Supporting Information

Enantioselective Addition of Diethylzinc to Aldehydes Catalyzed by *N*-(9-Phenylfluoren-9-yl) β-Amino Alcohols

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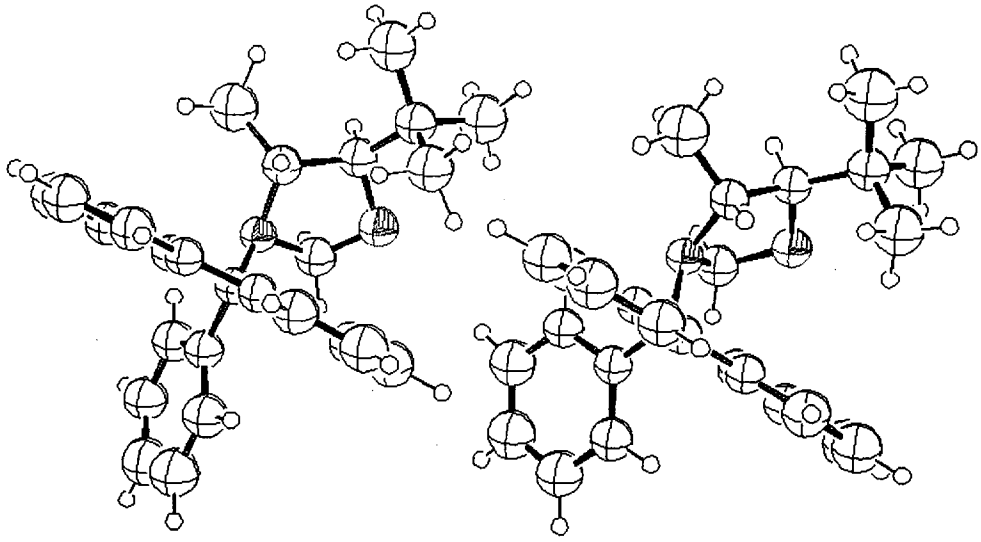
Crystal data of (4*S*, 5*R*)-5-(tert-butyl)-4-methyl-3-[*N*-(9'-phenylfluoren-9'-yl)amino]oxazolidine (6e).



Ortep diagram of **6e**. Ellipsoids drawn at 50% probability

The crystal structure has been deposited at the Cambridge Crystallographic Data Centre and allocated the deposition number: CCDC 136229

_symmetry_cell_setting	Orthorhombic
_symmetry_space_group_name_H-M	'P 2(1) 2(1) 2(1)'
_cell_length_a	9.417(2)
_cell_length_b	17.266(3)

_cell_length_c	27.143(5)
_cell_angle_alpha	90.00
_cell_angle_beta	90.00
_cell_angle_gamma	90.00
_cell_volume	4413.3(15)
_cell_formula_units_Z	8
_cell_measurement_temperature	293(2)
_cell_measurement_reflns_used	15
_cell_measurement_theta_min	10
_cell_measurement_theta_max	13
_exptl_crystal_description	prism
_exptl_crystal_colour	colorless
_exptl_crystal_size_max	.45
_exptl_crystal_size_mid	.20
_exptl_crystal_size_min	.15
_exptl_crystal_density_diffrn	1.154
_exptl_crystal_F_000	1648
_exptl_absorpt_coefficient_mu	0.069
_diffrn_ambient_temperature	293(2)
_diffrn_radiation_wavelength	0.71073
_diffrn_radiation_type	MoK\a
_diffrn_radiation_source	'fine-focus sealed tube'
_diffrn_radiation_monochromator	beta-filter
_diffrn_measurement_device_type	'Syntex P-1'
_diffrn_measurement_method	theta/2theta
_diffrn_standards_number	3
_diffrn_standards_interval_count	100
_diffrn_standards_decay_%	.8
_diffrn_reflns_number	2162
_diffrn_reflns_av_R_equivalents	0.0000
_diffrn_reflns_av_sigmaI/netI	0.0368
_diffrn_reflns_limit_h_min	0
_diffrn_reflns_limit_h_max	10
_diffrn_reflns_limit_k_min	0
_diffrn_reflns_limit_k_max	19
_diffrn_reflns_limit_l_min	0
_diffrn_reflns_limit_l_max	29
_diffrn_reflns_theta_min	1.91
_diffrn_reflns_theta_max	23.99
_reflns_number_total	2162
_reflns_number_gt	2050

_reflns_threshold_expression >2sigma(I)

_refine_special_details

Refinement of F^2^ against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2^, conventional R-factors R are based on F, with F set to zero for negative F^2^. The threshold expression of F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2^ are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

_refine_ls_structure_factor_coef Fsqd

_refine_ls_matrix_type fullcycle

_refine_ls_weighting_scheme

'calc w=1/[\s^2^(Fo^2^)+(0.0335P)^2^+2.1609P] where P=(Fo^2^+2Fc^2^)/3'

_atom_sites_solution_primary direct

_atom_sites_solution_secondary difmap

_atom_sites_solution_hydrogens difmap

_refine_ls_hydrogen_treatment refined

_refine_ls_extinction_method SHELXL

_refine_ls_extinction_coef 0.0017(2)

_refine_ls_extinction_expression

'Fc^*^=kFc[1+0.001xFc^2^\l^3^/sin(2\q)]^-1/4^'

_refine_ls_number_reflns 2162

_refine_ls_number_parameters 756

_refine_ls_number_restraints 0

_refine_ls_R_factor_all 0.0407

_refine_ls_R_factor_gt 0.0371

_refine_ls_wR_factor_ref 0.0870

_refine_ls_wR_factor_gt 0.0819

_refine_ls_goodness_of_fit_ref 1.054

_refine_ls_restrained_S_all 1.054

_refine_ls_shift/su_max 0.258

_refine_ls_shift/su_mean 0.154

Atomic coordinates:

O1A O 0.8213(4) 0.0377(2) 0.62218(14) 0.0590(10) Uani 1 d .

N1A N 0.6608(4) 0.1387(2) 0.62725(16) 0.0482(12) Uani 1 d .

C1A C 0.5371(6) 0.1384(3) 0.5937(2) 0.0479(15) Uani 1 d .

C2A C 0.4940(6) 0.0578(3) 0.5748(2) 0.0510(15) Uani 1 d .

C3A C 0.5646(7) 0.0097(4) 0.5425(2) 0.0636(17) Uani 1 d .

C4A C 0.5020(9) -0.0623(4) 0.5307(2) 0.074(2) Uani 1 d .

C5A C 0.3714(9) -0.0818(4) 0.5499(3) 0.078(2) Uani 1 d .

C6A C 0.2993(7) -0.0330(4) 0.5805(2) 0.0732(19) Uani 1 d .

C7A C 0.3600(6) 0.0373(3) 0.5926(2) 0.0501(15) Uani 1 d .

C8A C 0.3053(6) 0.1006(4) 0.6224(2) 0.0515(15) Uani 1 d .

C9A C 0.1768(7) 0.1090(4) 0.6475(2) 0.0679(18) Uani 1 d .
C10A C 0.1495(7) 0.1775(5) 0.6718(2) 0.0773(19) Uani 1 d .
C11A C 0.2464(8) 0.2370(4) 0.6713(2) 0.0772(19) Uani 1 d .
C12A C 0.3738(7) 0.2293(3) 0.6466(2) 0.0638(18) Uani 1 d .
C13A C 0.4039(6) 0.1602(3) 0.62350(19) 0.0463(14) Uani 1 d .
C14A C 0.5647(6) 0.1988(3) 0.5533(2) 0.0513(15) Uani 1 d .
C15A C 0.6411(7) 0.2653(3) 0.5639(2) 0.0594(16) Uani 1 d .
C16A C 0.6603(8) 0.3229(4) 0.5289(3) 0.078(2) Uani 1 d .
C17A C 0.6053(8) 0.3128(5) 0.4822(3) 0.086(2) Uani 1 d .
C18A C 0.5303(9) 0.2467(5) 0.4709(2) 0.081(2) Uani 1 d .
C19A C 0.5102(7) 0.1895(4) 0.5062(2) 0.0644(18) Uani 1 d .
C20A C 0.7931(6) 0.1146(4) 0.6049(2) 0.0623(17) Uani 1 d .
C21A C 0.7818(6) 0.0399(3) 0.6726(2) 0.0533(15) Uani 1 d .
C22A C 0.6498(6) 0.0942(3) 0.67407(19) 0.0525(15) Uani 1 d .
C23A C 0.6493(8) 0.1490(4) 0.7179(2) 0.090(2) Uani 1 d .
C24A C 0.7653(6) -0.0411(3) 0.6932(2) 0.0621(17) Uani 1 d .
C25A C 0.9049(8) -0.0846(4) 0.6844(3) 0.088(2) Uani 1 d .
C26A C 0.7389(8) -0.0373(4) 0.7480(2) 0.099(2) Uani 1 d .
C27A C 0.6478(8) -0.0855(3) 0.6679(3) 0.086(2) Uani 1 d .
O1B O 0.7514(4) 0.4968(2) 0.60467(15) 0.0624(11) Uani 1 d .
N1B N 0.6336(5) 0.6160(3) 0.60331(16) 0.0510(13) Uani 1 d .
C1B C 0.4861(6) 0.6158(3) 0.5836(2) 0.0499(16) Uani 1 d .
C2B C 0.4021(6) 0.5408(3) 0.5856(2) 0.0500(16) Uani 1 d .
C3B C 0.4295(8) 0.4709(4) 0.5618(3) 0.068(2) Uani 1 d .
C4B C 0.3328(9) 0.4105(4) 0.5664(3) 0.070(2) Uani 1 d .
C5B C 0.2107(9) 0.4204(5) 0.5942(3) 0.077(2) Uani 1 d .
C6B C 0.1835(8) 0.4901(4) 0.6175(3) 0.0689(19) Uani 1 d .
C7B C 0.2795(6) 0.5495(3) 0.6126(2) 0.0492(15) Uani 1 d .
C8B C 0.2750(6) 0.6289(3) 0.6319(2) 0.0503(15) Uani 1 d .
C9B C 0.1748(8) 0.6647(5) 0.6615(2) 0.0645(19) Uani 1 d .
C10B C 0.1954(9) 0.7423(5) 0.6735(3) 0.072(2) Uani 1 d .
C11B C 0.3117(10) 0.7822(5) 0.6571(3) 0.073(2) Uani 1 d .
C12B C 0.4127(9) 0.7457(4) 0.6275(3) 0.0637(19) Uani 1 d .
C13B C 0.3941(6) 0.6688(3) 0.61515(19) 0.0490(15) Uani 1 d .
C14B C 0.4910(7) 0.6502(3) 0.5307(2) 0.0561(16) Uani 1 d .
C15B C 0.5881(9) 0.7061(4) 0.5180(3) 0.068(2) Uani 1 d .
C16B C 0.5838(10) 0.7388(4) 0.4699(3) 0.076(2) Uani 1 d .
C17B C 0.4818(11) 0.7170(5) 0.4373(3) 0.088(3) Uani 1 d .
C18B C 0.3847(10) 0.6624(6) 0.4502(3) 0.091(3) Uani 1 d .
C19B C 0.3898(8) 0.6279(5) 0.4968(2) 0.074(2) Uani 1 d .
C20B C 0.7348(8) 0.5669(4) 0.5776(3) 0.0630(19) Uani 1 d .

C21B C 0.7533(7) 0.5234(3) 0.6546(2) 0.0575(17) Uani 1 d .
C22B C 0.6486(7) 0.5927(4) 0.6556(2) 0.0578(17) Uani 1 d .
C23B C 0.7057(12) 0.6607(6) 0.6859(4) 0.088(3) Uani 1 d .
C24B C 0.7258(7) 0.4543(4) 0.6890(2) 0.0639(18) Uani 1 d .
C25B C 0.8457(11) 0.3954(6) 0.6833(4) 0.089(3) Uani 1 d .
C26B C 0.7243(12) 0.4833(6) 0.7423(3) 0.084(3) Uani 1 d .
C27B C 0.5865(9) 0.4145(5) 0.6758(3) 0.078(2) Uani 1 d .
H3AA H 0.655(6) 0.022(2) 0.5257(16) 0.060(15) Uiso 1 d .
H4AA H 0.554(5) -0.098(3) 0.5060(18) 0.062(16) Uiso 1 d .
H5AA H 0.330(6) -0.133(3) 0.5418(19) 0.094(19) Uiso 1 d .
H6AA H 0.202(5) -0.045(3) 0.5957(17) 0.073(16) Uiso 1 d .
H9AA H 0.110(6) 0.062(3) 0.6440(17) 0.070(17) Uiso 1 d .
H10A H 0.069(7) 0.184(3) 0.687(2) 0.11(2) Uiso 1 d .
H11A H 0.215(6) 0.286(3) 0.6913(19) 0.093(18) Uiso 1 d .
H12A H 0.441(5) 0.274(2) 0.6473(16) 0.057(15) Uiso 1 d .
H15A H 0.674(7) 0.269(3) 0.5985(19) 0.092(19) Uiso 1 d .
H16A H 0.723(7) 0.368(3) 0.539(2) 0.12(2) Uiso 1 d .
H17A H 0.611(6) 0.347(3) 0.4587(19) 0.089(19) Uiso 1 d .
H18A H 0.492(6) 0.239(3) 0.4377(19) 0.093(19) Uiso 1 d .
H19A H 0.464(6) 0.140(3) 0.5002(18) 0.086(18) Uiso 1 d .
H20A H 0.787(5) 0.116(3) 0.5670(16) 0.056(14) Uiso 1 d .
H20B H 0.880(5) 0.148(2) 0.6157(16) 0.050(14) Uiso 1 d .
H21A H 0.852(6) 0.069(2) 0.6905(17) 0.058(15) Uiso 1 d .
H22A H 0.560(6) 0.068(3) 0.6729(18) 0.067(17) Uiso 1 d .
H23A H 0.553(8) 0.182(4) 0.716(2) 0.12(2) Uiso 1 d .
H23B H 0.661(6) 0.121(3) 0.7492(19) 0.083(18) Uiso 1 d .
H23C H 0.734(6) 0.182(3) 0.716(2) 0.093(19) Uiso 1 d .
H25A H 0.940(7) -0.089(4) 0.646(3) 0.14(3) Uiso 1 d .
H25B H 0.977(7) -0.053(3) 0.699(2) 0.11(2) Uiso 1 d .
H25C H 0.903(6) -0.136(3) 0.699(2) 0.09(2) Uiso 1 d .
H26A H 0.646(7) -0.010(4) 0.758(2) 0.11(2) Uiso 1 d .
H26B H 0.732(7) -0.086(3) 0.760(2) 0.11(2) Uiso 1 d .
H26C H 0.817(6) -0.006(3) 0.765(2) 0.084(18) Uiso 1 d .
H27A H 0.546(7) -0.059(4) 0.678(2) 0.12(2) Uiso 1 d .
H27B H 0.656(6) -0.081(3) 0.631(2) 0.10(2) Uiso 1 d .
H27C H 0.640(7) -0.138(3) 0.677(2) 0.11(2) Uiso 1 d .
H3BA H 0.504(6) 0.466(4) 0.543(2) 0.07(2) Uiso 1 d .
H4BA H 0.352(8) 0.357(4) 0.548(2) 0.12(3) Uiso 1 d .
H5BA H 0.143(8) 0.382(4) 0.596(2) 0.11(3) Uiso 1 d .
H6BA H 0.087(7) 0.498(4) 0.636(2) 0.08(2) Uiso 1 d .
H9BA H 0.093(7) 0.637(4) 0.670(2) 0.09(3) Uiso 1 d .

H10B H 0.126(8) 0.767(3) 0.697(2) 0.09(2) Uiso 1 d .
H11B H 0.340(7) 0.833(4) 0.669(2) 0.10(2) Uiso 1 d .
H12B H 0.498(6) 0.773(3) 0.6152(19) 0.054(18) Uiso 1 d .
H15B H 0.663(6) 0.721(3) 0.5415(19) 0.056(19) Uiso 1 d .
H16B H 0.657(8) 0.778(4) 0.466(2) 0.10(3) Uiso 1 d .
H17B H 0.481(7) 0.740(3) 0.405(2) 0.08(2) Uiso 1 d .
H18B H 0.302(8) 0.646(4) 0.428(3) 0.12(3) Uiso 1 d .
H19B H 0.326(7) 0.586(3) 0.507(2) 0.08(2) Uiso 1 d .
H20C H 0.701(5) 0.556(3) 0.5443(18) 0.041(16) Uiso 1 d .
H20D H 0.826(7) 0.596(3) 0.577(2) 0.073(19) Uiso 1 d .
H21B H 0.857(6) 0.547(3) 0.6633(18) 0.057(16) Uiso 1 d .
H22B H 0.555(5) 0.577(2) 0.6697(16) 0.025(13) Uiso 1 d .
H23D H 0.626(8) 0.701(4) 0.692(3) 0.11(3) Uiso 1 d .
H23E H 0.734(7) 0.640(4) 0.723(3) 0.11(2) Uiso 1 d .
H23F H 0.797(9) 0.676(5) 0.675(3) 0.13(4) Uiso 1 d .
H25D H 0.842(9) 0.351(4) 0.709(3) 0.12(3) Uiso 1 d .
H25E H 0.864(7) 0.386(4) 0.650(2) 0.08(3) Uiso 1 d .
H25F H 0.939(9) 0.424(5) 0.692(3) 0.15(4) Uiso 1 d .
H26D H 0.708(8) 0.443(4) 0.765(2) 0.10(3) Uiso 1 d .
H26E H 0.812(8) 0.518(4) 0.754(3) 0.11(3) Uiso 1 d .
H26F H 0.635(8) 0.520(4) 0.745(2) 0.10(3) Uiso 1 d .
H27D H 0.573(7) 0.378(4) 0.699(2) 0.08(2) Uiso 1 d .
H27E H 0.506(7) 0.458(4) 0.677(2) 0.10(3) Uiso 1 d .
H27F H 0.593(6) 0.387(3) 0.639(2) 0.067(18) Uiso 1 d .

Anisotropic thermal parameters:

O1A 0.053(2) 0.068(3) 0.056(3) 0.007(2) 0.003(2) 0.005(2)
N1A 0.036(3) 0.053(3) 0.056(3) 0.007(2) 0.001(3) 0.001(3)
C1A 0.046(4) 0.045(3) 0.053(4) -0.003(3) -0.006(3) -0.010(3)
C2A 0.046(4) 0.052(4) 0.055(4) 0.005(3) -0.004(3) -0.001(3)
C3A 0.057(4) 0.068(4) 0.066(4) -0.001(4) -0.011(4) 0.007(4)
C4A 0.090(6) 0.060(4) 0.073(5) -0.019(4) -0.023(5) 0.010(4)
C5A 0.080(5) 0.061(4) 0.092(5) -0.004(4) -0.037(5) -0.020(5)
C6A 0.073(5) 0.071(4) 0.075(5) 0.005(4) -0.010(4) -0.009(4)
C7A 0.053(4) 0.042(3) 0.055(4) 0.003(3) -0.019(3) -0.004(3)
C8A 0.038(3) 0.065(4) 0.052(4) 0.013(3) -0.004(3) -0.007(4)
C9A 0.053(4) 0.083(5) 0.068(4) 0.025(4) -0.003(4) -0.011(4)
C10A 0.059(4) 0.105(6) 0.068(4) 0.005(5) 0.006(4) 0.016(5)
C11A 0.075(5) 0.079(5) 0.077(5) -0.011(4) 0.015(4) 0.002(5)
C12A 0.062(5) 0.062(4) 0.068(4) -0.003(4) 0.013(4) -0.008(4)
C13A 0.044(4) 0.050(3) 0.045(3) 0.005(3) -0.001(3) 0.001(4)
C14A 0.046(4) 0.051(4) 0.057(4) 0.007(3) 0.005(3) 0.002(3)

C15A 0.057(4) 0.045(3) 0.076(4) 0.015(3) 0.001(4) -0.003(3)
C16A 0.065(5) 0.065(4) 0.103(5) 0.021(5) 0.014(5) 0.004(4)
C17A 0.077(6) 0.086(6) 0.095(6) 0.036(5) 0.033(5) 0.026(5)
C18A 0.092(6) 0.091(5) 0.060(4) 0.020(5) 0.004(4) 0.032(5)
C19A 0.063(4) 0.070(4) 0.060(4) 0.008(4) -0.001(4) 0.020(4)
C20A 0.045(4) 0.075(5) 0.066(4) 0.014(4) -0.009(3) -0.002(4)
C21A 0.044(3) 0.066(4) 0.050(4) 0.002(3) -0.006(3) -0.010(3)
C22A 0.051(4) 0.064(4) 0.043(3) 0.006(3) -0.002(3) 0.006(3)
C23A 0.113(6) 0.095(5) 0.062(4) -0.013(4) -0.018(5) 0.023(5)
C24A 0.050(4) 0.071(4) 0.065(4) 0.004(4) 0.004(4) -0.006(4)
C25A 0.087(5) 0.079(5) 0.097(5) 0.007(4) -0.016(5) 0.008(5)
C26A 0.120(6) 0.104(5) 0.073(5) 0.029(4) 0.001(5) 0.011(6)
C27A 0.078(5) 0.049(4) 0.129(6) 0.018(4) -0.015(5) -0.010(4)
O1B 0.066(3) 0.059(2) 0.062(3) 0.006(2) 0.011(2) 0.008(2)
N1B 0.046(3) 0.059(3) 0.048(3) -0.002(3) 0.002(3) 0.004(3)
C1B 0.044(4) 0.055(4) 0.051(4) -0.003(3) 0.005(3) -0.003(3)
C2B 0.043(4) 0.052(4) 0.055(4) -0.006(3) -0.005(3) 0.000(3)
C3B 0.062(5) 0.069(5) 0.073(5) -0.004(4) 0.003(4) -0.006(5)
C4B 0.080(6) 0.057(5) 0.074(5) -0.003(4) -0.007(5) -0.001(5)
C5B 0.073(6) 0.071(6) 0.086(6) 0.008(5) -0.013(5) -0.022(5)
C6B 0.064(5) 0.073(5) 0.070(5) 0.001(4) 0.004(4) -0.012(5)
C7B 0.041(4) 0.057(4) 0.050(4) 0.006(3) -0.003(3) -0.005(4)
C8B 0.044(4) 0.062(4) 0.045(3) 0.007(3) 0.002(3) 0.009(4)
C9B 0.053(5) 0.078(6) 0.062(4) 0.003(4) -0.006(4) 0.014(5)
C10B 0.076(6) 0.087(6) 0.053(4) -0.004(4) 0.000(4) 0.026(5)
C11B 0.087(6) 0.065(5) 0.068(5) -0.015(4) -0.015(5) 0.019(5)
C12B 0.065(5) 0.056(4) 0.070(5) -0.005(4) -0.001(4) 0.000(4)
C13B 0.047(4) 0.056(4) 0.044(3) -0.003(3) -0.002(3) 0.005(4)
C14B 0.064(4) 0.055(4) 0.049(4) -0.012(3) 0.014(4) -0.004(4)
C15B 0.072(5) 0.059(4) 0.075(6) -0.002(4) 0.008(5) -0.002(5)
C16B 0.089(6) 0.061(5) 0.077(6) 0.016(5) 0.032(6) 0.004(5)
C17B 0.091(7) 0.120(7) 0.052(5) 0.017(5) 0.010(5) 0.017(6)
C18B 0.080(6) 0.126(7) 0.067(6) 0.005(5) 0.004(5) -0.013(6)
C19B 0.079(5) 0.096(6) 0.048(5) 0.005(4) 0.000(4) -0.018(5)
C20B 0.053(5) 0.072(5) 0.064(5) -0.003(4) 0.004(4) -0.009(4)
C21B 0.051(4) 0.055(4) 0.066(5) 0.001(4) 0.004(4) -0.003(4)
C22B 0.052(4) 0.063(4) 0.058(4) -0.004(4) 0.001(4) 0.001(4)
C23B 0.094(8) 0.085(6) 0.085(7) -0.025(5) -0.024(6) -0.002(6)
C24B 0.050(4) 0.067(4) 0.074(5) 0.004(4) -0.007(4) -0.004(4)
C25B 0.085(6) 0.094(6) 0.089(7) 0.021(6) 0.000(6) 0.008(6)
C26B 0.096(7) 0.096(7) 0.060(5) 0.012(5) -0.008(5) -0.015(7)

C27B 0.092(6) 0.072(5) 0.070(6) 0.007(5) 0.004(5) -0.020(5)

Bond Distances:

O1A C21A 1.418(7)
O1A C20A 1.434(7)
N1A C20A 1.447(8)
N1A C1A 1.479(7) .
N1A C22A 1.489(7)
C1A C14A 1.534(8)
C1A C2A 1.537(8) .
C1A C13A 1.540(8)
C2A C3A 1.378(8) .
C2A C7A 1.398(8) .
C3A C4A 1.413(9) .
C4A C5A 1.377(10)
C5A C6A 1.365(10)
C6A C7A 1.381(8) .
C7A C8A 1.454(9) .
C8A C13A 1.386(8)
C8A C9A 1.396(9) .
C9A C10A 1.378(10) .
C10A C11A 1.373(10)
C11A C12A 1.380(9) .
C12A C13A 1.378(8) .
C14A C15A 1.385(8) .
C14A C19A 1.387(8) .
C15A C16A 1.388(9) .
C16A C17A 1.380(10)
C17A C18A 1.376(11)
C18A C19A 1.389(10)
C21A C24A 1.514(8) .
C21A C22A 1.558(8) .
C22A C23A 1.521(9) .
C24A C26A 1.509(9) .
C24A C27A 1.512(9) .
C24A C25A 1.533(9) .
O1B C20B 1.424(8) .
O1B C21B 1.431(8) .
N1B C20B 1.454(9) .
N1B C22B 1.483(8) .
N1B C1B 1.488(8) .
C1B C2B 1.519(9) .

C1B C13B 1.523(8) .
C1B C14B 1.555(9) .
C2B C7B 1.375(8) .
C2B C3B 1.393(10)
C3B C4B 1.389(10)
C4B C5B 1.387(11)
C5B C6B 1.382(11)
C6B C7B 1.374(9) .
C7B C8B 1.468(9) .
C8B C9B 1.384(9) .
C8B C13B 1.393(8)
C9B C10B 1.392(11) .
C10B C11B 1.368(11)
C11B C12B 1.396(11)
C12B C13B 1.381(9) .
C14B C19B 1.379(10)
C14B C15B 1.374(10)
C15B C16B 1.422(10)
C16B C17B 1.360(12) .
C17B C18B 1.358(12) .
C18B C19B 1.399(11) .
C21B C24B 1.537(9) .
C21B C22B 1.551(10) .
C22B C23B 1.530(11) .
C24B C27B 1.524(11) .
C24B C25B 1.529(12) .
C24B C26B 1.529(11) .

Bond Angles:

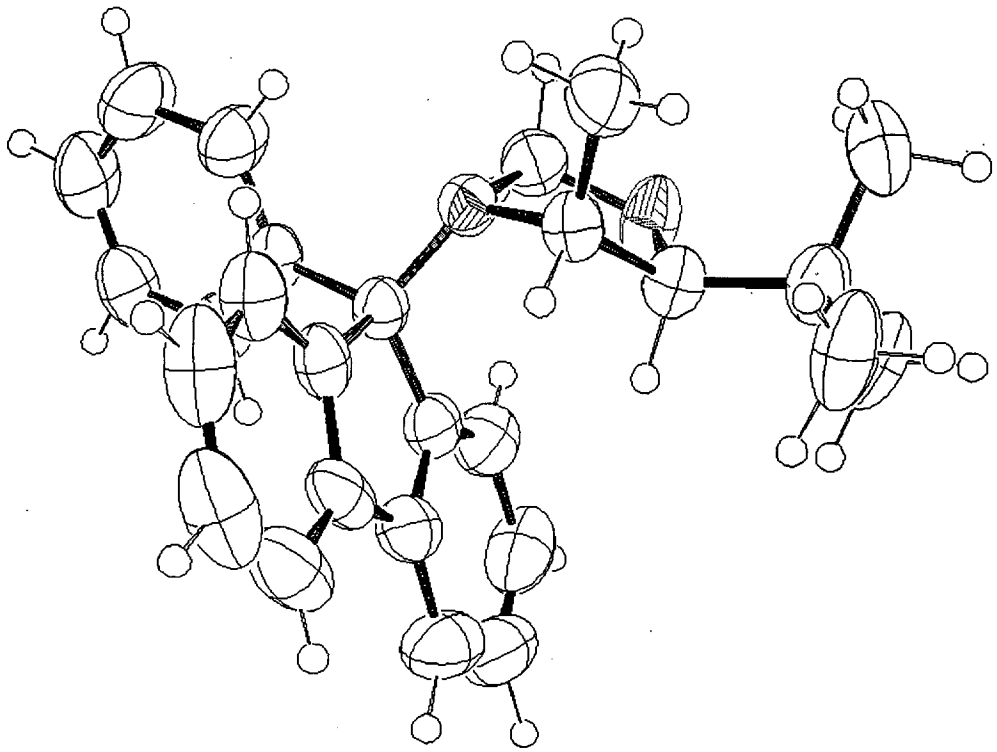
C21A O1A C20A 104.0(5)
C20A N1A C1A 114.8(5) .
C20A N1A C22A 105.6(5)
C1A N1A C22A 118.0(5) .
N1A C1A C14A 107.7(5) .
N1A C1A C2A 114.6(5) . .
C14A C1A C2A 115.0(5) .
N1A C1A C13A 108.4(4) .
C14A C1A C13A 110.3(5)
C2A C1A C13A 100.5(5) .
C3A C2A C7A 120.2(6) . .
C3A C2A C1A 129.1(6) . .
C7A C2A C1A 110.6(6) . .

C2A C3A C4A 118.3(7) . .
C5A C4A C3A 120.0(7) . .
C6A C5A C4A 121.7(7) . .
C5A C6A C7A 118.8(7) . .
C6A C7A C2A 120.9(7) . .
C6A C7A C8A 130.3(7) . .
C2A C7A C8A 108.8(6) . .
C13A C8A C9A 119.6(6) .
C13A C8A C7A 109.4(6) .
C9A C8A C7A 131.0(7) . .
C10A C9A C8A 118.9(7) .
C11A C10A C9A 120.9(7) .
C10A C11A C12A 120.7(7)
C13A C12A C11A 118.9(6)
C12A C13A C8A 121.0(6) .
C12A C13A C1A 128.3(6) .
C8A C13A C1A 110.7(5) . .
C15A C14A C19A 118.7(6)
C15A C14A C1A 120.2(6) .
C19A C14A C1A 121.1(6) .
C14A C15A C16A 121.3(6)
C15A C16A C17A 119.3(7)
C18A C17A C16A 120.1(7)
C17A C18A C19A 120.4(7)
C18A C19A C14A 120.2(7)
O1A C20A N1A 106.8(5) . .
O1A C21A C24A 111.0(5) .
O1A C21A C22A 104.5(5) .
C24A C21A C22A 117.7(5)
N1A C22A C23A 110.3(5) .
N1A C22A C21A 103.5(5) .
C23A C22A C21A 113.4(5)
C26A C24A C27A 110.5(7)
C26A C24A C21A 109.9(6)
C27A C24A C21A 112.0(6)
C26A C24A C25A 108.4(6)
C27A C24A C25A 108.0(6)
C21A C24A C25A 107.9(6)
C20B O1B C21B 102.6(5) .
C20B N1B C22B 103.9(6) .
C20B N1B C1B 116.0(6) . .

C22B N1B C1B 115.6(5) .
N1B C1B C2B 118.4(5) . .
N1B C1B C13B 109.2(5) .
C2B C1B C13B 101.3(5) .
N1B C1B C14B 107.7(5) .
C2B C1B C14B 111.9(5) .
C13B C1B C14B 107.8(5) .
C7B C2B C3B 119.8(7) . .
C7B C2B C1B 111.3(6) . .
C3B C2B C1B 128.8(6) . .
C2B C3B C4B 119.2(8) . .
C5B C4B C3B 120.0(8) . .
C4B C5B C6B 120.7(8) . .
C7B C6B C5B 118.9(8) . .
C6B C7B C2B 121.5(7) . .
C6B C7B C8B 130.0(7) . .
C2B C7B C8B 108.5(6) . .
C9B C8B C13B 121.1(7) .
C9B C8B C7B 130.1(7) . .
C13B C8B C7B 108.7(6) .
C8B C9B C10B 118.1(9) .
C11B C10B C9B 121.4(9) .
C10B C11B C12B 120.3(8)
C13B C12B C11B 119.1(8) .
C12B C13B C8B 119.9(7) . .
C12B C13B C1B 129.9(7) . .
C8B C13B C1B 110.2(6) . .
C19B C14B C15B 119.2(8) .
C19B C14B C1B 119.3(7) . .
C15B C14B C1B 121.4(7) . .
C14B C15B C16B 119.4(9) .
C17B C16B C15B 120.4(9) .
C18B C17B C16B 120.0(9) .
C17B C18B C19B 120.4(10)
C14B C19B C18B 120.5(9) .
O1B C20B N1B 108.6(6) . .
O1B C21B C24B 109.0(6) . .
O1B C21B C22B 104.8(6) . .
C24B C21B C22B 118.7(6) .
N1B C22B C23B 109.9(7) . .
N1B C22B C21B 104.6(5) . .

C23B C22B C21B 112.2(7) .
C27B C24B C25B 108.1(8) .
C27B C24B C26B 111.3(8) .
C25B C24B C26B 108.8(8) .
C27B C24B C21B 110.6(7) .
C25B C24B C21B 109.3(7) .
C26B C24B C21B 108.8(7) .

Crystal data of (4*S*, 5*S*)-5-(tert-butyl)-4-methyl-3-[*N*-(9'-phenylfluoren-9'-yl)amino]oxazolidine (7e).



Ortep diagram of **7e**. Ellipsoids drawn at 50% probability

The crystal structure has been deposited at the Cambridge Crystallographic Data Centre and allocated the deposition number: CCDC 136230

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_symmetry_space_group_name_H-M	' P 2(1)2(1)2(1)'
_cell_length_a	8.735(2)
_cell_length_b	8.941(2)
_cell_length_c	28.128(6)
_cell_angle_alpha	90.00
_cell_angle_beta	90.00

_cell_angle_gamma 90.00
_cell_volume 2196.8(8)
_cell_formula_units_Z 4
_cell_measurement_temperature 293(2)
_cell_measurement_reflns_used 24
_cell_measurement_theta_min 10
_cell_measurement_theta_max 15
_exptl_crystal_description prism
_exptl_crystal_colour colorless
_exptl_crystal_size_max .54
_exptl_crystal_size_mid .20
_exptl_crystal_size_min .18
_exptl_crystal_density_diffrn 1.160
_exptl_crystal_F_000 824
_exptl_absorpt_coefficient_mu 0.069
_diffrn_ambient_temperature 293(2)
_diffrn_radiation_wavelength 0.71073
_diffrn_radiation_type MoK\a
_diffrn_radiation_source 'fine-focus sealed tube'
_diffrn_radiation_monochromator beta-filter
_diffrn_measurement_device_type CAD-4
_diffrn_measurement_method theta/2theta
_diffrn_detector_area_resol_mean ?
_diffrn_standards_number 3
_diffrn_standards_interval_count ?
_diffrn_standards_interval_time 60
_diffrn_standards_decay_% .1
_diffrn_reflns_number 1080
_diffrn_reflns_av_R_equivalents 0.0000
_diffrn_reflns_av_sigmaI/netI 0.0230
_diffrn_reflns_limit_h_min 0
_diffrn_reflns_limit_h_max 10
_diffrn_reflns_limit_k_min 0
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_reflns_number_total 1080
_reflns_number_gt 1080
_reflns_threshold_expression >2sigma(I)

_refine_special_details

Refinement of F^2^ against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2^, conventional R-factors R are based on F, with F set to zero for negative F^2^. The threshold expression of F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2^ are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

_refine_ls_structure_factor_coef Fsqd
_refine_ls_matrix_type fullcycle
_refine_ls_weighting_scheme
'calc w=1/[\s^2^(Fo^2^)+(0.0306P)^2^+0.5997P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary direct
_atom_sites_solution_secondary difmap
_atom_sites_solution_hydrogens difmap
_refine_ls_hydrogen_treatment mixed
_refine_ls_extinction_method SHELXL
_refine_ls_extinction_coef 0.0008(8)
_refine_ls_extinction_expression
'Fc^*^=kFc[1+0.001xFc^2^\l^3^/sin(2\q)]^-1/4^'
_refine_ls_abs_structure_details
'Flack H D (1983), Acta Cryst. A39, 876-881'
_refine_ls_abs_structure_Flack -6(4)
_refine_ls_number_reflns 1080
_refine_ls_number_parameters 379
_refine_ls_number_restraints 0
_refine_ls_R_factor_all 0.0274
_refine_ls_R_factor_gt 0.0274
_refine_ls_wR_factor_ref 0.0650
_refine_ls_wR_factor_gt 0.0650
_refine_ls_goodness_of_fit_ref 1.090
_refine_ls_restrained_S_all 1.090
_refine_ls_shift/su_max 0.201
_refine_ls_shift/su_mean 0.127

Atomic coordinates:

O1 O 0.3127(4) 0.5782(3) 0.04626(11) 0.0652(10) Uani 1 d.
N1 N 0.3310(4) 0.3507(4) 0.08689(11) 0.0459(9) Uani 1 d.
C1 C 0.4052(5) 0.3598(5) 0.13374(13) 0.0430(10) Uani 1 d.
C2 C 0.4159(5) 0.5135(5) 0.15764(15) 0.0504(12) Uani 1 d.
C3 C 0.4924(6) 0.6403(7) 0.1435(2) 0.0663(14) Uani 1 d.
C4 C 0.4873(7) 0.7664(7) 0.1731(3) 0.0849(19) Uani 1 d.
C5 C 0.4144(8) 0.7618(9) 0.2164(3) 0.093(2) Uani 1 d.
C6 C 0.3396(7) 0.6352(8) 0.2310(2) 0.0799(17) Uani 1 d.

C7 C 0.3410(6) 0.5110(6) 0.20104(16) 0.0590(13) Uani 1 d.
C8 C 0.2745(5) 0.3648(7) 0.20922(15) 0.0570(12) Uani 1 d.
C9 C 0.1881(7) 0.3060(10) 0.24672(19) 0.0801(19) Uani 1 d.
C10 C 0.1400(7) 0.1629(11) 0.2449(3) 0.092(2) Uani 1 d.
C11 C 0.1758(7) 0.0723(9) 0.2066(3) 0.0848(18) Uani 1 d.
C12 C 0.2610(6) 0.1286(6) 0.1697(2) 0.0645(14) Uani 1 d.
C13 C 0.3099(5) 0.2744(5) 0.17048(14) 0.0491(11) Uani 1 d.
C14 C 0.5646(5) 0.2840(5) 0.13046(15) 0.0482(11) Uani 1 d.
C15 C 0.5840(6) 0.1616(6) 0.10160(18) 0.0644(14) Uani 1 d.
C16 C 0.7228(7) 0.0858(7) 0.1011(2) 0.0838(19) Uani 1 d.
C17 C 0.8413(6) 0.1310(8) 0.1287(2) 0.0781(17) Uani 1 d.
C18 C 0.8237(6) 0.2542(7) 0.15730(19) 0.0690(15) Uani 1 d.
C19 C 0.6858(6) 0.3316(6) 0.15750(16) 0.0546(12) Uani 1 d.
C20 C 0.3995(6) 0.4431(6) 0.05009(19) 0.0569(13) Uani 1 d.
C21 C 0.1773(5) 0.5631(5) 0.07456(17) 0.0514(11) Uani 1 d.
C22 C 0.1671(5) 0.3941(5) 0.08398(16) 0.0497(12) Uani 1 d.
C23 C 0.0922(8) 0.2965(7) 0.0468(2) 0.0693(15) Uani 1 d.
C24 C 0.0458(5) 0.6558(6) 0.05321(17) 0.0617(13) Uani 1 d.
C25 C 0.0189(10) 0.6188(9) 0.0002(3) 0.095(2) Uani 1 d.
C26 C 0.0903(9) 0.8204(6) 0.0564(3) 0.0853(19) Uani 1 d.
C27 C -0.0966(7) 0.6290(9) 0.0823(3) 0.094(2) Uani 1 d.
H3 H 0.535(4) 0.641(5) 0.1149(13) 0.040(13) Uiso 1 d.
H4 H 0.540(6) 0.854(6) 0.1640(16) 0.078(17) Uiso 1 d.
H5 H 0.415(7) 0.860(7) 0.238(2) 0.13(2) Uiso 1 d.
H6 H 0.268(8) 0.625(8) 0.264(2) 0.16(3) Uiso 1 d.
H9 H 0.171(7) 0.379(6) 0.2695(19) 0.086(19) Uiso 1 d.
H10 H 0.075(7) 0.112(6) 0.2714(19) 0.096(18) Uiso 1 d.
H11 H 0.135(6) -0.031(6) 0.2062(16) 0.084(18) Uiso 1 d.
H12 H 0.283(5) 0.070(4) 0.1428(14) 0.043(13) Uiso 1 d.
H15 H 0.500(4) 0.129(4) 0.0815(14) 0.050(12) Uiso 1 d.
H16 H 0.724(6) 0.005(6) 0.0802(17) 0.082(18) Uiso 1 d.
H17 H 0.943(6) 0.073(5) 0.1272(14) 0.074(15) Uiso 1 d.
H18 H 0.910(6) 0.294(5) 0.1794(16) 0.084(16) Uiso 1 d.
H19 H 0.675(5) 0.419(4) 0.1800(13) 0.046(11) Uiso 1 d.
H201 H 0.505(5) 0.475(4) 0.0583(12) 0.043(13) Uiso 1 d.
H202 H 0.392(5) 0.386(5) 0.0175(16) 0.070(15) Uiso 1 d.
H21 H 0.200(5) 0.610(5) 0.1093(16) 0.076(15) Uiso 1 d.
H22 H 0.117(5) 0.374(5) 0.1192(16) 0.082(16) Uiso 1 d.
H231 H 0.152(5) 0.319(5) 0.0145(17) 0.080(16) Uiso 1 d.
H232 H -0.019(7) 0.317(6) 0.0465(19) 0.11(2) Uiso 1 d.
H233 H 0.116(5) 0.188(5) 0.0536(15) 0.064(15) Uiso 1 d.

H251 H 0.123(12) 0.632(11) -0.015(3) 0.22(5) Uiso 1 d.
H252 H -0.052(8) 0.705(8) -0.011(2) 0.15(3) Uiso 1 d.
H253 H -0.034(7) 0.511(7) -0.002(2) 0.13(3) Uiso 1 d.
H261 H -0.001(7) 0.884(7) 0.044(2) 0.12(2) Uiso 1 d.
H262 H 0.180(7) 0.839(7) 0.033(2) 0.11(2) Uiso 1 d.
H263 H 0.122(7) 0.854(7) 0.095(2) 0.14(3) Uiso 1 d.
H271 H -0.169(6) 0.694(5) 0.0704(16) 0.077(15) Uiso 1 d.
H272 H -0.133(7) 0.520(7) 0.081(2) 0.13(2) Uiso 1 d.
H273 H -0.052(7) 0.663(7) 0.120(2) 0.12(2) Uiso 1 d.
Anisotropic thermal parameters:
O1 0.0481(17) 0.062(2) 0.085(2) 0.0258(19) 0.0200(19) 0.0121(17)
N1 0.0435(19) 0.050(2) 0.0444(18) 0.001(2) 0.0011(18) 0.007(2)
C1 0.039(2) 0.045(2) 0.045(3) 0.004(2) 0.002(2) 0.004(2)
C2 0.042(3) 0.054(3) 0.055(3) -0.001(2) -0.008(2) 0.005(2)
C3 0.058(3) 0.063(4) 0.078(4) -0.003(4) -0.008(3) 0.000(3)
C4 0.074(4) 0.051(4) 0.130(6) -0.012(4) -0.035(4) -0.003(3)
C5 0.085(4) 0.096(6) 0.098(5) -0.040(5) -0.026(4) 0.029(5)
C6 0.068(4) 0.092(5) 0.080(4) -0.032(4) -0.013(4) 0.010(4)
C7 0.045(3) 0.076(4) 0.056(3) -0.012(3) -0.016(3) 0.011(3)
C8 0.037(2) 0.092(4) 0.042(3) 0.003(3) -0.005(2) 0.009(3)
C9 0.057(3) 0.132(6) 0.052(3) 0.010(4) 0.003(3) 0.016(4)
C10 0.056(4) 0.134(7) 0.087(5) 0.051(5) -0.002(3) 0.000(4)
C11 0.054(3) 0.087(4) 0.113(5) 0.046(5) -0.004(4) 0.001(4)
C12 0.053(3) 0.068(4) 0.072(4) 0.017(4) -0.003(3) 0.005(3)
C13 0.036(2) 0.060(3) 0.051(3) 0.015(2) 0.000(2) 0.004(2)
C14 0.041(2) 0.052(3) 0.052(3) 0.010(2) -0.001(2) 0.005(2)
C15 0.050(3) 0.066(3) 0.078(4) -0.009(3) -0.003(3) 0.012(3)
C16 0.066(4) 0.087(5) 0.099(5) -0.015(4) 0.004(3) 0.032(4)
C17 0.047(3) 0.101(5) 0.087(4) 0.017(4) 0.005(3) 0.026(4)
C18 0.044(3) 0.092(4) 0.071(3) 0.020(3) -0.007(3) 0.001(3)
C19 0.046(3) 0.066(3) 0.052(3) 0.007(3) 0.002(2) 0.002(3)
C20 0.051(3) 0.066(3) 0.054(3) 0.001(3) 0.008(3) 0.006(3)
C21 0.044(2) 0.050(3) 0.061(3) 0.009(2) 0.007(3) 0.001(2)
C22 0.045(2) 0.052(3) 0.053(3) 0.006(2) -0.002(3) 0.002(2)
C23 0.070(4) 0.062(4) 0.076(4) -0.002(3) -0.019(4) -0.002(3)
C24 0.049(3) 0.065(3) 0.071(3) 0.012(3) 0.009(3) 0.012(3)
C25 0.106(6) 0.096(6) 0.081(4) 0.022(4) -0.023(4) 0.032(5)
C26 0.080(4) 0.051(4) 0.126(6) 0.013(4) 0.011(5) 0.019(3)
C27 0.053(3) 0.094(5) 0.136(6) 0.035(5) 0.013(4) 0.025(4)
Bond lengths:
O1 C20 1.430(6).

O1 C21 1.432(5).
N1 C20 1.453(6).
N1 C1 1.471(5).
N1 C22 1.485(5).
C1 C2 1.532(6).
C1 C13 1.531(6).
C1 C14 1.551(6).
C2 C3 1.375(7).
C2 C7 1.385(6).
C3 C4 1.403(8).
C4 C5 1.375(9).
C5 C6 1.370(9).
C6 C7 1.395(7).
C7 C8 1.450(7).
C8 C13 1.391(6).
C8 C9 1.399(7).
C9 C10 1.347(10).
C10 C11 1.384(9).
C11 C12 1.373(8).
C12 C13 1.372(7).
C14 C15 1.373(6).
C14 C19 1.371(6).
C15 C16 1.389(8).
C16 C17 1.356(8).
C17 C18 1.373(8).
C18 C19 1.389(7).
C21 C22 1.536(6).
C21 C24 1.539(6).
C22 C23 1.511(7).
C24 C27 1.507(8).
C24 C26 1.525(8).
C24 C25 1.547(8).

Bond angles:

C20 O1 C21 108.4(4).
C20 N1 C1 115.1(4).
C20 N1 C22 102.1(3).
C1 N1 C22 117.4(3).
N1 C1 C2 118.0(3).
N1 C1 C13 109.7(3).
C2 C1 C13 100.6(3).
N1 C1 C14 108.5(3).

C2 C1 C14 111.3(4).
C13 C1 C14 108.1(4).
C3 C2 C7 119.9(5).
C3 C2 C1 129.9(4).
C7 C2 C1 110.1(4).
C2 C3 C4 118.3(6).
C5 C4 C3 121.2(7).
C4 C5 C6 120.8(6).
C5 C6 C7 118.2(6).
C2 C7 C6 121.6(6).
C2 C7 C8 110.1(4).
C6 C7 C8 128.2(6).
C13 C8 C9 119.5(6).
C13 C8 C7 108.1(4).
C9 C8 C7 132.4(6).
C10 C9 C8 119.7(7).
C9 C10 C11 121.0(7).
C12 C11 C10 119.7(7).
C11 C12 C13 120.4(7).
C12 C13 C8 119.7(5).
C12 C13 C1 129.2(5).
C8 C13 C1 111.1(4).
C15 C14 C19 118.7(5).
C15 C14 C1 119.6(4).
C19 C14 C1 121.6(4).
C14 C15 C16 120.1(6).
C17 C16 C15 121.1(6).
C16 C17 C18 119.2(6).
C17 C18 C19 120.0(6).
C14 C19 C18 120.9(5).
O1 C20 N1 108.4(4).
O1 C21 C22 103.7(4).
O1 C21 C24 110.4(4).
C22 C21 C24 123.6(4).
N1 C22 C23 107.7(4).
N1 C22 C21 102.2(4).
C23 C22 C21 118.3(4).
C27 C24 C26 109.4(6).
C27 C24 C21 108.6(4).
C26 C24 C21 107.8(5).
C27 C24 C25 111.3(6).

C26 C24 C25 107.6(6).

C21 C24 C25 112.0(5).