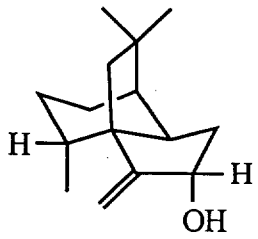
JOC The Journal of Organic Chemistry

J. Org. Chem., 1998, 63(25), 9166-9176, DOI:10.1021/jo971579v

Data Set 2 for β-terrecyclen-3α-OH (31, R=H)

Contents



31

W47N Crystal

Space group[1] $P\bar{1}$ (C_i^1) No. 2 triclinic

Conditions limiting possible reflections[1] none

Cell parameters[2] Molybdenum radiation, $\lambda(K\bar{\alpha}) = 0.71073$ Å
range of intensities, $18.8 < 2\theta < 20.5$ °
temperature, $t = -75$ °C

$\underline{a} = 12.586(2)$ Å $\alpha = 102.98(2)°$

$\underline{b} = 14.167(3)$ $\beta = 94.59(1)$

$\underline{c} = 15.013(3)$ $\gamma = 90.12(2)$

$V = 2600(11)$ Å^3

Formula[3] $C_{15}H_{24}O$ Formula weight[3] 220.36

Formula/unit cell[3] 8 Electrons/unit cell, $F_{000} = 976$

Density calculated, $\rho = 1.126$ g/cm^3

Linear absorption coefficient[4a], $\mu = 0.63$ cm^{-1}

Approximate size 0.4 × 0.5 × 0.7 mm

Comments The colorless, translucent equidimensional data crystal was cut from a large parent crystal with poorly developed faces. The excised sample uniformly extinguished plane-polarized light. The crystal was mounted using epoxy to a thin glass fiber with the (1 -6 -1) scattering planes roughly normal to the spindle axis. The data crystal was approximately bound by the {0 0 1}, {1 0 0} and {0 1 0} forms. Distances from the crystal center to these facial boundaries were 0.23, 0.24 and 0.35, respectively

W47N Data Collection and Reduction

Instrument Enraf-Nonius CAD4 automated κ-axis diffractometer

Radiation Molybdenum $K\alpha_1$ = 0.70930, $K\alpha_2$ = 0.71359, $K\bar{\alpha}$ = 0.71073 Å

no filters were used, attenuator (factor 20.13) used when required

graphite crystal monochromator, 2θ monochromator = 12°

Shell				
1:	2.0 < 2θ < 28.0°	for	±h-k±l
2:	28.0	38.0	
3:	38.0	44.0	
4:	44.0	48.0	(limited observed data, shell not used)

Scan mode ω/θ

range ω-scan angle = 1.50[1.00 + 0.35tan(θ)]°

rate variable, from 3 to 16°/min

Total background time per scan time 0.33

Standard intensities measured per 5400 sec exposure time 3

Miller indices of standard reflections (-2 -4 -4), (-2 6 0), (3 6 -2)

Orientation test on 3 reflections per 1000 intensities measured

Intensities measured (including standards and non-unique) 6786 (see comments)

Crystal exposure 46.58 hr.

Intensities processed (excluding standards and non-unique data) 6352

"Observed" reflections ($I > 2.58\sigma(I)$)[5] 4767

"Ignorance" factor[5], p = 0.01

Typical ω-scan width at half maximum < 0.3°

Corrections applied to the data

Lorentz and polarization effects[6a] applied

anomalous dispersion effects[4c,6b] applied

crystal decay[7] not applied, no significant change

non-unique data averaged 323 equivalent intensities were measured, internal consistency index, R_i = 0.029

absorption[4a,6c,8a] not applied

extinction[6d,9] not applied

questionable reflections deleted none

Comments Data were measured at -75°C. The fourth shell had very few observed data and a minor problem with the cooling stream resulted in some crystal movement, so only the first three data shells were reduced for structure solution and refinement. No other problems were encountered collecting these data and there was no change in the appearance of the sample during the experiment.

W47N Solution and Refinement

Methods[10a,6f,11b,6h,6i,11a] direct methods, SHELXS-86; unweighted difference Fourier syntheses, block-diagonal matrix least-squares refinement, SHELX-76

Space group confirmation average values of normalized structure factors and successful refinement of the proposed model in the centric space group

Final agreement factors[15] $R = 0.045$ $R_w = 0.049$ E,k = 2.56,1.00

NO = 4767 NV = 617 (464/block) NP = 961 NALS = 76 NASF = 160

Maximum shift/error in final least squares cycles[4b,4c,6i,16] 0.002

Final difference Fourier[6h,17] $+0.27 > e/Å^3 > -0.28$

Tables

1 symmetry[18] no crystallographic symmetry was imposed on the four independent molecules

2 positional parameters[19] first tables lists refined coordinates, second table lists "idealized" H atom coordinates (note - hydroxyl and vinyl H atom positions, H1, H5 and H6, were independently refined)

1 thermal parameters[21] non-H atoms were refined with anisotropic thermal coefficients, common isotropic thermal parameters for H atoms of each independent molecule were refined

5 selected distances and angles[22,23a] first table includes refined positions, tables 2 through 5 include all positions for molecules 1 through 4, respectively

1 van der Waals contacts[22,23b] includes all positions, there were 4 strong intermolecular H···O contacts

4 torsion angles[24] one table including all positions for each independent molecule

0 planes[25] available on request

1 selected hydrogen interactions[26] describing 4 strong H bonds that form two polymeric chains

1 observed and calculated structure factor amplitudes[6j,27b] 32 pages

Comments The structure was solved by direct methods, SHELXS-86; correct positions for all non-H atoms were deduced from an E-map. A subsequent

isotropic least-squares refinement cycle followed by a difference Fourier synthesis revealed positions for hydroxyl and vinyl H atoms. The remaining H atoms were included as fixed contributors in "idealized" positions. The four independent molecules were refined in blocks representing all possible combinations of three molecules. In the final cycles of least-squares refinement, hydroxyl and vinyl H atom positions were independently refined, common isotropic H atom thermal parameters were refined for each molecule, and non-H atoms were refined with anisotropic thermal coefficients. Successful convergence was indicated by the maximum shift/error for the last cycles. The final difference Fourier map had no significant features. A final analysis of variance between obsereved and calculated structure factors showed no systematic errors.

(Although there are four indepepndent moleucles, there are only different basic conformations represented by molecules A and B or molecules C and D.)

W47N Graphics[10a,29]

View of one molecule (35% probability ellipsoids) Thermal ellipsoid representations of the four independent molecules with unique nonhydrogen atoms labelled were plotted roughly parallel to the best-plane normals.

Packing diagram available on request

Comments Stereo plots of the views mentioned, single or stereo plots in specific orientations, and liquid ink diagrams suitable for publication of any of the above are available on request.

Equivalent Positions

1	x	y	z
2	-x	-y	-z

Table S1a. Refined Positional Parameters

	x/a	y/b	z/c
O2A	0.0712(2)	0.4286(1)	0.1005(1)
C1A	0.1516(2)	0.4593(2)	0.2536(2)
C2A	0.1679(2)	0.4648(2)	0.1560(2)
C3A	0.2598(2)	0.3983(2)	0.1306(2)
C3'A	0.3227(3)	0.4031(3)	0.0652(2)
C3aA	0.2690(2)	0.3299(2)	0.1945(2)
C4A	0.2679(2)	0.2215(2)	0.1483(2)
C5A	0.2699(3)	0.1628(2)	0.2230(2)
C6A	0.2035(3)	0.2034(2)	0.3039(2)
C7A	0.2123(2)	0.3143(2)	0.3372(2)
C7aA	0.1739(2)	0.3528(2)	0.2529(2)
C8A	0.3290(2)	0.3513(2)	0.3623(2)
C9A	0.3660(2)	0.3569(2)	0.2675(2)
C10A	0.1761(3)	0.1895(2)	0.0758(2)
C11A	0.3358(3)	0.4508(2)	0.4293(2)
C12A	0.3991(3)	0.2866(3)	0.4111(2)
O2B	0.0805(2)	0.4371(1)	-0.0795(1)
C1B	0.1786(2)	0.3055(2)	-0.1676(2)
C2B	0.0746(2)	0.3607(2)	-0.1601(2)
C3B	-0.0099(2)	0.2828(2)	-0.1636(2)
C3'B	-0.0901(2)	0.2914(2)	-0.1113(2)
C3aB	0.0241(2)	0.1963(2)	-0.2331(2)
C4B	-0.0174(2)	0.0944(2)	-0.2319(2)
C5B	0.0332(2)	0.0210(2)	-0.3078(2)
C6B	0.1518(2)	0.0402(2)	-0.3167(2)
C7B	0.1802(2)	0.1480(2)	-0.3086(2)

Table S1a. (continued)

	x/a	y/b	z/c
C7aB	0.1471(2)	0.1991(2)	-0.2144(2)
C8B	0.1126(2)	0.1931(2)	-0.3785(2)
C9B	0.0065(2)	0.2130(2)	-0.3324(2)
C10B	0.0006(2)	0.0659(2)	-0.1398(2)
C11B	0.1639(2)	0.2880(2)	-0.3897(2)
C12B	0.0991(3)	0.1276(2)	-0.4746(2)
O2C	0.4290(2)	0.8794(1)	0.8977(1)
C1C	0.3479(2)	0.8315(2)	0.7441(2)
C2C	0.3324(2)	0.8864(2)	0.8411(2)
C3C	0.2409(2)	0.8325(2)	0.8685(2)
C3'C	0.1778(3)	0.8698(3)	0.9328(2)
C3aC	0.2328(2)	0.7318(2)	0.8077(2)
C4C	0.2363(2)	0.6479(2)	0.8574(2)
C5C	0.2358(3)	0.5521(2)	0.7860(2)
C6C	0.3017(3)	0.5515(2)	0.7046(2)
C7C	0.2901(2)	0.6439(2)	0.6668(2)
C7aC	0.3271(2)	0.7262(2)	0.7486(2)
C8C	0.1728(2)	0.6658(2)	0.6407(2)
C9C	0.1352(2)	0.7189(2)	0.7349(2)
C10C	0.3295(3)	0.6557(2)	0.9306(2)
C11C	0.1645(3)	0.7300(2)	0.5713(2)
C12C	0.1034(2)	0.5752(2)	0.5946(2)
O2D	0.4197(2)	0.9738(1)	0.0797(1)
C1D	0.3216(2)	0.8855(2)	0.1689(2)
C2D	0.4253(2)	0.9378(2)	0.1609(2)
C3D	0.5102(2)	0.8631(2)	0.1671(2)

Table S1a. (continued)

	x/a	y/b	z/c
C3'D	0.5908(2)	0.8465(2)	0.1154(2)
C3aD	0.4760(2)	0.8109(2)	0.2371(2)
C4D	0.5193(2)	0.7098(2)	0.2391(2)
C5D	0.4690(2)	0.6737(2)	0.3160(2)
C6D	0.3496(2)	0.6949(2)	0.3226(2)
C7D	0.3193(2)	0.7973(2)	0.3121(2)
C7aD	0.3536(2)	0.8033(2)	0.2183(2)
C8D	0.3846(2)	0.8784(2)	0.3814(2)
C9D	0.4920(2)	0.8777(2)	0.3362(2)
C10D	0.5016(2)	0.6348(2)	0.1479(2)
C11D	0.3307(2)	0.9765(2)	0.3890(2)
C12D	0.3983(3)	0.8618(2)	0.4790(2)
H1A	0.079(2)	0.419(2)	0.045(2)
H5A	0.384(2)	0.354(2)	0.056(2)
H6A	0.312(2)	0.452(2)	0.029(2)
H1B	0.038(2)	0.479(2)	-0.087(2)
H5B	-0.139(2)	0.235(2)	-0.112(2)
H6B	-0.102(2)	0.351(2)	-0.065(2)
H1C	0.416(3)	0.898(2)	0.952(2)
H5C	0.122(2)	0.830(2)	0.949(2)
H6C	0.185(2)	0.937(2)	0.970(2)
H1D	0.465(2)	1.024(2)	0.089(2)
H5D	0.641(2)	0.797(2)	0.119(2)
H6D	0.602(2)	0.884(2)	0.068(2)

Table S1b. Idealized Positional Parameters

	x/a	y/b	z/c
H2A	0.2007	0.5016	0.2963
H3A	0.0800	0.4754	0.2686
H4A	0.1826	0.5287	0.1479
H7A	0.3306	0.2093	0.1150
H8A	0.3425	0.1599	0.2464
H9A	0.2436	0.0986	0.1950
H10A	0.1302	0.1859	0.2856
H11A	0.2271	0.1748	0.3539
H12A	0.1731	0.3347	0.3905
H13A	0.1038	0.3244	0.2364
H14A	0.3910	0.4214	0.2694
H15A	0.4224	0.3122	0.2516
H16A	0.1773	0.2276	0.0304
H17A	0.1098	0.1985	0.1041
H18A	0.1833	0.1224	0.0471
H19A	0.2937	0.4961	0.4038
H20A	0.4087	0.4732	0.4397
H21A	0.3094	0.4454	0.4864
H22A	0.3992	0.2223	0.3733
H23A	0.3713	0.2848	0.4685
H24A	0.4706	0.3126	0.4218
H2B	0.2252	0.3318	-0.2042
H3B	0.2133	0.3091	-0.1079
H4B	0.0581	0.3940	-0.2084
H7B	-0.0935	0.0946	-0.2425
H8B	-0.0051	0.0222	-0.3651

Table S1b. (continued)

	x/a	y/b	z/c
H9B	0.0261	-0.0422	-0.2952
H10B	0.1928	0.0181	-0.2692
H11B	0.1704	0.0041	-0.3755
H12B	0.2540	0.1545	-0.3188
H13B	0.1834	0.1666	-0.1718
H14B	-0.0140	0.2787	-0.3301
H15B	-0.0482	0.1696	-0.3665
H16B	-0.0317	0.1126	-0.0935
H17B	0.0756	0.0640	-0.1239
H18B	-0.0310	0.0031	-0.1442
H19B	0.1742	0.3321	-0.3309
H20B	0.1180	0.3165	-0.4299
H21B	0.2315	0.2745	-0.4152
H22B	0.0672	0.0669	-0.4716
H23B	0.1676	0.1163	-0.4990
H24B	0.0542	0.1583	-0.5137
H2C	0.2979	0.8514	0.7009
H3C	0.4191	0.8406	0.7281
H4C	0.3180	0.9540	0.8470
H7C	0.1739	0.6512	0.8910
H8C	0.1633	0.5362	0.7628
H9C	0.2628	0.5032	0.8162
H10C	0.3754	0.5454	0.7236
H11C	0.2794	0.4968	0.6564
H12C	0.3289	0.6370	0.6130
H13C	0.3978	0.7079	0.7655

Table S1b. (continued)

	x/a	y/b	z/c
H14C	0.1082	0.7812	0.7308
H15C	0.0802	0.6812	0.7525
H16C	0.3270	0.7167	0.9740
H17C	0.3956	0.6515	0.9019
H18C	0.3241	0.6039	0.9618
H19C	0.2058	0.7884	0.5950
H20C	0.0913	0.7459	0.5604
H21C	0.1911	0.6960	0.5148
H22C	0.1045	0.5307	0.6343
H23C	0.1313	0.5445	0.5376
H24C	0.0315	0.5944	0.5832
H2D	0.2742	0.9293	0.2043
H3D	0.2875	0.8588	0.1092
H4D	0.4411	0.9951	0.2080
H7D	0.5952	0.7169	0.2504
H8D	0.5061	0.7044	0.3733
H9D	0.4777	0.6049	0.3053
H10D	0.3102	0.6486	0.2752
H11D	0.3302	0.6876	0.3815
H12D	0.2450	0.8065	0.3211
H13D	0.3176	0.7496	0.1765
H14D	0.5114	0.9422	0.3328
H15D	0.5470	0.8524	0.3716
H16D	0.5334	0.6583	0.1006
H17D	0.4266	0.6242	0.1322
H18D	0.5338	0.5749	0.1538

Table S1b. (continued)

	x/a	y/b	z/c
H19D	0.3203	0.9902	0.3292
H20D	0.3750	1.0263	0.4283
H21D	0.2630	0.9744	0.4142
H22D	0.4319	0.8008	0.4779
H23D	0.3297	0.8611	0.5031
H24D	0.4418	0.9130	0.5172

Table S2. Thermal Parameters

	U11	U22	U33	U23	U13	U12
O2A	0.041(1)	0.039(1)	0.030(1)	0.006(1)	-0.002(1)	0.0124(9)
C1A	0.042(2)	0.034(2)	0.031(2)	0.006(1)	0.004(1)	0.013(1)
C2A	0.046(2)	0.023(2)	0.032(2)	0.007(1)	-0.003(1)	0.003(1)
C3A	0.030(2)	0.027(2)	0.025(2)	0.004(1)	-0.002(1)	-0.008(1)
C3'A	0.042(2)	0.052(2)	0.036(2)	0.017(2)	0.001(2)	-0.008(2)
C3aA	0.025(2)	0.027(2)	0.028(2)	0.008(1)	0.005(1)	0.004(1)
C4A	0.048(2)	0.030(2)	0.043(2)	0.007(1)	0.011(2)	0.013(1)
C5A	0.066(2)	0.029(2)	0.062(2)	0.017(2)	0.003(2)	0.011(2)
C6A	0.050(2)	0.051(2)	0.067(2)	0.039(2)	0.006(2)	0.004(2)
C7A	0.035(2)	0.049(2)	0.035(2)	0.020(2)	0.013(1)	0.012(1)
C7aA	0.027(2)	0.030(2)	0.036(2)	0.014(1)	0.010(1)	0.006(1)
C8A	0.037(2)	0.052(2)	0.031(2)	0.017(2)	0.004(1)	0.009(1)
C9A	0.030(2)	0.051(2)	0.036(2)	0.016(2)	0.003(1)	0.005(1)
C10A	0.080(3)	0.027(2)	0.055(2)	0.001(2)	-0.002(2)	-0.003(2)
C11A	0.064(2)	0.081(3)	0.034(2)	0.012(2)	-0.009(2)	0.007(2)
C12A	0.047(2)	0.090(3)	0.043(2)	0.031(2)	0.002(2)	0.015(2)
O2B	0.035(1)	0.024(1)	0.030(1)	-0.0010(9)	0.0005(9)	0.0089(8)
C1B	0.024(2)	0.025(2)	0.034(2)	0.001(1)	0.000(1)	-0.001(1)
C2B	0.026(2)	0.020(1)	0.026(2)	-0.001(1)	0.004(1)	0.002(1)
C3B	0.020(2)	0.029(2)	0.026(2)	0.008(1)	0.001(1)	0.003(1)
C3'B	0.026(2)	0.039(2)	0.038(2)	0.010(2)	0.007(1)	0.002(1)
C3aB	0.021(1)	0.024(2)	0.028(2)	0.004(1)	0.003(1)	-0.000(1)
C4B	0.029(2)	0.027(2)	0.037(2)	0.005(1)	0.002(1)	-0.006(1)
C5B	0.049(2)	0.023(2)	0.045(2)	0.004(1)	0.000(2)	-0.005(1)
C6B	0.044(2)	0.026(2)	0.044(2)	-0.005(1)	0.004(2)	0.007(1)
C7B	0.025(2)	0.028(2)	0.040(2)	-0.002(1)	0.008(1)	0.001(1)

Table S2. (continued)

	U11	U22	U33	U23	U13	U12
C7aB	0.020(2)	0.022(2)	0.034(2)	0.001(1)	-0.000(1)	0.002(1)
C8B	0.038(2)	0.027(2)	0.029(2)	-0.002(1)	0.008(1)	-0.001(1)
C9B	0.032(2)	0.027(2)	0.029(2)	0.001(1)	-0.001(1)	-0.001(1)
C10B	0.052(2)	0.030(2)	0.051(2)	0.012(2)	0.007(2)	-0.006(1)
C11B	0.055(2)	0.043(2)	0.040(2)	0.006(2)	0.019(2)	-0.003(2)
C12B	0.058(2)	0.047(2)	0.034(2)	0.002(2)	0.011(2)	0.001(2)
O2C	0.041(1)	0.041(1)	0.037(1)	0.009(1)	0.000(1)	-0.0122(10)
C1C	0.045(2)	0.035(2)	0.038(2)	0.012(1)	0.005(1)	-0.012(1)
C2C	0.050(2)	0.025(2)	0.038(2)	0.009(1)	0.002(2)	-0.003(1)
C3C	0.031(2)	0.027(2)	0.031(2)	0.007(1)	0.001(1)	0.005(1)
C3'C	0.047(2)	0.044(2)	0.043(2)	0.003(2)	0.003(2)	0.009(2)
C3aC	0.024(2)	0.025(2)	0.034(2)	0.007(1)	0.006(1)	-0.001(1)
C4C	0.046(2)	0.030(2)	0.041(2)	0.012(1)	0.006(2)	-0.009(1)
C5C	0.063(2)	0.032(2)	0.061(2)	0.014(2)	0.003(2)	-0.005(2)
C6C	0.048(2)	0.030(2)	0.060(2)	-0.002(2)	0.001(2)	0.001(2)
C7C	0.035(2)	0.033(2)	0.040(2)	-0.001(1)	0.013(1)	-0.003(1)
C7aC	0.023(2)	0.027(2)	0.039(2)	0.005(1)	0.007(1)	-0.003(1)
C8C	0.035(2)	0.037(2)	0.037(2)	0.002(1)	0.003(1)	-0.004(1)
C9C	0.028(2)	0.039(2)	0.048(2)	0.003(2)	0.004(1)	-0.001(1)
C10C	0.081(3)	0.039(2)	0.052(2)	0.024(2)	-0.004(2)	0.000(2)
C11C	0.066(2)	0.064(2)	0.044(2)	0.008(2)	-0.007(2)	-0.005(2)
C12C	0.043(2)	0.058(2)	0.053(2)	-0.004(2)	0.002(2)	-0.010(2)
O2D	0.036(1)	0.031(1)	0.037(1)	0.0129(10)	0.0020(9)	-0.0090(9)
C1D	0.024(2)	0.029(2)	0.040(2)	0.012(1)	0.001(1)	0.001(1)
C2D	0.025(2)	0.025(2)	0.032(2)	0.009(1)	0.004(1)	-0.004(1)
C3D	0.019(2)	0.023(2)	0.031(2)	0.000(1)	0.000(1)	-0.004(1)

Table S2. (continued)

	U11	U22	U33	U23	U13	U12
C3'D	0.024(2)	0.035(2)	0.044(2)	0.007(2)	0.005(2)	-0.001(1)
C3aD	0.022(2)	0.024(2)	0.031(2)	0.004(1)	0.000(1)	-0.000(1)
C4D	0.028(2)	0.026(2)	0.040(2)	0.007(1)	0.002(1)	0.004(1)
C5D	0.048(2)	0.027(2)	0.045(2)	0.013(1)	-0.002(2)	0.004(1)
C6D	0.042(2)	0.036(2)	0.040(2)	0.016(1)	0.002(1)	-0.005(1)
C7D	0.023(2)	0.033(2)	0.043(2)	0.015(1)	0.003(1)	-0.000(1)
C7aD	0.020(2)	0.025(2)	0.033(2)	0.009(1)	-0.002(1)	-0.005(1)
C8D	0.034(2)	0.035(2)	0.033(2)	0.009(1)	0.007(1)	0.004(1)
C9D	0.029(2)	0.028(2)	0.033(2)	0.006(1)	-0.001(1)	0.001(1)
C10D	0.046(2)	0.027(2)	0.055(2)	0.006(2)	0.004(2)	0.006(1)
C11D	0.044(2)	0.040(2)	0.049(2)	0.003(2)	0.015(2)	0.005(2)
C12D	0.052(2)	0.057(2)	0.039(2)	0.007(2)	0.010(2)	0.001(2)

	Uiso	
H(common)	0.055(2)	molecule A
H(common)	0.046(2)	molecule B
H(common)	0.059(2)	molecule C
H(common)	0.043(2)	molecule D

	Atom	x/a	y/b	z/c	S.O.F.	Radius	Minimum	Diagram	Elevation
1	O2A	0.0712	0.4286	0.1005	1.0000	0.76	0.10	1	0.90
2	H1A	0.0795	0.4193	0.0447	1.0000	0.47	0.10	1	1.30
3	C1A	0.1516	0.4593	0.2536	1.0000	0.87	0.10	1	0.72
4	C2A	0.1679	0.4648	0.1560	1.0000	0.87	0.10	1	1.51
5	C3A	0.2598	0.3983	0.1306	1.0000	0.87	0.10	1	2.26
6	C3'A	0.3227	0.4031	0.0652	1.0000	0.87	0.10	1	3.25
7	H5A	0.3844	0.3540	0.0564	1.0000	0.47	0.10	1	3.68
8	H6A	0.3122	0.4516	0.0289	1.0000	0.47	0.10	1	3.55
9	C3aA	0.2690	0.3299	0.1945	1.0000	0.87	0.10	1	1.70
10	C4A	0.2679	0.2215	0.1483	1.0000	0.87	0.10	1	1.63
11	C5A	0.2699	0.1628	0.2230	1.0000	0.87	0.10	1	0.97
12	C6A	0.2035	0.2034	0.3039	1.0000	0.87	0.10	1	0.00
13	C7A	0.2123	0.3143	0.3372	1.0000	0.87	0.10	1	0.23
14	C7aA	0.1739	0.3528	0.2529	1.0000	0.87	0.10	1	0.57
15	C8A	0.3290	0.3513	0.3623	1.0000	0.87	0.10	1	1.22
16	C9A	0.3660	0.3569	0.2675	1.0000	0.87	0.10	1	2.17
17	C10A	0.1761	0.1895	0.0758	1.0000	0.87	0.10	1	1.18
18	C11A	0.3358	0.4508	0.4293	1.0000	0.87	0.10	1	1.18
19	C12A	0.3991	0.2866	0.4110	1.0000	0.87	0.10	1	1.30
20	O2B	0.0805	0.4371	-0.0795	1.0000	0.76	0.10	2	1.87
21	H1B	0.0377	0.4786	-0.0874	1.0000	0.47	0.10	2	1.38
22	C1B	0.1786	0.3055	-0.1676	1.0000	0.87	0.10	2	2.50
23	C2B	0.0746	0.3607	-0.1601	1.0000	0.87	0.10	2	1.51
24	C3B	-0.0099	0.2828	-0.1636	1.0000	0.87	0.10	2	0.84
25	C3'B	-0.0901	0.2914	-0.1113	1.0000	0.87	0.10	2	0.37
26	H5B	-0.1393	0.2355	-0.1122	1.0000	0.47	0.10	2	0.00
27	H6B	-0.1019	0.3513	-0.0649	1.0000	0.47	0.10	2	0.42
28	C3aB	0.0241	0.1963	-0.2331	1.0000	0.87	0.10	2	0.91
29	C4B	-0.0174	0.0944	-0.2319	1.0000	0.87	0.10	2	0.69
30	C5B	0.0332	0.0210	-0.3078	1.0000	0.87	0.10	2	0.86
31	C6B	0.1518	0.0402	-0.3167	1.0000	0.87	0.10	2	1.86
32	C7B	0.1802	0.1480	-0.3086	1.0000	0.87	0.10	2	2.00
33	C7aB	0.1471	0.1991	-0.2144	1.0000	0.87	0.10	2	2.12
34	C8B	0.1126	0.1931	-0.3785	1.0000	0.87	0.10	2	0.95
35	C9B	0.0065	0.2130	-0.3324	1.0000	0.87	0.10	2	0.20
36	C10B	0.0006	0.0659	-0.1398	1.0000	0.87	0.10	2	1.38
37	C11B	0.1639	0.2880	-0.3897	1.0000	0.87	0.10	2	1.22
38	C12B	0.0991	0.1276	-0.4746	1.0000	0.87	0.10	2	0.42
39	O2C	0.4290	0.8794	0.8977	1.0000	0.76	0.10	3	0.88
40	H1C	0.4161	0.8979	0.9522	1.0000	0.47	0.10	3	1.31
41	C1C	0.3479	0.8315	0.7441	1.0000	0.87	0.10	3	0.71
42	C2C	0.3324	0.8864	0.8411	1.0000	0.87	0.10	3	1.49
43	C3C	0.2409	0.8325	0.8685	1.0000	0.87	0.10	3	2.25
44	C3'C	0.1778	0.8698	0.9328	1.0000	0.87	0.10	3	3.24
45	H5C	0.1220	0.8299	0.9487	1.0000	0.47	0.10	3	3.68
46	H6C	0.1851	0.9367	0.9701	1.0000	0.47	0.10	3	3.58
47	C3aC	0.2328	0.7318	0.8077	1.0000	0.87	0.10	3	1.70
48	C4C	0.2363	0.6479	0.8573	1.0000	0.87	0.10	3	1.63
49	C5C	0.2358	0.5521	0.7860	1.0000	0.87	0.10	3	0.97
50	C6C	0.3017	0.5515	0.7046	1.0000	0.87	0.10	3	0.00

51	C7C	0.2901	0.6439	0.6668	1.0000	0.87	0.10	3	0.23
52	C7aC	0.3271	0.7262	0.7485	1.0000	0.87	0.10	3	0.56
53	C8C	0.1728	0.6658	0.6407	1.0000	0.87	0.10	3	1.22
54	C9C	0.1352	0.7189	0.7349	1.0000	0.87	0.10	3	2.18
55	C10C	0.3295	0.6557	0.9306	1.0000	0.87	0.10	3	1.18
56	C11C	0.1645	0.7300	0.5713	1.0000	0.87	0.10	3	1.18
57	C12C	0.1034	0.5752	0.5946	1.0000	0.87	0.10	3	1.31
58	O2D	0.4197	0.9738	0.0797	1.0000	0.76	0.10	4	1.91
59	H1D	0.4650	1.0240	0.0885	1.0000	0.47	0.10	4	1.38
60	C1D	0.3216	0.8855	0.1689	1.0000	0.87	0.10	4	2.53
61	C2D	0.4253	0.9378	0.1609	1.0000	0.87	0.10	4	1.54
62	C3D	0.5102	0.8631	0.1671	1.0000	0.87	0.10	4	0.86
63	C3'D	0.5908	0.8465	0.1154	1.0000	0.87	0.10	4	0.39
64	H5D	0.6409	0.7967	0.1190	1.0000	0.47	0.10	4	0.00
65	H6D	0.6020	0.8840	0.0684	1.0000	0.47	0.10	4	0.45
66	C3aD	0.4760	0.8109	0.2371	1.0000	0.87	0.10	4	0.93
67	C4D	0.5193	0.7098	0.2391	1.0000	0.87	0.10	4	0.69
68	C5D	0.4690	0.6737	0.3160	1.0000	0.87	0.10	4	0.85
69	C6D	0.3496	0.6949	0.3227	1.0000	0.87	0.10	4	1.87
70	C7D	0.3193	0.7973	0.3121	1.0000	0.87	0.10	4	2.03
71	C7aD	0.3536	0.8033	0.2183	1.0000	0.87	0.10	4	2.14
72	C8D	0.3846	0.8784	0.3814	1.0000	0.87	0.10	4	0.99
73	C9D	0.4920	0.8777	0.3362	1.0000	0.87	0.10	4	0.23
74	C10D	0.5016	0.6348	0.1479	1.0000	0.87	0.10	4	1.38
75	C11D	0.3307	0.9765	0.3890	1.0000	0.87	0.10	4	1.30
76	C12D	0.3983	0.8618	0.4790	1.0000	0.87	0.10	4	0.45

Distances

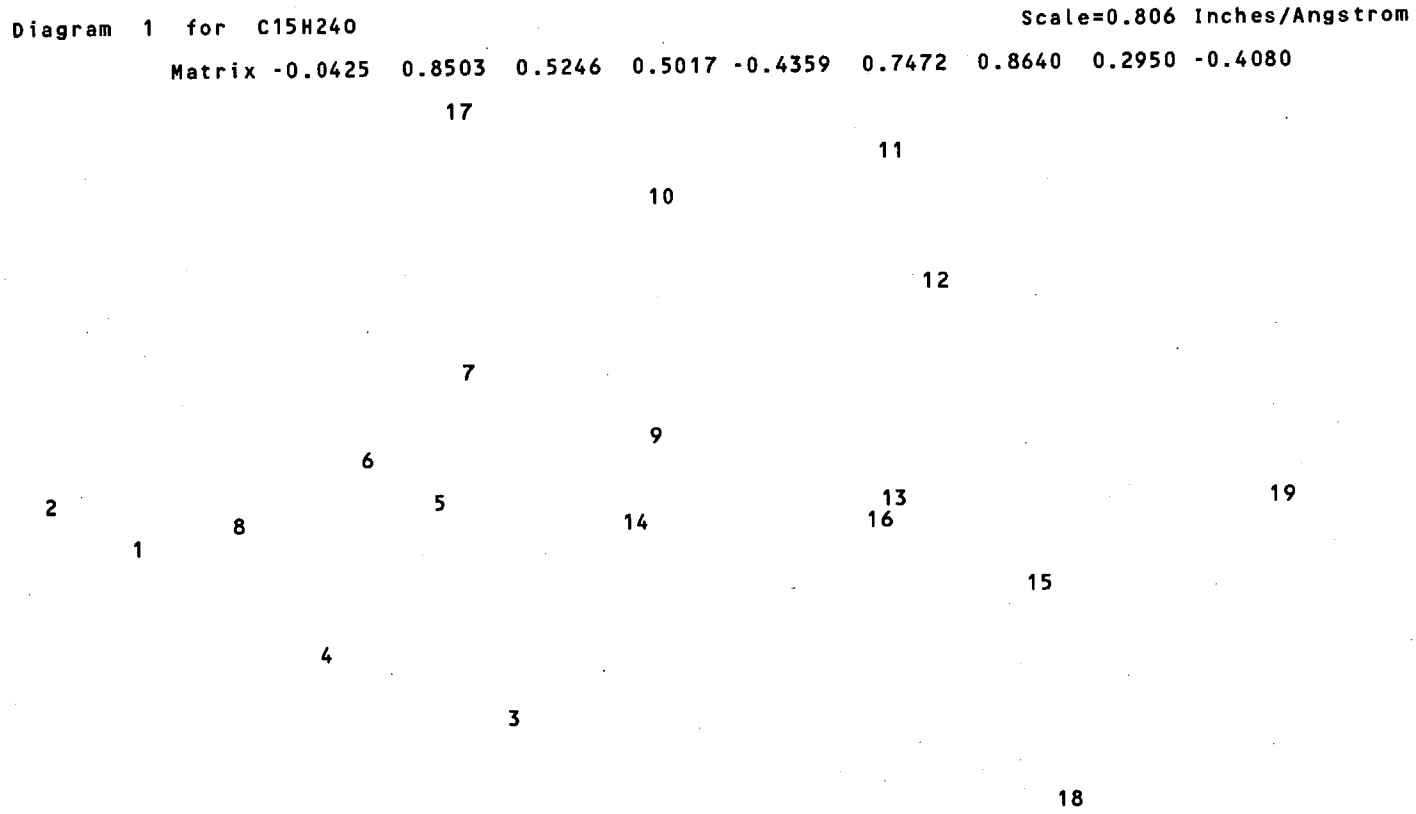
O2A -H1A	0.83(3)	O2A -C2A	1.443(3)	C1A -C2A	1.514(4)
C2A -C3A	1.511(4)	C3A -C3'A	1.322(4)	C3'A-H5A	1.04(3)
C3'A-H6A	0.97(3)	C3A -C3aA	1.507(4)	C3aA-C4A	1.536(4)
C4A -C5A	1.537(4)	C5A -C6A	1.534(5)	C6A -C7A	1.538(4)
C1A -C7aA	1.533(4)	C3aA-C7aA	1.533(4)	C7A -C7aA	1.532(4)
C7A -C8A	1.547(4)	C3aA-C9A	1.560(4)	C8A -C9A	1.552(4)
C4A -C10A	1.517(4)	C8A -C11A	1.536(4)	C8A -C12A	1.534(4)
O2B -H1B	0.82(3)	O2B -C2B	1.428(3)	C1B -C2B	1.524(3)
C2B -C3B	1.520(3)	C3B -C3'B	1.318(4)	C3'B-H5B	1.00(3)
C3'B-H6B	0.99(3)	C3B -C3aB	1.507(4)	C3aB-C4B	1.540(4)
C4B -C5B	1.540(4)	C5B -C6B	1.538(4)	C6B -C7B	1.544(4)
C1B -C7aB	1.549(3)	C3aB-C7aB	1.550(3)	C7B -C7aB	1.527(4)
C7B -C8B	1.546(4)	C3aB-C9B	1.559(4)	C8B -C9B	1.549(4)
C4B -C10B	1.524(4)	C8B -C11B	1.538(4)	C8B -C12B	1.528(4)
O2C -H1C	0.83(3)	O2C -C2C	1.445(3)	C1C -C2C	1.516(4)
C2C -C3C	1.514(4)	C3C -C3'C	1.319(4)	C3'C-H5C	0.98(3)
C3'C-H6C	0.99(3)	C3C -C3aC	1.509(4)	C3aC-C4C	1.538(4)
C4C -C5C	1.528(4)	C5C -C6C	1.530(5)	C6C -C7C	1.543(4)
C1C -C7aC	1.531(4)	C3aC-C7aC	1.530(4)	C7C -C7aC	1.532(4)
C7C -C8C	1.547(4)	C3aC-C9C	1.559(4)	C8C -C9C	1.555(4)

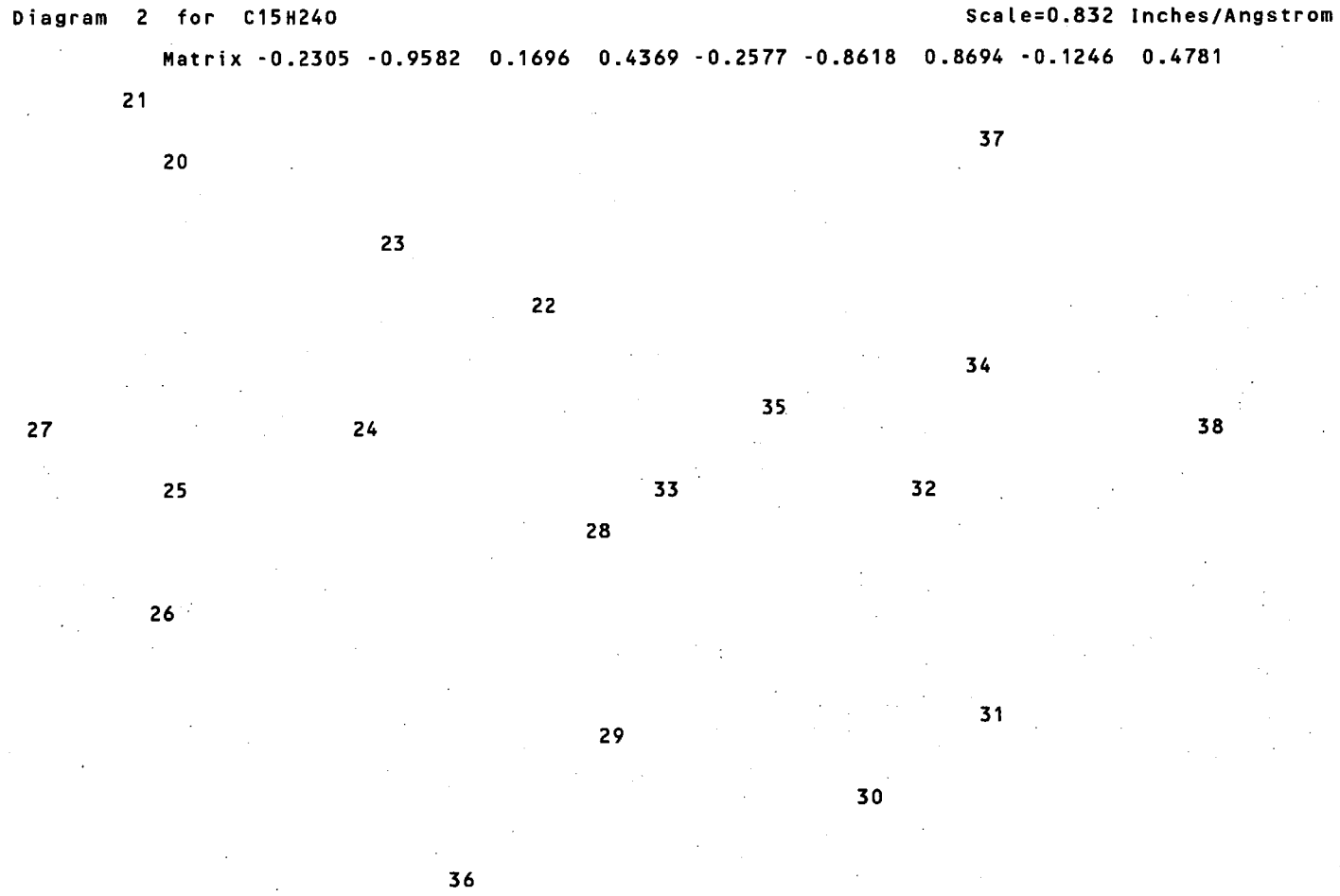
C4C -C10C	1.528(4)	C8C -C11C	1.528(4)	C8C -C12C	1.545(4)
O2D -H1D	0.89(3)	O2D -C2D	1.420(3)	C1D -C2D	1.526(4)
C2D -C3D	1.517(4)	C3D -C3'D	1.317(4)	C3'D-H5D	0.95(3)
C3'D-H6D	0.99(3)	C3D -C3aD	1.502(4)	C3aD-C4D	1.539(4)
C4D -C5D	1.541(4)	C5D -C6D	1.540(4)	C6D -C7D	1.540(4)
C1D -C7aD	1.552(4)	C3aD-C7aD	1.543(3)	C7D -C7aD	1.525(4)
C7D -C8D	1.549(4)	C3aD-C9D	1.571(4)	C8D -C9D	1.560(4)
C4D -C10D	1.533(4)	C8D -C11D	1.532(4)	C8D -C12D	1.532(4)

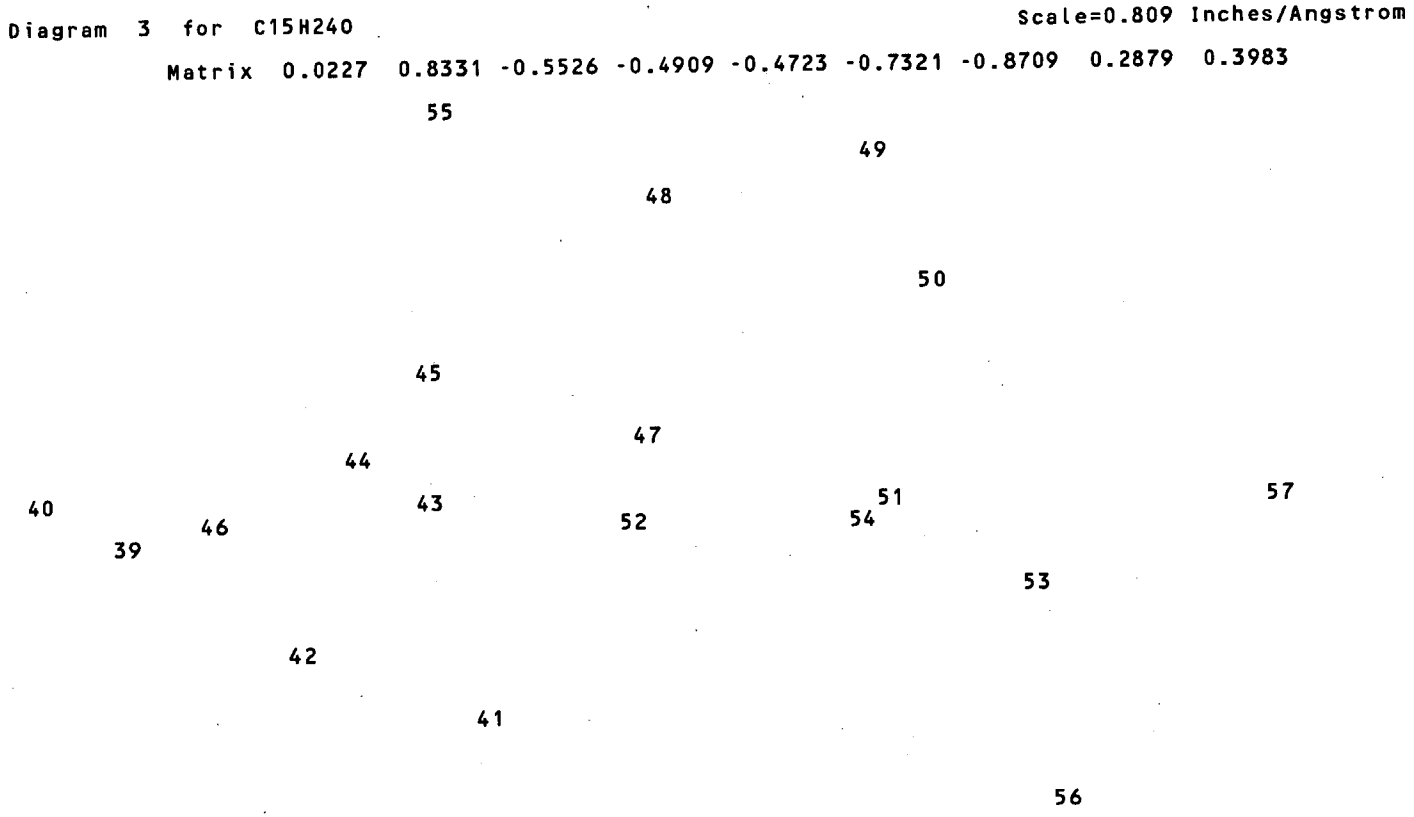
Angles

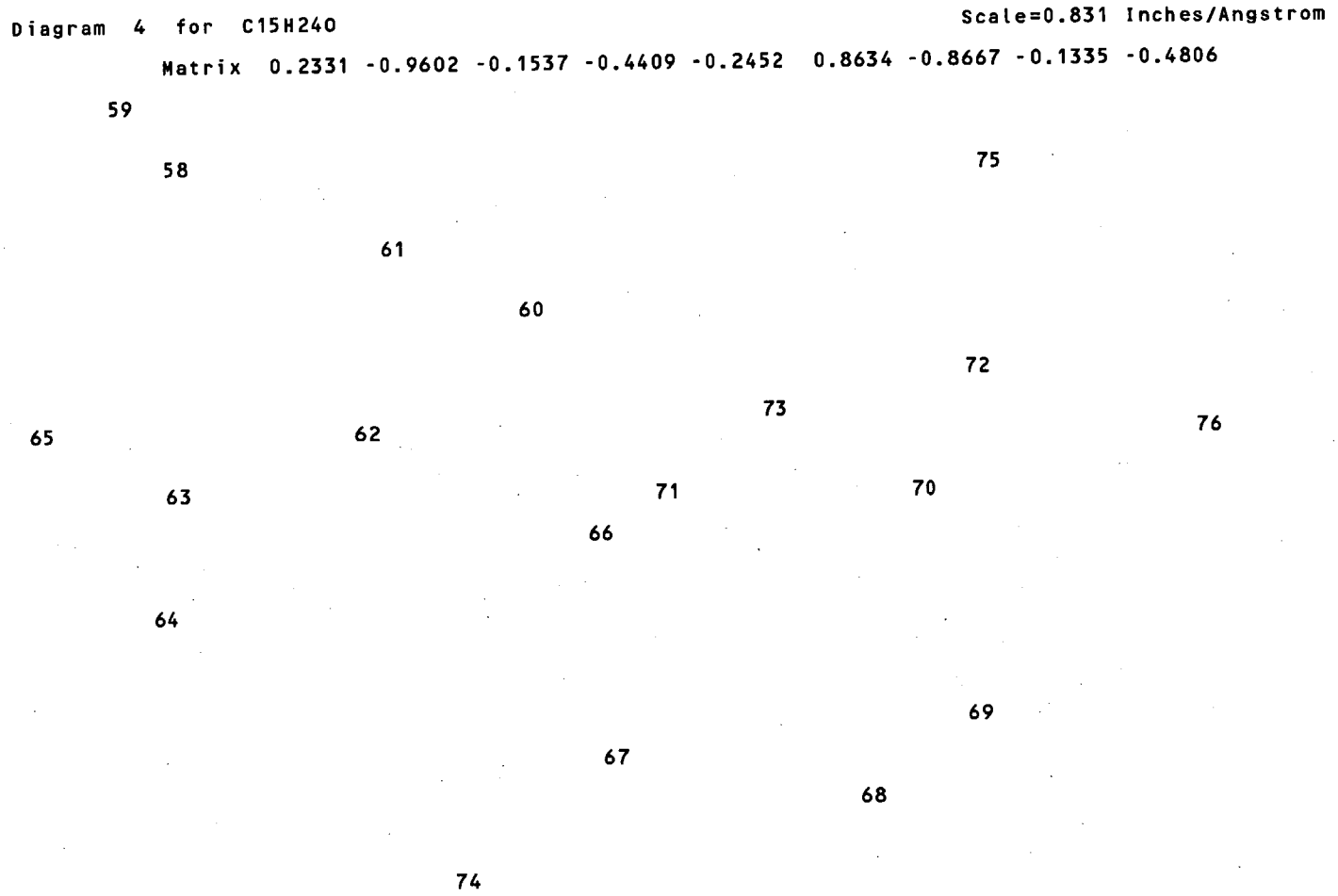
H1A -O2A -C2A	112(2)	C2A -C1A -C7aA	102.6(2)	O2A -C2A -C1A	107.3(2)
O2A -C2A -C3A	111.2(2)	C1A -C2A -C3A	104.2(2)	C2A -C3A -C3'A	124.8(3)
C2A -C3A -C3aA	108.3(2)	C3'A-C3A -C3aA	126.8(3)	C3A -C3'A-H5A	117(2)
C3A -C3'A-H6A	121(2)	H5A -C3'A-H6A	122(2)	C3A -C3aA-C4A	115.9(2)
C3A -C3aA-C7aA	104.8(2)	C3A -C3aA-C9A	111.9(2)	C4A -C3aA-C7aA	110.0(2)
C4A -C3aA-C9A	110.8(2)	C7aA-C3aA-C9A	102.4(2)	C3aA-C4A -C5A	108.8(2)
C3aA-C4A -C10A	114.1(2)	C5A -C4A -C10A	111.6(2)	C4A -C5A -C6A	115.5(2)
C5A -C6A -C7A	113.7(2)	C6A -C7A -C7aA	104.4(2)	C6A -C7A -C8A	112.6(2)
C7aA-C7A -C8A	105.6(2)	C1A -C7aA-C3aA	103.8(2)	C1A -C7aA-C7A	125.0(2)
C3aA-C7aA-C7A	101.2(2)	C7A -C8A -C9A	102.0(2)	C7A -C8A -C11A	111.8(2)
C7A -C8A -C12A	114.2(2)	C9A -C8A -C11A	111.6(2)	C9A -C8A -C12A	113.2(2)
C11A-C8A -C12A	104.3(2)	C3aA-C9A -C8A	108.4(2)	H1B -O2B -C2B	109(2)
C2B -C1B -C7aB	106.0(2)	O2B -C2B -C1B	110.8(2)	O2B -C2B -C3B	115.0(2)
C1B -C2B -C3B	104.1(2)	C2B -C3B -C3'B	125.2(2)	C2B -C3B -C3aB	104.9(2)
C3'B-C3B -C3aB	129.8(2)	C3B -C3'B-H5B	122(2)	C3B -C3'B-H6B	122(2)
H5B -C3'B-H6B	116(2)	C3B -C3aB-C4B	119.6(2)	C3B -C3aB-C7aB	103.1(2)
C3B -C3aB-C9B	111.2(2)	C4B -C3aB-C7aB	108.4(2)	C4B -C3aB-C9B	109.5(2)
C7aB-C3aB-C9B	103.5(2)	C3aB-C4B -C5B	108.0(2)	C3aB-C4B -C10B	115.2(2)
C5B -C4B -C10B	111.0(2)	C4B -C5B -C6B	115.1(2)	C5B -C6B -C7B	113.7(2)
C6B -C7B -C7aB	104.4(2)	C6B -C7B -C8B	112.9(2)	C7aB-C7B -C8B	105.6(2)
C1B -C7aB-C3aB	106.1(2)	C1B -C7aB-C7B	123.5(2)	C3aB-C7aB-C7B	100.8(2)
C7B -C8B -C9B	101.9(2)	C7B -C8B -C11B	111.5(2)	C7B -C8B -C12B	113.4(2)
C9B -C8B -C11B	110.9(2)	C9B -C8B -C12B	113.6(2)	C11B-C8B -C12B	105.8(2)
C3aB-C9B -C8B	108.3(2)	H1C -O2C -C2C	108(2)	C2C -C1C -C7aC	102.6(2)
O2C -C2C -C1C	108.0(2)	O2C -C2C -C3C	110.9(2)	C1C -C2C -C3C	103.9(2)
C2C -C3C -C3'C	124.8(3)	C2C -C3C -C3aC	108.4(2)	C3'C-C3C -C3aC	126.7(3)
C3C -C3'C-H5C	120(2)	C3C -C3'C-H6C	124(2)	H5C -C3'C-H6C	116(2)
C3C -C3aC-C4C	115.9(2)	C3C -C3aC-C7aC	104.7(2)	C3C -C3aC-C9C	112.3(2)
C4C -C3aC-C7aC	110.0(2)	C4C -C3aC-C9C	110.5(2)	C7aC-C3aC-C9C	102.4(2)
C3aC-C4C -C5C	108.9(2)	C3aC-C4C -C10C	113.7(2)	C5C -C4C -C10C	111.9(2)
C4C -C5C -C6C	115.7(2)	C5C -C6C -C7C	113.5(2)	C6C -C7C -C7aC	104.3(2)
C6C -C7C -C8C	112.9(2)	C7aC-C7C -C8C	105.3(2)	C1C -C7aC-C3aC	104.1(2)
C1C -C7aC-C7C	125.5(2)	C3aC-C7aC-C7C	101.4(2)	C7C -C8C -C9C	102.0(2)
C7C -C8C -C11C	111.7(2)	C7C -C8C -C12C	114.4(2)	C9C -C8C -C11C	111.7(2)
C9C -C8C -C12C	112.9(2)	C11C-C8C -C12C	104.5(2)	C3aC-C9C -C8C	108.3(2)
H1D -O2D -C2D	108(2)	C2D -C1D -C7aD	106.0(2)	O2D -C2D -C1D	111.0(2)
O2D -C2D -C3D	115.5(2)	C1D -C2D -C3D	104.0(2)	C2D -C3D -C3'D	124.9(2)
C2D -C3D -C3aD	105.3(2)	C3'D-C3D -C3aD	129.7(2)	C3D -C3'D-H5D	123(2)

C3D -C3'D-H6D	122(2)	H5D -C3'D-H6D	116(2)	C3D -C3aD-C4D	120.0(2)
C3D -C3aD-C7aD	103.6(2)	C3D -C3aD-C9D	110.8(2)	C4D -C3aD-C7aD	109.0(2)
C4D -C3aD-C9D	109.1(2)	C7aD-C3aD-C9D	103.0(2)	C3aD-C4D -C5D	108.4(2)
C3aD-C4D -C10D	114.7(2)	C5D -C4D -C10D	110.5(2)	C4D -C5D -C6D	114.6(2)
C5D -C6D -C7D	113.9(2)	C6D -C7D -C7aD	104.9(2)	C6D -C7D -C8D	113.0(2)
C7aD-C7D -C8D	105.1(2)	C1D -C7aD-C3aD	106.1(2)	C1D -C7aD-C7D	124.2(2)
C3aD-C7aD-C7D	101.5(2)	C7D -C8D -C9D	101.9(2)	C7D -C8D -C11D	111.0(2)
C7D -C8D -C12D	113.9(2)	C9D -C8D -C11D	110.8(2)	C9D -C8D -C12D	113.1(2)
C11D-C8D -C12D	106.1(2)	C3aD-C9D -C8D	107.9(2)		









	Atom	x/a	y/b	z/c	S.O.F.	Radius	Minimum	Diagram	Elevation
1	O2A	0.0712	0.4286	0.1005	1.0000	0.76	0.10	1	1.03
2	H1A	0.0795	0.4193	0.0447	1.0000	0.47	0.10	1	1.36
3	C1A	0.1516	0.4593	0.2536	1.0000	0.87	0.10	1	1.00
4	H2A	0.2007	0.5016	0.2963	1.0000	0.47	0.10	1	1.30
5	H3A	0.0800	0.4754	0.2686	1.0000	0.47	0.10	1	0.35
6	C2A	0.1679	0.4648	0.1560	1.0000	0.87	0.10	1	1.66
7	H4A	0.1826	0.5287	0.1479	1.0000	0.47	0.10	1	1.98
8	C3A	0.2598	0.3983	0.1306	1.0000	0.87	0.10	1	2.42
9	C3'A	0.3227	0.4031	0.0652	1.0000	0.87	0.10	1	3.30
10	H5A	0.3844	0.3540	0.0564	1.0000	0.47	0.10	1	3.76
11	H6A	0.3122	0.4516	0.0289	1.0000	0.47	0.10	1	3.52
12	C3aA	0.2690	0.3299	0.1945	1.0000	0.87	0.10	1	2.00
13	C4A	0.2679	0.2215	0.1483	1.0000	0.87	0.10	1	1.97
14	H7A	0.3306	0.2093	0.1150	1.0000	0.47	0.10	1	2.65
15	C5A	0.2699	0.1628	0.2230	1.0000	0.87	0.10	1	1.47
16	H8A	0.3425	0.1599	0.2464	1.0000	0.47	0.10	1	1.96
17	H9A	0.2436	0.0986	0.1949	1.0000	0.47	0.10	1	1.23
18	C6A	0.2035	0.2034	0.3039	1.0000	0.87	0.10	1	0.58
19	H10A	0.1302	0.1859	0.2855	1.0000	0.47	0.10	1	0.00
20	H11A	0.2271	0.1748	0.3539	1.0000	0.47	0.10	1	0.45
21	C7A	0.2123	0.3143	0.3372	1.0000	0.87	0.10	1	0.74
22	H12A	0.1731	0.3347	0.3905	1.0000	0.47	0.10	1	0.18
23	C7aA	0.1739	0.3528	0.2529	1.0000	0.87	0.10	1	0.94
24	H13A	0.1038	0.3244	0.2364	1.0000	0.47	0.10	1	0.36
25	C8A	0.3290	0.3513	0.3623	1.0000	0.87	0.10	1	1.70
26	C9A	0.3660	0.3569	0.2675	1.0000	0.87	0.10	1	2.52
27	H14A	0.3910	0.4214	0.2694	1.0000	0.47	0.10	1	2.88
28	H15A	0.4224	0.3122	0.2516	1.0000	0.47	0.10	1	2.98
29	C10A	0.1761	0.1895	0.0758	1.0000	0.87	0.10	1	1.48
30	H16A	0.1773	0.2276	0.0304	1.0000	0.47	0.10	1	1.82
31	H17A	0.1098	0.1985	0.1041	1.0000	0.47	0.10	1	0.79
32	H18A	0.1833	0.1223	0.0471	1.0000	0.47	0.10	1	1.53
33	C11A	0.3358	0.4508	0.4293	1.0000	0.87	0.10	1	1.66
34	H19A	0.2937	0.4961	0.4038	1.0000	0.47	0.10	1	1.53
35	H20A	0.4087	0.4732	0.4397	1.0000	0.47	0.10	1	2.28
36	H21A	0.3094	0.4454	0.4864	1.0000	0.47	0.10	1	1.12
37	C12A	0.3991	0.2866	0.4110	1.0000	0.87	0.10	1	1.90
38	H22A	0.3992	0.2222	0.3733	1.0000	0.47	0.10	1	1.94
39	H23A	0.3713	0.2848	0.4685	1.0000	0.47	0.10	1	1.36
40	H24A	0.4706	0.3126	0.4218	1.0000	0.47	0.10	1	2.52

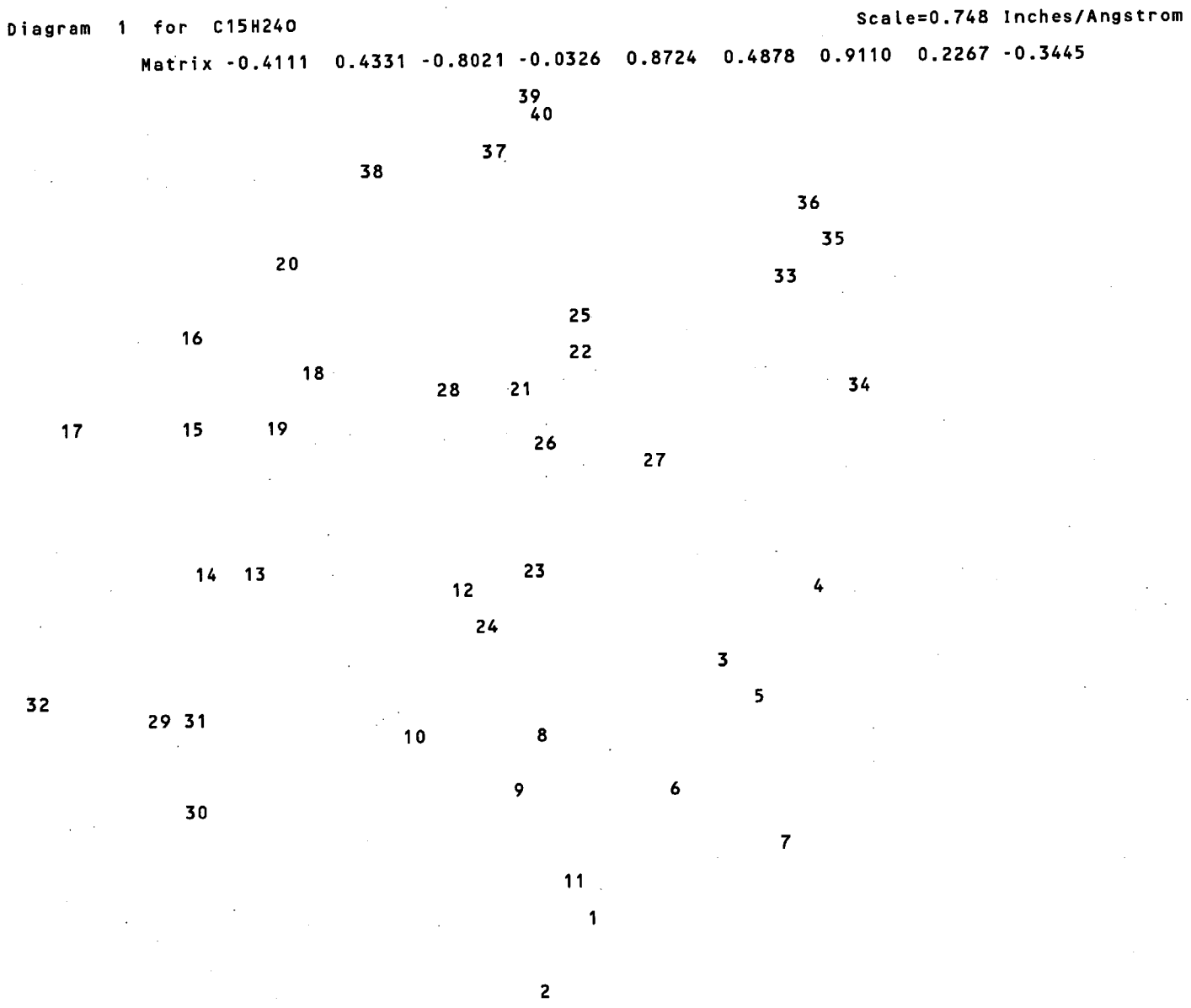
Distances

O2A -H1A	0.83(3)	C1A -H2A	0.957(4)	C1A -H3A	0.962(4)
O2A -C2A	1.443(3)	C1A -C2A	1.514(4)	C2A -H4A	0.960(4)
C2A -C3A	1.511(4)	C3A -C3'A	1.322(4)	C3'A-H5A	1.04(3)
C3'A-H6A	0.97(3)	C3A -C3aA	1.507(4)	C3aA-C4A	1.536(4)

C4A -H7A	0.963(4)	C4A -C5A	1.537(4)	C5A -H8A	0.957(5)
C5A -H9A	0.959(4)	C5A -C6A	1.534(5)	C6A -H10A	0.958(5)
C6A -H11A	0.958(5)	C6A -C7A	1.538(4)	C7A -H12A	0.963(4)
C1A -C7aA	1.533(4)	C3aA-C7aA	1.533(4)	C7A -C7aA	1.532(4)
C7aA-H13A	0.958(4)	C7A -C8A	1.547(4)	C3aA-C9A	1.560(4)
C8A -C9A	1.552(4)	C9A -H14A	0.960(4)	C9A -H15A	0.961(4)
C4A -C10A	1.517(4)	C10A-H16A	0.960(4)	C10A-H17A	0.963(5)
C10A-H18A	0.960(4)	C8A -C11A	1.536(4)	C11A-H19A	0.958(5)
C11A-H20A	0.959(5)	C11A-H21A	0.962(4)	C8A -C12A	1.534(4)
C12A-H22A	0.960(5)	C12A-H23A	0.963(4)	C12A-H24A	0.959(4)

Angles

H1A -O2A -C2A	112(2)	H2A -C1A -H3A	109.3(3)	H2A -C1A -C2A	110.9(3)
H2A -C1A -C7aA	111.3(3)	H3A -C1A -C2A	111.5(3)	H3A -C1A -C7aA	111.1(3)
C2A -C1A -C7aA	102.6(2)	O2A -C2A -C1A	107.3(2)	O2A -C2A -H4A	108.0(3)
O2A -C2A -C3A	111.2(2)	C1A -C2A -H4A	114.9(3)	C1A -C2A -C3A	104.2(2)
H4A -C2A -C3A	111.2(3)	C2A -C3A -C3'A	124.8(3)	C2A -C3A -C3aA	108.3(2)
C3'A-C3A -C3aA	126.8(3)	C3A -C3'A-H5A	117(2)	C3A -C3'A-H6A	121(2)
H5A -C3'A-H6A	122(2)	C3A -C3aA-C4A	115.9(2)	C3A -C3aA-C7aA	104.8(2)
C3A -C3aA-C9A	111.9(2)	C4A -C3aA-C7aA	110.0(2)	C4A -C3aA-C9A	110.8(2)
C7aA-C3aA-C9A	102.4(2)	C3aA-C4A -H7A	107.6(3)	C3aA-C4A -C5A	108.8(2)
C3aA-C4A -C10A	114.1(2)	H7A -C4A -C5A	110.4(3)	H7A -C4A -C10A	104.2(3)
C5A -C4A -C10A	111.6(2)	C4A -C5A -H8A	107.7(3)	C4A -C5A -H9A	108.1(3)
C4A -C5A -C6A	115.5(2)	H8A -C5A -H9A	109.3(4)	H8A -C5A -C6A	108.2(3)
H9A -C5A -C6A	107.9(3)	C5A -C6A -H10A	108.7(4)	C5A -C6A -H11A	108.4(3)
C5A -C6A -C7A	113.7(2)	H10A-C6A -H11A	109.1(4)	H10A-C6A -C7A	108.3(3)
H11A-C6A -C7A	108.5(3)	C6A -C7A -H12A	109.7(3)	C6A -C7A -C7aA	104.4(2)
C6A -C7A -C8A	112.6(2)	H12A-C7A -C7aA	116.1(3)	H12A-C7A -C8A	108.4(3)
C7aA-C7A -C8A	105.6(2)	C1A -C7aA-C3aA	103.8(2)	C1A -C7aA-C7A	125.0(2)
C1A -C7aA-H13A	100.9(3)	C3aA-C7aA-C7A	101.2(2)	C3aA-C7aA-H13A	125.0(3)
C7A -C7aA-H13A	103.4(3)	C7A -C8A -C9A	102.0(2)	C7A -C8A -C11A	111.8(2)
C7A -C8A -C12A	114.2(2)	C9A -C8A -C11A	111.6(2)	C9A -C8A -C12A	113.2(2)
C11A-C8A -C12A	104.3(2)	C3aA-C9A -C8A	108.4(2)	C3aA-C9A -H14A	109.7(3)
C3aA-C9A -H15A	109.6(3)	C8A -C9A -H14A	109.8(3)	C8A -C9A -H15A	110.0(3)
H14A-C9A -H15A	109.4(4)	C4A -C10A-H16A	109.3(3)	C4A -C10A-H17A	109.4(3)
C4A -C10A-H18A	109.4(3)	H16A-C10A-H17A	109.7(4)	H16A-C10A-H18A	109.4(4)
H17A-C10A-H18A	109.6(4)	C8A -C11A-H19A	109.7(3)	C8A -C11A-H20A	109.2(3)
C8A -C11A-H21A	109.5(3)	H19A-C11A-H20A	109.3(4)	H19A-C11A-H21A	109.3(4)
H20A-C11A-H21A	109.8(4)	C8A -C12A-H22A	109.7(3)	C8A -C12A-H23A	109.3(3)
C8A -C12A-H24A	109.3(4)	H22A-C12A-H23A	109.5(4)	H22A-C12A-H24A	109.2(4)
H23A-C12A-H24A	109.8(4)				



	Atom	x/a	y/b	z/c	S.O.F.	Radius	Minimum	Diagram	Elevation
1	O2B	0.0805	0.4371	-0.0795	1.0000	0.76	0.10	1	0.88
2	H1B	0.0377	0.4786	-0.0874	1.0000	0.47	0.10	1	1.24
3	C1B	0.1786	0.3055	-0.1676	1.0000	0.87	0.10	1	0.57
4	H2B	0.2252	0.3318	-0.2042	1.0000	0.47	0.10	1	0.35
5	H3B	0.2133	0.3091	-0.1079	1.0000	0.47	0.10	1	0.00
6	C2B	0.0746	0.3607	-0.1601	1.0000	0.87	0.10	1	1.34
7	H4B	0.0581	0.3940	-0.2084	1.0000	0.47	0.10	1	1.69
8	C3B	-0.0099	0.2828	-0.1636	1.0000	0.87	0.10	1	2.08
9	C3'B	-0.0901	0.2914	-0.1113	1.0000	0.87	0.10	1	2.48
10	H5B	-0.1393	0.2355	-0.1122	1.0000	0.47	0.10	1	2.91
11	H6B	-0.1019	0.3513	-0.0649	1.0000	0.47	0.10	1	2.32
12	C3aB	0.0241	0.1963	-0.2331	1.0000	0.87	0.10	1	2.18
13	C4B	-0.0174	0.0944	-0.2319	1.0000	0.87	0.10	1	2.56
14	H7B	-0.0935	0.0946	-0.2425	1.0000	0.47	0.10	1	3.23
15	C5B	0.0332	0.0210	-0.3078	1.0000	0.87	0.10	1	2.55
16	H8B	-0.0051	0.0222	-0.3651	1.0000	0.47	0.10	1	3.13
17	H9B	0.0261	-0.0422	-0.2952	1.0000	0.47	0.10	1	2.58
18	C6B	0.1518	0.0402	-0.3167	1.0000	0.87	0.10	1	1.62
19	H10B	0.1928	0.0181	-0.2692	1.0000	0.47	0.10	1	1.07
20	H11B	0.1704	0.0041	-0.3755	1.0000	0.47	0.10	1	1.77
21	C7B	0.1802	0.1480	-0.3086	1.0000	0.87	0.10	1	1.30
22	H12B	0.2540	0.1545	-0.3188	1.0000	0.47	0.10	1	0.75
23	C7aB	0.1471	0.1991	-0.2144	1.0000	0.87	0.10	1	1.10
24	H13B	0.1834	0.1666	-0.1718	1.0000	0.47	0.10	1	0.61
25	C8B	0.1126	0.1931	-0.3785	1.0000	0.87	0.10	1	2.16
26	C9B	0.0065	0.2130	-0.3324	1.0000	0.87	0.10	1	2.79
27	H14B	-0.0140	0.2787	-0.3301	1.0000	0.47	0.10	1	2.91
28	H15B	-0.0482	0.1696	-0.3665	1.0000	0.47	0.10	1	3.41
29	C10B	0.0006	0.0659	-0.1398	1.0000	0.87	0.10	1	1.99
30	H16B	-0.0317	0.1126	-0.0935	1.0000	0.47	0.10	1	2.01
31	H17B	0.0756	0.0641	-0.1239	1.0000	0.47	0.10	1	1.31
32	H18B	-0.0310	0.0031	-0.1442	1.0000	0.47	0.10	1	2.30
33	C11B	0.1639	0.2880	-0.3897	1.0000	0.87	0.10	1	1.75
34	H19B	0.1742	0.3321	-0.3309	1.0000	0.47	0.10	1	1.37
35	H20B	0.1180	0.3165	-0.4299	1.0000	0.47	0.10	1	2.30
36	H21B	0.2315	0.2745	-0.4152	1.0000	0.47	0.10	1	1.33
37	C12B	0.0991	0.1276	-0.4746	1.0000	0.87	0.10	1	2.76
38	H22B	0.0672	0.0669	-0.4716	1.0000	0.47	0.10	1	3.03
39	H23B	0.1676	0.1163	-0.4990	1.0000	0.47	0.10	1	2.32
40	H24B	0.0542	0.1583	-0.5137	1.0000	0.47	0.10	1	3.29

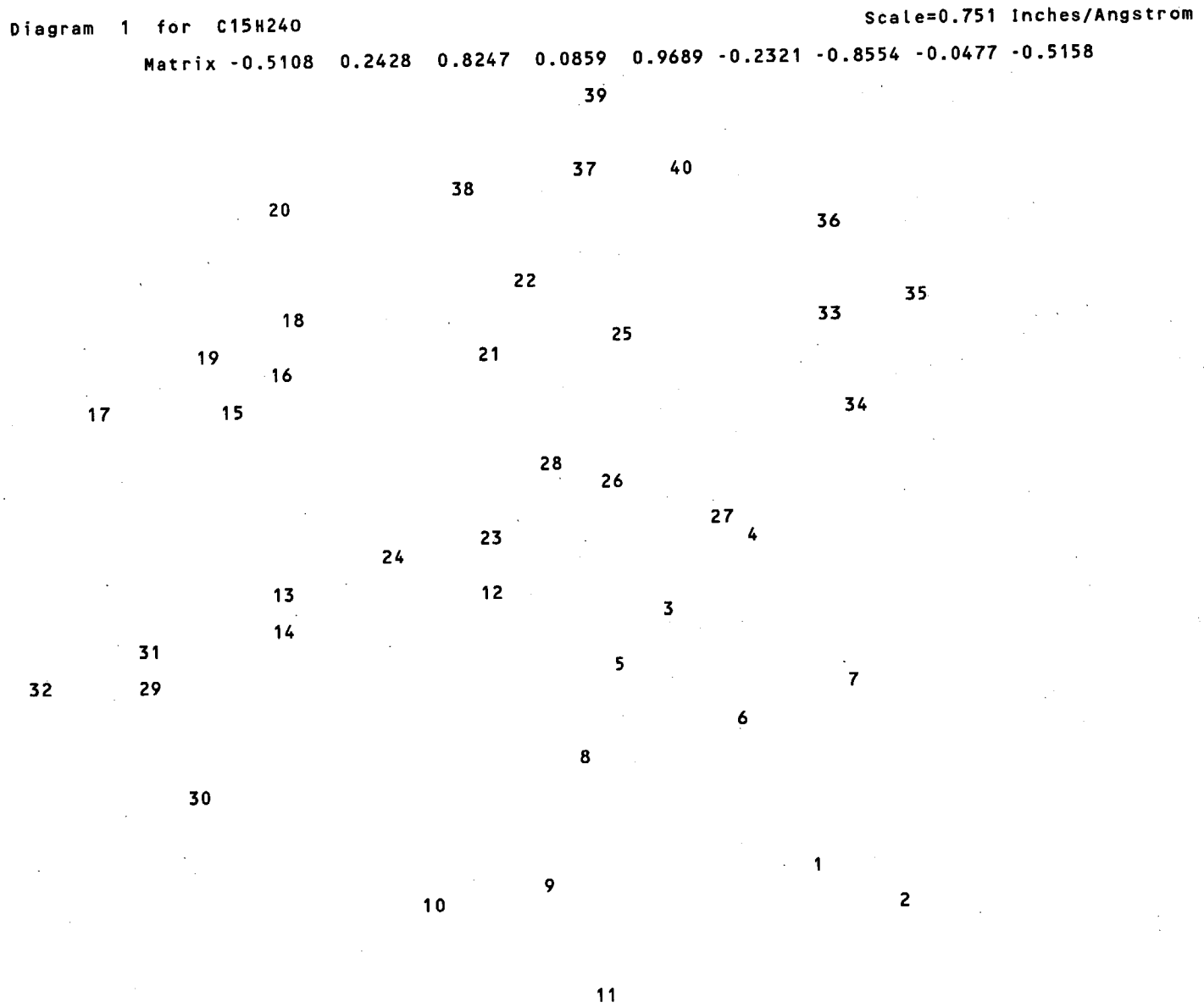
Distances

O2B -H1B	0.82(3)	C1B -H2B	0.963(4)	C1B -H3B	0.957(4)
O2B -C2B	1.428(3)	C1B -C2B	1.524(3)	C2B -H4B	0.959(3)
C2B -C3B	1.520(3)	C3B -C3'B	1.318(4)	C3'B-H5B	1.00(3)
C3'B-H6B	0.99(3)	C3B -C3aB	1.507(4)	C3aB-C4B	1.540(4)

C4B -H7B	0.959(4)	C4B -C5B	1.540(4)	C5B -H8B	0.956(4)
C5B -H9B	0.960(4)	C5B -C6B	1.538(4)	C6B -H10B	0.957(4)
C6B -H11B	0.962(4)	C6B -C7B	1.544(4)	C7B -H12B	0.961(4)
C1B -C7aB	1.549(3)	C3aB-C7aB	1.550(3)	C7B -C7aB	1.527(4)
C7aB-H13B	0.958(4)	C7B -C8B	1.546(4)	C3aB-C9B	1.559(4)
C8B -C9B	1.549(4)	C9B -H14B	0.960(4)	C9B -H15B	0.957(4)
C4B -C10B	1.524(4)	C10B-H16B	0.962(4)	C10B-H17B	0.958(4)
C10B-H18B	0.960(4)	C8B -C11B	1.538(4)	C11B-H19B	0.959(4)
C11B-H20B	0.957(4)	C11B-H21B	0.963(4)	C8B -C12B	1.528(4)
C12B-H22B	0.960(4)	C12B-H23B	0.963(4)	C12B-H24B	0.957(4)

Angles

H1B -O2B -C2B	109(2)	H2B -C1B -H3B	109.6(3)	H2B -C1B -C2B	110.6(3)
H2B -C1B -C7aB	110.3(3)	H3B -C1B -C2B	110.1(3)	H3B -C1B -C7aB	110.2(3)
C2B -C1B -C7aB	106.0(2)	O2B -C2B -C1B	110.8(2)	O2B -C2B -H4B	103.1(2)
O2B -C2B -C3B	115.0(2)	C1B -C2B -H4B	114.3(3)	C1B -C2B -C3B	104.1(2)
H4B -C2B -C3B	110.0(3)	C2B -C3B -C3'B	125.2(2)	C2B -C3B -C3aB	104.9(2)
C3'B-C3B -C3aB	129.8(2)	C3B -C3'B-H5B	122(2)	C3B -C3'B-H6B	122(2)
H5B -C3'B-H6B	116(2)	C3B -C3aB-C4B	119.6(2)	C3B -C3aB-C7aB	103.1(2)
C3B -C3aB-C9B	111.2(2)	C4B -C3aB-C7aB	108.4(2)	C4B -C3aB-C9B	109.5(2)
C7aB-C3aB-C9B	103.5(2)	C3aB-C4B -H7B	107.0(3)	C3aB-C4B -C5B	108.0(2)
C3aB-C4B -C10B	115.2(2)	H7B -C4B -C5B	111.8(3)	H7B -C4B -C10B	103.7(3)
C5B -C4B -C10B	111.0(2)	C4B -C5B -H8B	108.1(3)	C4B -C5B -H9B	108.0(3)
C4B -C5B -C6B	115.1(2)	H8B -C5B -H9B	109.5(4)	H8B -C5B -C6B	107.8(3)
H9B -C5B -C6B	108.2(3)	C5B -C6B -H10B	108.1(3)	C5B -C6B -H11B	108.8(3)
C5B -C6B -C7B	113.7(2)	H10B-C6B -H11B	109.3(4)	H10B-C6B -C7B	108.6(3)
H11B-C6B -C7B	108.3(3)	C6B -C7B -H12B	109.5(3)	C6B -C7B -C7aB	104.4(2)
C6B -C7B -C8B	112.9(2)	H12B-C7B -C7aB	116.4(3)	H12B-C7B -C8B	108.1(3)
C7aB-C7B -C8B	105.6(2)	C1B -C7aB-C3aB	106.1(2)	C1B -C7aB-C7B	123.5(2)
C1B -C7aB-H13B	99.9(3)	C3aB-C7aB-C7B	100.8(2)	C3aB-C7aB-H13B	122.8(3)
C7B -C7aB-H13B	105.6(3)	C7B -C8B -C9B	101.9(2)	C7B -C8B -C11B	111.5(2)
C7B -C8B -C12B	113.4(2)	C9B -C8B -C11B	110.9(2)	C9B -C8B -C12B	113.6(2)
C11B-C8B -C12B	105.8(2)	C3aB-C9B -C8B	108.3(2)	C3aB-C9B -H14B	109.7(3)
C3aB-C9B -H15B	109.6(3)	C8B -C9B -H14B	109.9(3)	C8B -C9B -H15B	109.8(3)
H14B-C9B -H15B	109.6(3)	C4B -C10B-H16B	109.6(3)	C4B -C10B-H17B	109.1(3)
C4B -C10B-H18B	109.7(3)	H16B-C10B-H17B	109.8(4)	H16B-C10B-H18B	109.3(4)
H17B-C10B-H18B	109.4(4)	C8B -C11B-H19B	109.3(3)	C8B -C11B-H20B	109.6(3)
C8B -C11B-H21B	109.5(3)	H19B-C11B-H20B	109.2(4)	H19B-C11B-H21B	109.8(4)
H20B-C11B-H21B	109.3(4)	C8B -C12B-H22B	109.3(3)	C8B -C12B-H23B	109.8(3)
C8B -C12B-H24B	109.2(3)	H22B-C12B-H23B	109.5(4)	H22B-C12B-H24B	109.6(4)
H23B-C12B-H24B	109.3(4)				



	Atom	x/a	y/b	z/c	S.O.F.	Radius	Minimum	Diagram	Elevation
1	O2C	0.4290	0.8794	0.8977	1.0000	0.76	0.10	1	1.00
2	H1C	0.4161	0.8979	0.9522	1.0000	0.47	0.10	1	1.37
3	C1C	0.3479	0.8315	0.7441	1.0000	0.87	0.10	1	0.98
4	H2C	0.2979	0.8514	0.7009	1.0000	0.47	0.10	1	1.29
5	H3C	0.4191	0.8406	0.7281	1.0000	0.47	0.10	1	0.33
6	C2C	0.3324	0.8864	0.8411	1.0000	0.87	0.10	1	1.63
7	H4C	0.3180	0.9540	0.8470	1.0000	0.47	0.10	1	1.94
8	C3C	0.2409	0.8325	0.8685	1.0000	0.87	0.10	1	2.41
9	C3'C	0.1778	0.8698	0.9328	1.0000	0.87	0.10	1	3.29
10	H5C	0.1220	0.8299	0.9487	1.0000	0.47	0.10	1	3.75
11	H6C	0.1851	0.9367	0.9701	1.0000	0.47	0.10	1	3.53
12	C3aC	0.2328	0.7318	0.8077	1.0000	0.87	0.10	1	2.00
13	C4C	0.2363	0.6479	0.8573	1.0000	0.87	0.10	1	1.97
14	H7C	0.1739	0.6512	0.8910	1.0000	0.47	0.10	1	2.65
15	C5C	0.2358	0.5521	0.7860	1.0000	0.87	0.10	1	1.47
16	H8C	0.1633	0.5362	0.7628	1.0000	0.47	0.10	1	1.97
17	H9C	0.2629	0.5032	0.8162	1.0000	0.47	0.10	1	1.24
18	C6C	0.3017	0.5515	0.7046	1.0000	0.87	0.10	1	0.58
19	H10C	0.3754	0.5454	0.7236	1.0000	0.47	0.10	1	0.00
20	H11C	0.2794	0.4967	0.6564	1.0000	0.47	0.10	1	0.45
21	C7C	0.2901	0.6439	0.6668	1.0000	0.87	0.10	1	0.74
22	H12C	0.3289	0.6370	0.6130	1.0000	0.47	0.10	1	0.18
23	C7aC	0.3271	0.7262	0.7485	1.0000	0.87	0.10	1	0.94
24	H13C	0.3978	0.7078	0.7655	1.0000	0.47	0.10	1	0.35
25	C8C	0.1728	0.6658	0.6407	1.0000	0.87	0.10	1	1.70
26	C9C	0.1352	0.7189	0.7349	1.0000	0.87	0.10	1	2.53
27	H14C	0.1082	0.7812	0.7308	1.0000	0.47	0.10	1	2.89
28	H15C	0.0802	0.6812	0.7524	1.0000	0.47	0.10	1	2.98
29	C10C	0.3295	0.6557	0.9306	1.0000	0.87	0.10	1	1.47
30	H16C	0.3270	0.7167	0.9740	1.0000	0.47	0.10	1	1.81
31	H17C	0.3956	0.6515	0.9019	1.0000	0.47	0.10	1	0.78
32	H18C	0.3241	0.6039	0.9618	1.0000	0.47	0.10	1	1.52
33	C11C	0.1645	0.7300	0.5713	1.0000	0.87	0.10	1	1.65
34	H19C	0.2058	0.7884	0.5950	1.0000	0.47	0.10	1	1.52
35	H20C	0.0913	0.7459	0.5604	1.0000	0.47	0.10	1	2.28
36	H21C	0.1911	0.6960	0.5148	1.0000	0.47	0.10	1	1.12
37	C12C	0.1034	0.5752	0.5946	1.0000	0.87	0.10	1	1.91
38	H22C	0.1045	0.5307	0.6343	1.0000	0.47	0.10	1	1.96
39	H23C	0.1313	0.5445	0.5376	1.0000	0.47	0.10	1	1.37
40	H24C	0.0315	0.5944	0.5832	1.0000	0.47	0.10	1	2.53

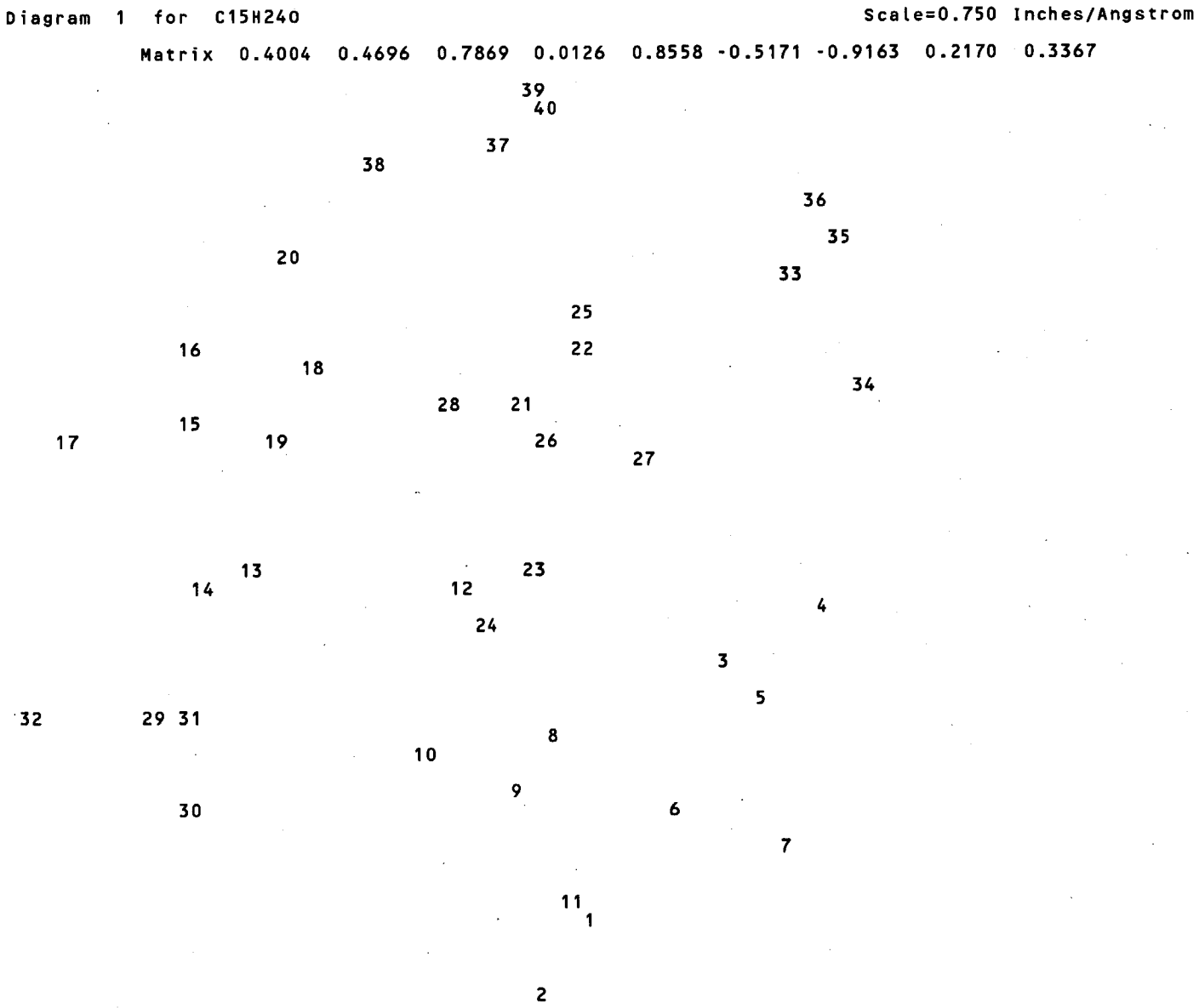
Distances

O2C -H1C	0.83(3)	C1C -H2C	0.956(4)	C1C -H3C	0.962(4)
O2C -C2C	1.445(3)	C1C -C2C	1.516(4)	C2C -H4C	0.960(4)
C2C -C3C	1.514(4)	C3C -C3'C	1.319(4)	C3'C-H5C	0.98(3)
C3'C-H6C	0.99(3)	C3C -C3aC	1.509(4)	C3aC-C4C	1.538(4)

C4C -H7C	0.963(4)	C4C -C5C	1.528(4)	C5C -H8C	0.957(5)
C5C -H9C	0.959(4)	C5C -C6C	1.530(5)	C6C -H10C	0.958(4)
C6C -H11C	0.958(4)	C6C -C7C	1.543(4)	C7C -H12C	0.963(4)
C1C -C7aC	1.531(4)	C3aC-C7aC	1.530(4)	C7C -C7aC	1.532(4)
C7aC-H13C	0.958(4)	C7C -C8C	1.547(4)	C3aC-C9C	1.559(4)
C8C -C9C	1.555(4)	C9C -H14C	0.960(4)	C9C -H15C	0.961(4)
C4C -C10C	1.528(4)	C10C-H16C	0.960(4)	C10C-H17C	0.963(5)
C10C-H18C	0.960(4)	C8C -C11C	1.528(4)	C11C-H19C	0.958(5)
C11C-H20C	0.959(5)	C11C-H21C	0.963(5)	C8C -C12C	1.545(4)
C12C-H22C	0.960(4)	C12C-H23C	0.963(4)	C12C-H24C	0.959(4)

Angles

H1C -O2C -C2C	108(2)	H2C -C1C -H3C	109.3(4)	H2C -C1C -C2C	110.9(3)
H2C -C1C -C7aC	111.3(3)	H3C -C1C -C2C	111.5(3)	H3C -C1C -C7aC	111.1(3)
C2C -C1C -C7aC	102.6(2)	O2C -C2C -C1C	108.0(2)	O2C -C2C -H4C	107.6(3)
O2C -C2C -C3C	110.9(2)	C1C -C2C -H4C	114.5(3)	C1C -C2C -C3C	103.9(2)
H4C -C2C -C3C	111.9(3)	C2C -C3C -C3'C	124.8(3)	C2C -C3C -C3aC	108.4(2)
C3'C-C3C -C3aC	126.7(3)	C3C -C3'C-H5C	120(2)	C3C -C3'C-H6C	124(2)
H5C -C3'C-H6C	116(2)	C3C -C3aC-C4C	115.9(2)	C3C -C3aC-C7aC	104.7(2)
C3C -C3aC-C9C	112.3(2)	C4C -C3aC-C7aC	110.0(2)	C4C -C3aC-C9C	110.5(2)
C7aC-C3aC-C9C	102.4(2)	C3aC-C4C -H7C	107.9(3)	C3aC-C4C -C5C	108.9(2)
C3aC-C4C -C10C	113.7(2)	H7C -C4C -C5C	110.0(3)	H7C -C4C -C10C	104.3(3)
C5C -C4C -C10C	111.9(2)	C4C -C5C -H8C	107.7(3)	C4C -C5C -H9C	108.1(3)
C4C -C5C -C6C	115.7(2)	H8C -C5C -H9C	109.3(4)	H8C -C5C -C6C	108.2(3)
H9C -C5C -C6C	107.9(3)	C5C -C6C -H10C	108.7(3)	C5C -C6C -H11C	108.5(3)
C5C -C6C -C7C	113.5(2)	H10C-C6C -H11C	109.2(4)	H10C-C6C -C7C	108.3(3)
H11C-C6C -C7C	108.6(3)	C6C -C7C -H12C	109.5(3)	C6C -C7C -C7aC	104.3(2)
C6C -C7C -C8C	112.9(2)	H12C-C7C -C7aC	116.5(3)	H12C-C7C -C8C	108.4(3)
C7aC-C7C -C8C	105.3(2)	C1C -C7aC-C3aC	104.1(2)	C1C -C7aC-C7C	125.5(2)
C1C -C7aC-H13C	100.4(3)	C3aC-C7aC-C7C	101.4(2)	C3aC-C7aC-H13C	125.1(3)
C7C -C7aC-H13C	103.0(3)	C7C -C8C -C9C	102.0(2)	C7C -C8C -C11C	111.7(2)
C7C -C8C -C12C	114.4(2)	C9C -C8C -C11C	111.7(2)	C9C -C8C -C12C	112.9(2)
C11C-C8C -C12C	104.5(2)	C3aC-C9C -C8C	108.3(2)	C3aC-C9C -H14C	109.7(3)
C3aC-C9C -H15C	109.6(3)	C8C -C9C -H14C	109.8(3)	C8C -C9C -H15C	110.0(3)
H14C-C9C -H15C	109.4(3)	C4C -C10C-H16C	109.3(3)	C4C -C10C-H17C	109.4(3)
C4C -C10C-H18C	109.4(3)	H16C-C10C-H17C	109.7(4)	H16C-C10C-H18C	109.4(4)
H17C-C10C-H18C	109.6(4)	C8C -C11C-H19C	109.7(3)	C8C -C11C-H20C	109.2(3)
C8C -C11C-H21C	109.5(3)	H19C-C11C-H20C	109.3(4)	H19C-C11C-H21C	109.3(4)
H20C-C11C-H21C	109.8(4)	C8C -C12C-H22C	109.7(3)	C8C -C12C-H23C	109.3(3)
C8C -C12C-H24C	109.3(3)	H22C-C12C-H23C	109.5(4)	H22C-C12C-H24C	109.2(4)
H23C-C12C-H24C	109.8(4)				



	Atom	x/a	y/b	z/c	S.O.F.	Radius	Minimum Diagram		Elevation
1	O2D	0.4197	0.9738	0.0797	1.0000	0.76	0.10	1	2.20
2	H1D	0.4650	1.0240	0.0885	1.0000	0.47	0.10	1	1.71
3	C1D	0.3216	0.8855	0.1689	1.0000	0.87	0.10	1	2.68
4	H2D	0.2742	0.9293	0.2043	1.0000	0.47	0.10	1	2.79
5	H3D	0.2875	0.8588	0.1092	1.0000	0.47	0.10	1	3.29
6	C2D	0.4253	0.9378	0.1609	1.0000	0.87	0.10	1	1.83
7	H4D	0.4411	0.9951	0.2080	1.0000	0.47	0.10	1	1.37
8	C3D	0.5102	0.8631	0.1671	1.0000	0.87	0.10	1	1.29
9	C3'D	0.5908	0.8465	0.1154	1.0000	0.87	0.10	1	0.95
10	H5D	0.6409	0.7967	0.1190	1.0000	0.47	0.10	1	0.65
11	H6D	0.6020	0.8840	0.0684	1.0000	0.47	0.10	1	1.03
12	C3aD	0.4760	0.8109	0.2371	1.0000	0.87	0.10	1	1.30
13	C4D	0.5193	0.7098	0.2391	1.0000	0.87	0.10	1	1.15
14	H7D	0.5952	0.7168	0.2504	1.0000	0.47	0.10	1	0.50
15	C5D	0.4690	0.6737	0.3160	1.0000	0.87	0.10	1	1.23
16	H8D	0.5061	0.7044	0.3733	1.0000	0.47	0.10	1	0.61
17	H9D	0.4777	0.6049	0.3053	1.0000	0.47	0.10	1	1.35
18	C6D	0.3496	0.6949	0.3227	1.0000	0.87	0.10	1	2.07
19	H10D	0.3102	0.6486	0.2752	1.0000	0.47	0.10	1	2.69
20	H11D	0.3302	0.6876	0.3815	1.0000	0.47	0.10	1	1.95
21	C7D	0.3193	0.7973	0.3121	1.0000	0.87	0.10	1	2.16
22	H12D	0.2450	0.8065	0.3211	1.0000	0.47	0.10	1	2.67
23	C7aD	0.3536	0.8033	0.2183	1.0000	0.87	0.10	1	2.35
24	H13D	0.3176	0.7496	0.1765	1.0000	0.47	0.10	1	2.93
25	C8D	0.3846	0.8784	0.3814	1.0000	0.87	0.10	1	1.17
26	C9D	0.4920	0.8777	0.3362	1.0000	0.87	0.10	1	0.57
27	H14D	0.5114	0.9422	0.3328	1.0000	0.47	0.10	1	0.32
28	H15D	0.5470	0.8524	0.3716	1.0000	0.47	0.10	1	0.02
29	C10D	0.5016	0.6348	0.1479	1.0000	0.87	0.10	1	1.88
30	H16D	0.5334	0.6583	0.1006	1.0000	0.47	0.10	1	1.82
31	H17D	0.4266	0.6242	0.1322	1.0000	0.47	0.10	1	2.55
32	H18D	0.5338	0.5749	0.1538	1.0000	0.47	0.10	1	1.71
33	C11D	0.3307	0.9765	0.3890	1.0000	0.87	0.10	1	1.36
34	H19D	0.3203	0.9902	0.3292	1.0000	0.47	0.10	1	1.71
35	H20D	0.3750	1.0263	0.4283	1.0000	0.47	0.10	1	0.73
36	H21D	0.2630	0.9744	0.4142	1.0000	0.47	0.10	1	1.76
37	C12D	0.3983	0.8618	0.4790	1.0000	0.87	0.10	1	0.62
38	H22D	0.4319	0.8008	0.4779	1.0000	0.47	0.10	1	0.48
39	H23D	0.3297	0.8611	0.5031	1.0000	0.47	0.10	1	1.03
40	H24D	0.4418	0.9130	0.5172	1.0000	0.47	0.10	1	0.00

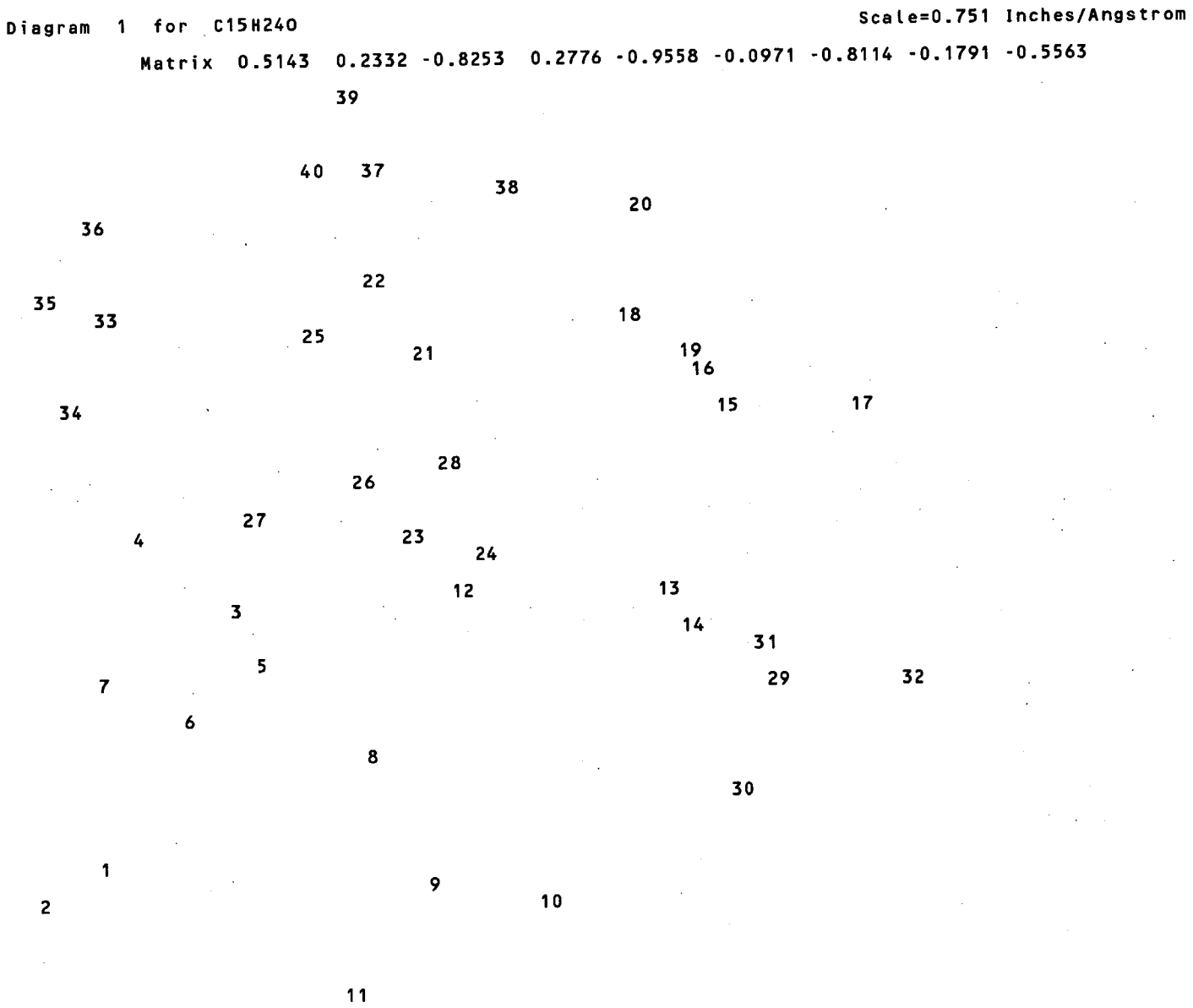
Distances

O2D -H1D	0.89(3)	C1D -H2D	0.963(4)	C1D -H3D	0.957(4)
O2D -C2D	1.420(3)	C1D -C2D	1.526(4)	C2D -H4D	0.959(4)
C2D -C3D	1.517(4)	C3D -C3'D	1.317(4)	C3'D-H5D	0.95(3)
C3'D-H6D	0.99(3)	C3D -C3aD	1.502(4)	C3aD-C4D	1.539(4)

C4D -H7D	0.959(4)	C4D -C5D	1.541(4)	C5D -H8D	0.956(4)
C5D -H9D	0.960(4)	C5D -C6D	1.540(4)	C6D -H10D	0.957(4)
C6D -H11D	0.962(4)	C6D -C7D	1.540(4)	C7D -H12D	0.961(4)
C1D -C7aD	1.552(4)	C3aD-C7aD	1.543(3)	C7D -C7aD	1.525(4)
C7aD-H13D	0.958(4)	C7D -C8D	1.549(4)	C3aD-C9D	1.571(4)
C8D -C9D	1.560(4)	C9D -H14D	0.960(4)	C9D -H15D	0.957(4)
C4D -C10D	1.533(4)	C10D-H16D	0.962(4)	C10D-H17D	0.958(4)
C10D-H18D	0.960(4)	C8D -C11D	1.532(4)	C11D-H19D	0.959(4)
C11D-H20D	0.957(4)	C11D-H21D	0.963(4)	C8D -C12D	1.532(4)
C12D-H22D	0.960(5)	C12D-H23D	0.963(4)	C12D-H24D	0.957(4)

Angles

H1D -O2D -C2D	108(2)	H2D -C1D -H3D	109.6(3)	H2D -C1D -C2D	110.6(3)
H2D -C1D -C7aD	110.3(3)	H3D -C1D -C2D	110.1(3)	H3D -C1D -C7aD	110.3(3)
C2D -C1D -C7aD	106.0(2)	O2D -C2D -C1D	111.0(2)	O2D -C2D -H4D	102.6(3)
O2D -C2D -C3D	115.5(2)	C1D -C2D -H4D	114.5(3)	C1D -C2D -C3D	104.0(2)
H4D -C2D -C3D	109.8(3)	C2D -C3D -C3'D	124.9(2)	C2D -C3D -C3aD	105.3(2)
C3'D-C3D -C3aD	129.7(2)	C3D -C3'D-H5D	123(2)	C3D -C3'D-H6D	122(2)
H5D -C3'D-H6D	116(2)	C3D -C3aD-C4D	120.0(2)	C3D -C3aD-C7aD	103.6(2)
C3D -C3aD-C9D	110.8(2)	C4D -C3aD-C7aD	109.0(2)	C4D -C3aD-C9D	109.1(2)
C7aD-C3aD-C9D	103.0(2)	C3aD-C4D -H7D	107.0(3)	C3aD-C4D -C5D	108.4(2)
C3aD-C4D -C10D	114.7(2)	H7D -C4D -C5D	111.7(3)	H7D -C4D -C10D	104.5(3)
C5D -C4D -C10D	110.5(2)	C4D -C5D -H8D	108.3(3)	C4D -C5D -H9D	108.1(3)
C4D -C5D -C6D	114.6(2)	H8D -C5D -H9D	109.6(4)	H8D -C5D -C6D	107.9(3)
H9D -C5D -C6D	108.3(3)	C5D -C6D -H10D	108.0(3)	C5D -C6D -H11D	108.7(3)
C5D -C6D -C7D	113.9(2)	H10D-C6D -H11D	109.3(4)	H10D-C6D -C7D	108.5(3)
H11D-C6D -C7D	108.2(3)	C6D -C7D -H12D	108.9(3)	C6D -C7D -C7aD	104.9(2)
C6D -C7D -C8D	113.0(2)	H12D-C7D -C7aD	116.5(3)	H12D-C7D -C8D	108.5(3)
C7aD-C7D -C8D	105.1(2)	C1D -C7aD-C3aD	106.1(2)	C1D -C7aD-C7D	124.2(2)
C1D -C7aD-H13D	99.6(3)	C3aD-C7aD-C7D	101.5(2)	C3aD-C7aD-H13D	122.9(3)
C7D -C7aD-H13D	104.6(3)	C7D -C8D -C9D	101.9(2)	C7D -C8D -C11D	111.0(2)
C7D -C8D -C12D	113.9(2)	C9D -C8D -C11D	110.8(2)	C9D -C8D -C12D	113.1(2)
C11D-C8D -C12D	106.1(2)	C3aD-C9D -C8D	107.9(2)	C3aD-C9D -H14D	109.9(3)
C3aD-C9D -H15D	109.7(3)	C8D -C9D -H14D	110.0(3)	C8D -C9D -H15D	109.9(3)
H14D-C9D -H15D	109.6(3)	C4D -C10D-H16D	109.6(3)	C4D -C10D-H17D	109.1(3)
C4D -C10D-H18D	109.7(3)	H16D-C10D-H17D	109.8(4)	H16D-C10D-H18D	109.3(4)
H17D-C10D-H18D	109.4(4)	C8D -C11D-H19D	109.3(3)	C8D -C11D-H20D	109.6(3)
C8D -C11D-H21D	109.5(3)	H19D-C11D-H20D	109.2(4)	H19D-C11D-H21D	109.8(4)
H20D-C11D-H21D	109.3(4)	C8D -C12D-H22D	109.3(3)	C8D -C12D-H23D	109.8(3)
C8D -C12D-H24D	109.2(3)	H22D-C12D-H23D	109.5(4)	H22D-C12D-H24D	109.7(4)
H23D-C12D-H24D	109.3(4)				



	Atom	x/a	y/b	z/c	S.O.F.	Radius	Minimum	Diagram	Elevation
1	O2A	0.0712	0.4286	0.1005	1.0000	1.46	0.76	1	0.59
2	H1A	0.0795	0.4193	0.0447	1.0000	1.17	0.47	1	0.61
3	C1A	0.1516	0.4593	0.2536	1.0000	1.57	0.87	1	0.88
4	H2A	0.2007	0.5016	0.2963	1.0000	1.17	0.47	1	1.02
5	H3A	0.0800	0.4754	0.2686	1.0000	1.17	0.47	1	0.65
6	C2A	0.1679	0.4648	0.1560	1.0000	1.57	0.87	1	0.89
7	H4A	0.1826	0.5287	0.1479	1.0000	1.17	0.47	1	0.88
8	C3A	0.2598	0.3983	0.1306	1.0000	1.57	0.87	1	1.22
9	C3'A	0.3227	0.4031	0.0652	1.0000	1.57	0.87	1	1.39
10	H5A	0.3844	0.3540	0.0564	1.0000	1.17	0.47	1	1.61
11	H6A	0.3122	0.4516	0.0289	1.0000	1.17	0.47	1	1.30
12	C3aA	0.2690	0.3299	0.1945	1.0000	1.57	0.87	1	1.32
13	C4A	0.2679	0.2215	0.1483	1.0000	1.57	0.87	1	1.38
14	H7A	0.3306	0.2093	0.1150	1.0000	1.17	0.47	1	1.58
15	C5A	0.2699	0.1628	0.2230	1.0000	1.57	0.87	1	1.46
16	H8A	0.3425	0.1599	0.2464	1.0000	1.17	0.47	1	1.70
17	H9A	0.2436	0.0986	0.1949	1.0000	1.17	0.47	1	1.42
18	C6A	0.2035	0.2034	0.3039	1.0000	1.57	0.87	1	1.26
19	H10A	0.1302	0.1859	0.2855	1.0000	1.17	0.47	1	1.03
20	H11A	0.2271	0.1748	0.3539	1.0000	1.17	0.47	1	1.37
21	C7A	0.2123	0.3143	0.3372	1.0000	1.57	0.87	1	1.21
22	H12A	0.1731	0.3347	0.3905	1.0000	1.17	0.47	1	1.10
23	C7aA	0.1739	0.3528	0.2529	1.0000	1.57	0.87	1	1.03
24	H13A	0.1038	0.3244	0.2364	1.0000	1.17	0.47	1	0.83
25	C8A	0.3290	0.3513	0.3623	1.0000	1.57	0.87	1	1.56
26	C9A	0.3660	0.3569	0.2675	1.0000	1.57	0.87	1	1.63
27	H14A	0.3910	0.4214	0.2694	1.0000	1.17	0.47	1	1.66
28	H15A	0.4224	0.3122	0.2516	1.0000	1.17	0.47	1	1.84
29	C10A	0.1761	0.1895	0.0758	1.0000	1.57	0.87	1	1.09
30	H16A	0.1773	0.2276	0.0304	1.0000	1.17	0.47	1	1.05
31	H17A	0.1098	0.1985	0.1041	1.0000	1.17	0.47	1	0.89
32	H18A	0.1833	0.1223	0.0471	1.0000	1.17	0.47	1	1.16
33	C11A	0.3358	0.4508	0.4293	1.0000	1.57	0.87	1	1.53
34	H19A	0.2937	0.4961	0.4038	1.0000	1.17	0.47	1	1.36
35	H20A	0.4087	0.4732	0.4397	1.0000	1.17	0.47	1	1.75
36	H21A	0.3094	0.4454	0.4864	1.0000	1.17	0.47	1	1.47
37	C12A	0.3991	0.2866	0.4110	1.0000	1.57	0.87	1	1.85
38	H22A	0.3992	0.2222	0.3733	1.0000	1.17	0.47	1	1.88
39	H23A	0.3713	0.2848	0.4685	1.0000	1.17	0.47	1	1.78
40	H24A	0.4706	0.3126	0.4218	1.0000	1.17	0.47	1	2.05
41	O2B	0.0805	0.4371	-0.0795	1.0000	1.46	0.76	1	0.55
42	H1B	0.0377	0.4786	-0.0874	1.0000	1.17	0.47	1	0.38
43	C1B	0.1786	0.3055	-0.1676	1.0000	1.57	0.87	1	0.92
44	H2B	0.2252	0.3318	-0.2042	1.0000	1.17	0.47	1	1.03
45	H3B	0.2133	0.3091	-0.1079	1.0000	1.17	0.47	1	1.05
46	C2B	0.0746	0.3607	-0.1601	1.0000	1.57	0.87	1	0.56
47	H4B	0.0581	0.3940	-0.2084	1.0000	1.17	0.47	1	0.46
48	C3B	-0.0099	0.2828	-0.1636	1.0000	1.57	0.87	1	0.35
49	C3'B	-0.0901	0.2914	-0.1113	1.0000	1.57	0.87	1	0.11
50	H5B	-0.1393	0.2355	-0.1122	1.0000	1.17	0.47	1	0.00

51	H6B	-0.1019	0.3513	-0.0649	1.0000	1.17	0.47	1	0.05
52	C3aB	0.0241	0.1963	-0.2331	1.0000	1.57	0.87	1	0.49
53	C4B	-0.0174	0.0944	-0.2319	1.0000	1.57	0.87	1	0.44
54	H7B	-0.0935	0.0946	-0.2425	1.0000	1.17	0.47	1	0.20
55	C5B	0.0332	0.0210	-0.3078	1.0000	1.57	0.87	1	0.63
56	H8B	-0.0051	0.0222	-0.3651	1.0000	1.17	0.47	1	0.48
57	H9B	0.0261	-0.0422	-0.2952	1.0000	1.17	0.47	1	0.66
58	C6B	0.1518	0.0402	-0.3167	1.0000	1.57	0.87	1	0.98
59	H10B	0.1928	0.0181	-0.2692	1.0000	1.17	0.47	1	1.14
60	H11B	0.1704	0.0041	-0.3755	1.0000	1.17	0.47	1	1.04
61	C7B	0.1802	0.1480	-0.3086	1.0000	1.57	0.87	1	0.99
62	H12B	0.2540	0.1545	-0.3188	1.0000	1.17	0.47	1	1.21
63	C7aB	0.1471	0.1991	-0.2144	1.0000	1.57	0.87	1	0.88
64	H13B	0.1834	0.1666	-0.1718	1.0000	1.17	0.47	1	1.04
65	C8B	0.1126	0.1931	-0.3785	1.0000	1.57	0.87	1	0.72
66	C9B	0.0065	0.2130	-0.3324	1.0000	1.57	0.87	1	0.39
67	H14B	-0.0140	0.2787	-0.3301	1.0000	1.17	0.47	1	0.28
68	H15B	-0.0482	0.1696	-0.3665	1.0000	1.17	0.47	1	0.24
69	C10B	0.0006	0.0659	-0.1398	1.0000	1.57	0.87	1	0.55
70	H16B	-0.0317	0.1126	-0.0935	1.0000	1.17	0.47	1	0.44
71	H17B	0.0756	0.0641	-0.1239	1.0000	1.17	0.47	1	0.80
72	H18B	-0.0310	0.0031	-0.1442	1.0000	1.17	0.47	1	0.50
73	C11B	0.1639	0.2880	-0.3897	1.0000	1.57	0.87	1	0.80
74	H19B	0.1742	0.3321	-0.3309	1.0000	1.17	0.47	1	0.82
75	H20B	0.1180	0.3165	-0.4299	1.0000	1.17	0.47	1	0.62
76	H21B	0.2315	0.2745	-0.4152	1.0000	1.17	0.47	1	1.01
77	C12B	0.0991	0.1276	-0.4746	1.0000	1.57	0.87	1	0.69
78	H22B	0.0672	0.0669	-0.4716	1.0000	1.17	0.47	1	0.63
79	H23B	0.1676	0.1163	-0.4990	1.0000	1.17	0.47	1	0.90
80	H24B	0.0542	0.1583	-0.5137	1.0000	1.17	0.47	1	0.51
81	O2C	0.4290	0.8794	0.8977	1.0000	1.46	0.76	1	1.68
82	H1C	0.4161	0.8979	0.9522	1.0000	1.17	0.47	1	1.65
83	C1C	0.3479	0.8315	0.7441	1.0000	1.57	0.87	1	1.40
84	H2C	0.2979	0.8514	0.7009	1.0000	1.17	0.47	1	1.21
85	H3C	0.4191	0.8406	0.7281	1.0000	1.17	0.47	1	1.61
86	C2C	0.3324	0.8864	0.8411	1.0000	1.57	0.87	1	1.35
87	H4C	0.3180	0.9540	0.8470	1.0000	1.17	0.47	1	1.26
88	C3C	0.2409	0.8325	0.8685	1.0000	1.57	0.87	1	1.11
89	C3'C	0.1778	0.8698	0.9328	1.0000	1.57	0.87	1	0.91
90	H5C	0.1220	0.8299	0.9487	1.0000	1.17	0.47	1	0.78
91	H6C	0.1851	0.9367	0.9701	1.0000	1.17	0.47	1	0.90
92	C3aC	0.2328	0.7318	0.8077	1.0000	1.57	0.87	1	1.14
93	C4C	0.2363	0.6479	0.8573	1.0000	1.57	0.87	1	1.24
94	H7C	0.1739	0.6512	0.8910	1.0000	1.17	0.47	1	1.05
95	C5C	0.2358	0.5521	0.7860	1.0000	1.57	0.87	1	1.28
96	H8C	0.1633	0.5362	0.7628	1.0000	1.17	0.47	1	1.06
97	H9C	0.2629	0.5032	0.8162	1.0000	1.17	0.47	1	1.41
98	C6C	0.3017	0.5515	0.7046	1.0000	1.57	0.87	1	1.45
99	H10C	0.3754	0.5454	0.7236	1.0000	1.17	0.47	1	1.70
100	H11C	0.2794	0.4967	0.6564	1.0000	1.17	0.47	1	1.41
101	C7C	0.2901	0.6439	0.6668	1.0000	1.57	0.87	1	1.33
102	H12C	0.3289	0.6370	0.6130	1.0000	1.17	0.47	1	1.44