

@<TRIPOS>MOLECULE

Molecule Name

80 86

SMALL

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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(S₀) = -1191.20182558 A.U.

No imaginary frequencies.

@<TRIPOS>MOLECULE

Molecule Name

55 59

SMALL

NO_CHARGES

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1 C1	-5.4617	-0.7329	-0.9136 C
2 C2	-5.7909	1.7610	-0.8750 C
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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E(S₀) = -1191.20102850 A.U.

E(S₁) = -1191.09228404 A.U.

@<TRIPOS>MOLECULE

Molecule Name

55 59

SMALL

NO_CHARGES

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1 C1	5.3803	-0.5907	1.0884 C
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

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E(S₀) = -1191.20140998 A.U.

E(S₁) = -1191.09737350 A.U.

@<TRIPOS>MOLECULE

Molecule Name

55 59

SMALL

NO_CHARGES

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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 3 2 1
 8 2 3 3 1
 9 3 4 1
 10 3 5 1
 11 3 9 2
 12 4 3 6 1
 13 4 3 7 1
 14 5 1 5 1
 15 5 2 9 1
 16 6 3 0 1
 17 6 3 1 1
 18 7 8 1
 19 7 1 2 1
 20 7 1 4 1
 21 8 9 1
 22 8 1 0 2
 23 9 4 3 1
 24 10 1 1 1
 25 11 1 2 1
 26 11 1 6 2
 27 12 1 3 2
 28 14 1 5 1
 29 14 4 4 1
 30 14 4 5 1
 31 15 4 1 1
 32 15 4 2 1
 33 16 1 7 1
 34 16 2 3 1
 35 17 1 9 Ar
 36 17 2 0 Ar
 37 18 2 1 Ar
 38 18 2 2 Ar
 39 18 5 3 1
 40 19 2 2 Ar
 41 19 5 5 1
 42 20 2 1 Ar
 43 20 5 1 1
 44 21 5 2 1
 45 22 5 4 1
 46 23 2 5 Ar
 47 23 2 6 Ar
 48 24 2 7 Ar
 49 24 2 8 Ar
 50 24 4 8 1
 51 25 2 8 Ar
 52 25 5 0 1
 53 26 2 7 Ar
 54 26 4 6 1
 55 27 4 7 1
 56 28 4 9 1
 57 29 3 8 1
 58 29 3 9 1
 59 29 4 0 1

DAIN 1'' (30 °):
 E(S₀) = -1191.19673202 A.U.
 E(S₁) = -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 3 4 1
 4 1 3 5 1
 5 2 4 1
 6 2 6 1
 7 2 3 2 1
 8 2 3 3 1
 9 3 4 1
 10 3 5 1
 11 3 9 2
 12 4 3 6 1
 13 4 3 7 1
 14 5 1 5 1
 15 5 2 9 1
 16 6 3 0 1
 17 6 3 1 1
 18 7 8 1
 19 7 1 2 1
 20 7 1 4 1
 21 8 9 1
 22 8 1 0 2

23 9 4 3 1
 24 10 1 1 1
 25 11 1 2 1
 26 11 1 6 2
 27 12 1 3 2
 28 14 1 5 1
 29 14 4 4 1
 30 14 4 5 1
 31 15 4 1 1
 32 15 4 2 1
 33 16 1 7 1
 34 16 2 3 1
 35 17 1 9 Ar
 36 17 2 0 Ar
 37 18 2 1 Ar
 38 18 2 2 Ar
 39 18 5 3 1
 40 19 2 2 Ar
 41 19 5 5 1
 42 20 2 1 Ar
 43 20 5 1 1
 44 21 5 2 1
 45 22 5 4 1
 46 23 2 5 Ar
 47 23 2 6 Ar
 48 24 2 7 Ar
 49 24 2 8 Ar
 50 24 4 8 1
 51 25 2 8 Ar
 52 25 5 0 1
 53 26 2 7 Ar
 54 26 4 6 1
 55 27 4 7 1
 56 28 4 9 1
 57 29 3 8 1
 58 29 3 9 1
 59 29 4 0 1

DAIN 1'' (45 °):
 E(S₀) = -1191.18669796 A.U.
 E(S₁) = -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(S₀) = -1191.17215637 A.U.

E(S₁) = -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(S₀) = -1191.15589306 A.U.

E(S_i) = -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
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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(S₀) = -1191.13262730 A.U.

E(S_i) = -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(S₀) = -1191.20160978 A.U.

E(S_i) = -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(S₀) = -1191.19685665 A.U.

E(S_i) = -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(S₀) = -1191.18679423 A.U.

E(S₁) = -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(S₀) = -1191.17241609 A.U.

E(S₁) = -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(S₀) = -1191.15603685 A.U.

E(S₁) = -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

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2 1 6 1
3 1 34 1
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5 2 4 1
6 2 6 1
7 2 32 1
8 2 33 1
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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
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 34 16 23 1
 35 17 19 Ar
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 37 18 21 Ar
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 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
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 54 26 46 1
 55 27 47 1
 56 28 49 1
 57 29 38 1
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 59 29 40 1

DAIN 1** (-90 °):

E(S₀) = -1191.13967958 A.U.
 E(S₁) = -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

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 2 1 6 1
 3 1 34 1
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 5 2 4 1
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 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
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 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
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 55 27 47 1
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 59 29 40 1

DAIN 2a** (optimized):

E(S₀) = -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

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 19 6 12 1
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 49 23 26 Ar
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 51 24 25 Ar
 52 24 43 1
 53 25 44 1
 54 26 46 1
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60 53 56 1
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DAIN 2a'' (0 °):

E(S₀) = -1192.42164740 A.U.

E(S₁) = -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

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 7 2 3 0 1
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 10 3 3 5 1
 11 3 5 4 1
 12 4 1 3 1
 13 4 2 7 1
 14 4 5 4 1
 15 5 2 8 1
 16 5 2 9 1
 17 6 7 1
 18 6 10 1
 19 6 12 1
 20 7 8 2
 21 7 5 3 1
 22 8 9 1
 23 9 10 1
 24 9 14 2
 25 10 11 2
 26 12 13 1
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 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
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DAIN 2a'' (15 °):

E(S₀) = -1192.42200716 A.U.

E(S₁) = -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

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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
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22 8 9 1
23 9 10 1
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25 10 11 2
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39 17 52 1
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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
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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(S₀) = -1192.41694522 A.U.

E(S₁) = -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(S₀) = -1192.40594926 A.U.

E(S₁) = -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(S₀) = -1192.39101366 A.U.

E(S₁) = -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
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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 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
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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(S₀) = -1192.37333383 A.U.

E(S₁) = -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
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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(S₀) = -1192.35552554 A.U.
E(S₁) = -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(S₀) = -1192.42197063 A.U.
E(S₁) = -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(S₀) = -1192.41683577 A.U.
 E(S₁) = -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(S₀) = -1192.40596285 A.U.
 E(S₁) = -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(S₀) = -1192.39086015 A.U.

E(S₁) = -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
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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 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(S₀) = -1192.36497223 A.U.
 E(S₁) = -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
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 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
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 11 3 54 1
 12 4 13 1
 13 4 27 1
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 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(S₀) = -1192.34787565 A.U.
 E(S₁) = -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(S₀) = -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

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 3 1 32 1
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 5 2 3 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 2
 25 10 11 2
 26 12 13 1
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 28 12 42 1
 29 13 39 1
 30 13 40 1
 31 14 15 1
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 34 15 18 Ar
 35 16 19 Ar
 36 16 20 Ar
 37 16 50 1
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 39 17 52 1
 40 18 19 Ar
 41 18 48 1
 42 19 49 1
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 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(S₀) = -1192.41687050 A.U.
 E(S₁) = -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
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 11 3 54 1
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 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(S₀) = -1192.41702092 A.U.

E(S_i) = -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

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 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
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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
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 26 12 13 1
 27 12 41 1
 28 12 42 1
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 31 14 15 1
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 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(S₀) = -1192.41190845 A.U.

E(S₁) = -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
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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 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(S₀) = -1192.40127043 A.U.

E(S₁) = -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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 16 5 2 9 1
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 23 9 1 0 1
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 30 13 4 0 1
 31 14 1 5 1
 32 14 2 1 1
 33 15 1 7 Ar
 34 15 1 8 Ar
 35 16 1 9 Ar
 36 16 2 0 Ar
 37 16 5 0 1
 38 17 2 0 Ar
 39 17 5 2 1
 40 18 1 9 Ar
 41 18 4 8 1
 42 19 4 9 1
 43 20 5 1 1
 44 21 2 3 Ar
 45 21 2 4 Ar
 46 22 2 5 Ar
 47 22 2 6 Ar
 48 22 4 5 1
 49 23 2 6 Ar
 50 23 4 7 1
 51 24 2 5 Ar
 52 24 4 3 1
 53 25 4 4 1
 54 26 4 6 1
 55 27 3 6 1
 56 27 3 7 1
 57 27 3 8 1
 58 53 5 4 1
 59 53 5 6 1
 60 53 5 7 1
 61 54 5 5 1

DAIN 2b** (60 °):
 E(S₀) = -1192.38606534 A.U.
 E(S₁) = -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

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 13 4 2 7 1

14 4 5 4 1
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 16 5 2 9 1
 17 6 7 Ar
 18 6 1 0 1
 19 6 1 2 1
 20 7 8 2
 21 7 5 3 1
 22 8 9 1
 23 9 1 0 1
 24 9 1 4 Ar
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 28 12 4 2 1
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 30 13 4 0 1
 31 14 1 5 1
 32 14 2 1 1
 33 15 1 7 Ar
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 35 16 1 9 Ar
 36 16 2 0 Ar
 37 16 5 0 1
 38 17 2 0 Ar
 39 17 5 2 1
 40 18 1 9 Ar
 41 18 4 8 1
 42 19 4 9 1
 43 20 5 1 1
 44 21 2 3 Ar
 45 21 2 4 Ar
 46 22 2 5 Ar
 47 22 2 6 Ar
 48 22 4 5 1
 49 23 2 6 Ar
 50 23 4 7 1
 51 24 2 5 Ar
 52 24 4 3 1
 53 25 4 4 1
 54 26 4 6 1
 55 27 3 6 1
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 57 27 3 8 1
 58 53 5 4 1
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 60 53 5 7 1
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DAIN 2b** (75 °):
 E(S₀) = -1192.36820362 A.U.
 E(S₁) = -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

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2 1 5 1
3 1 32 1
4 1 33 1
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6 2 5 1
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8 2 31 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 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
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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(S₀) = -1192.35093358 A.U.

E(S₁) = -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

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14 4 54 1
15 5 28 1
16 5 29 1
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18 6 10 1
19 6 12 1
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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(S₀) = -1192.41700021 A.U.

E(S₁) = -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(S₀) = -1192.41183076 A.U.

E(S₁) = -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
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 11 3 54 1
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 15 5 28 1
 16 5 29 1
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 18 6 10 1
 19 6 12 1
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 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(S₀) = -1192.40125484 A.U.
 E(S₁) = -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(S₀) = -1192.38611605 A.U.
 E(S₁) = -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(S₀) = -1192.36857075 A.U.

E(S₁) = -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
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(S₀) = -1192.34316399 A.U.

E(S₁) = -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

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 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