Supporting Information

**Rh(III)-Catalyzed Oxidative Annulation of Sulfoximines with Arylalkynyl Silanes via
Desilylation**

Vinayak Hanchate, Nachimuthu Muniraj and Kandikere Ramaiah Prabhu*

Department of Organic Chemistry,
Indian Institute of Science,
Bangalore 560 012, Karnataka, India

*E-mail: prabhu@iisc.ac.in

Contents

2	Deuterium incorporation studies	SI-3
3	Competitive experiment	SI-4
4	Crystal structure for compound 4ai	SI-5
5	Crystal data for compound 4ai	SI-6
5	^1H and ^{13}C NMR spectra for sulfoximines	SI-17
6	^1H and ^{13}C NMR spectra for sulfoximine derivatives	SI-25

Deuterium incorporation studies

Mechanistic investigation (H/D) exchange reaction:

In a 8-mL screw cap reaction vial, sulfoximine **1a** (0.2 mmol), D_2O (10 equiv), rhodium catalyst (5 mol %), $Cu(OAc)_2 \cdot H_2O$ (20 mol %), $AgSbF_6$ (20 mol %) were added followed by the addition of toluene (2 mL). This vial was sealed with a screw cap, placed in a pre-heated metal block at 100 °C for 4 h. After completion of the reaction, the reaction mixture was cooled to room temperature. The crude reaction mixture was purified on a flash column using EtOAc/ petroleum (1:1) ether to give the desired product **deuterio-1a** in 99% yield. The deuterium incorporation was calculated from 1H NMR spectroscopy (see the following 1H NMR spectra).

Competitive experiment:

In a 8-mL screw cap reaction vial, 1:1 ratio of **1a-d₂** (100% D) [ie. by weighing 0.125 mmol of **deuterio-1a** 80% D, which contains 0.1 mmol of **1a-d₂** (100% D) and 0.025 mmol of **1a**] and **1a** (0.075 mmol) were taken. (Now the reaction vial contains 0.1 mmol of each of **1a** and **1a-d₂** (100% D)). Then were added **2a** (0.1 mmol), rhodium catalyst (5 mol %), Cu(OAc)₂.H₂O (0.2 equiv), AgSbF₆ (20 mol %) and toluene (2 mL) and the vial was flushed with O₂ and sealed with a screw cap immediately. Then the reaction mixture was stirred at 100 °C for 4 h and concentrated under vacuum. The crude reaction mixture was purified on a column chromatography using EtOAc/petroleum ether mixture (1:1). The obtained product was subjected to ¹H NMR measurement to calculate the kinetic isotopic effect (See the following ¹H NMR spectrum).

Crystal structure for compound 4ai (50% ellipsoid probability): **Crystal data for compound 4ai:**

Bond precision: C-C = 0.0036 Å Wavelength: 0.71073

Cell: a= 15.6015(5) b= 10.7198 (4) c= 10.2858 (4)

alpha= 90 beta= 98.036 (4) gamma= 90

Temperature: 293K

	Calculated
Volume	1703.36(11)
Space group	P 21/c
Hall group	-P 2ybc
Moiety formula	C ₂₁ H ₁₅ N O ₂ S

Sum formula	C ₂₁ H ₁₅ N O ₂ S
Mr	345.40
D _x , g cm ⁻³	1.347
Z	4
Mu (mm ⁻¹)	0.204
F ₀₀₀	720.0
F ₀₀₀ '	720.79
h, k, l _{max}	20,13,13
N _{ref}	3912

Data completeness= 0.998 Theta (max)= 27.474

R (reflections) = 0.0549 (2934) wR₂ (reflections) = 0.1618 (3905)

S = 1.054 N_{par}= 230

The ORTEP diagram and Crystal Parameters of **4ai** in thermal ellipsoids are drawn at 50% probability level. The crystal of suitable quality was obtained from slow evaporation of solution of **4ai** in ethyl acetate, and was analyzed by single crystal diffractometer. Atomic coordinates, bond lengths, bond angles, and thermal parameters for this compound have been deposited at the Cambridge Crystallographic Data Centre. CCDC 1914164 contains supplementary crystallographic data.

data_shelx

```

_audit_creation_method      'SHELXL-2016/6'
_shelx_SHELXL_version_number '2016/6'
_chemical_name_systematic   4-(1-oxido-1-phenylbenzo[e]
                             [1,2]thiazin-3-yl)benzaldehyde
_chemical_name_common       ?
_chemical_melting_point     ?
_chemical_formula_moiety    ?
_chemical_formula_sum       'C21 H15 N1 O2 S1'
_chemical_formula_weight    345.40

```

```

loop_
  _atom_type_symbol
  _atom_type_description
  _atom_type_scatter_dispersion_real
  _atom_type_scatter_dispersion_imag
  _atom_type_scatter_source
  'C' 'C' 0.0033 0.0016
  'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
  'H' 'H' 0.0000 0.0000
  'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
  'N' 'N' 0.0061 0.0033
  'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
  'O' 'O' 0.0106 0.0060
  'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
  'S' 'S' 0.1246 0.1234
  'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

_space_group_crystal_system      monoclinic
_space_group_IT_number           14
_space_group_name_H-M_alt        'P 21/c'
_space_group_name_Hall           '-P 2ybc'

_shelx_space_group_comment
;
The symmetry employed for this shelxl refinement is uniquely defined
by the following loop, which should always be used as a source of
symmetry information in preference to the above space-group names.
They are only intended as comments.
;

loop_
  _space_group_symop_operation_xyz
  'x, y, z'
  '-x, y+1/2, -z+1/2'
  '-x, -y, -z'
  'x, -y-1/2, z-1/2'

_cell_length_a      15.6015(5)
_cell_length_b      10.7198(4)
_cell_length_c      10.2858(4)
_cell_angle_alpha    90
_cell_angle_beta     98.036(4)
_cell_angle_gamma     90
_cell_volume         1703.36(11)
_cell_formula_units_Z 4
_cell_measurement_temperature 293(2)
_cell_measurement_reflns_used 6529
_cell_measurement_theta_min 3.7980
_cell_measurement_theta_max 26.1780

_exptl_crystal_description BLOCK

```

```

_exptl_crystal_colour          YELLOW
_exptl_crystal_density_meas    ?
_exptl_crystal_density_method  ?
_exptl_crystal_density_diffrn  1.347
_exptl_crystal_F_000           720
_exptl_transmission_factor_min  ?
_exptl_transmission_factor_max  ?
_exptl_crystal_size_max        ?
_exptl_crystal_size_mid        ?
_exptl_crystal_size_min        ?
_exptl_absorpt_coefficient_mu   0.204
_shelx_estimated_absorpt_T_min  ?
_shelx_estimated_absorpt_T_max  ?
_exptl_absorpt_correction_type  multi-scan
_exptl_absorpt_correction_T_min 0.90115
_exptl_absorpt_correction_T_max 1.00000
_exptl_absorpt_process_details  CrysAlisPro
_exptl_absorpt_special_details  ?
_diffn_ambient_temperature      293(2)
_diffn_radiation_wavelength     0.71073
_diffn_radiation_type           MoK\alpha
_diffn_source                    'micro-focus sealed X-ray tube'
_diffn_measurement_device_type   'Xcalibur, Eos, Nova'
_diffn_measurement_method        ?
_diffn_detector_area_resol_mean  ?
_diffn_reflns_number            22740
_diffn_reflns_av_unetI/netI      0.0338
_diffn_reflns_av_R_equivalents   0.0457
_diffn_reflns_limit_h_min        -20
_diffn_reflns_limit_h_max        20
_diffn_reflns_limit_k_min        -13
_diffn_reflns_limit_k_max        13
_diffn_reflns_limit_l_min        -13
_diffn_reflns_limit_l_max        13
_diffn_reflns_theta_min          3.251
_diffn_reflns_theta_max          27.474
_diffn_reflns_theta_full         25.242
_diffn_measured_fraction_theta_max 0.998
_diffn_measured_fraction_theta_full 0.998
_diffn_reflns_Laue_measured_fraction_max 0.998
_diffn_reflns_Laue_measured_fraction_full 0.998
_diffn_reflns_point_group_measured_fraction_max 0.998
_diffn_reflns_point_group_measured_fraction_full 0.998
_reflns_number_total             3905
_reflns_number_gt                2934
_reflns_threshold_expression      'I > 2\sigma(I)'
_reflns_Friedel_coverage         0.000
_reflns_Friedel_fraction_max     .
_reflns_Friedel_fraction_full    .

_reflns_special_details
;

```


Reflections were merged by SHELXL according to the crystal class for the calculation of statistics and refinement.

_reflns_Friedel_fraction is defined as the number of unique Friedel pairs measured divided by the number that would be possible theoretically, ignoring centric projections and systematic absences.

```
;
_computing_data_collection      ?
_computing_cell_refinement     ?
_computing_data_reduction      ?
_computing_structure_solution  ?
_computing_structure_refinement 'SHELXL-2016/6 (Sheldrick, 2016)'
_computing_molecular_graphics  ?
_computing_publication_material ?
_refine_special_details        ?
_refine_ls_structure_factor_coef Fsqd
_refine_ls_matrix_type         full
_refine_ls_weighting_scheme    calc
_refine_ls_weighting_details
'w=1/[\s^2^(Fo^2^)+(0.0736P)^2^+0.5669P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary   ?
_atom_sites_solution_secondary ?
_atom_sites_solution_hydrogens mixed
_refine_ls_hydrogen_treatment mixed
_refine_ls_extinction_method   none
_refine_ls_extinction_coef     .
_refine_ls_number_reflns      3905
_refine_ls_number_parameters   230
_refine_ls_number_restraints   0
_refine_ls_R_factor_all        0.0746
_refine_ls_R_factor_gt         0.0549
_refine_ls_wR_factor_ref       0.1618
_refine_ls_wR_factor_gt        0.1457
_refine_ls_goodness_of_fit_ref 1.054
_refine_ls_restrained_S_all    1.054
_refine_ls_shift/su_max        0.000
_refine_ls_shift/su_mean       0.000

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_U_iso_or_equiv
  _atom_site_adp_type
  _atom_site_occupancy
  _atom_site_site_symmetry_order
  _atom_site_calc_flag
  _atom_site_refinement_flags_posn
```

```

_atom_site_refinement_flags_adp
_atom_site_refinement_flags_occupancy
_atom_site_disorder_assembly
_atom_site_disorder_group
C1 C 0.5174(2) 0.9240(4) 0.7631(3) 0.0822(9) Uani 1 1 d . . . . .
H1 H 0.556381 0.859328 0.785991 0.099 Uiso 1 1 calc R U . . .
C2 C 0.45517(16) 0.9093(3) 0.6423(2) 0.0612(7) Uani 1 1 d . . . . .
C3 C 0.40308(17) 1.0066(3) 0.5890(3) 0.0625(7) Uani 1 1 d . . . . .
H3 H 0.407379 1.084559 0.629040 0.075 Uiso 1 1 calc R U . . .
C4 C 0.34483(16) 0.9880(2) 0.4765(2) 0.0565(6) Uani 1 1 d . . . . .
H4 H 0.310566 1.054054 0.441227 0.068 Uiso 1 1 calc R U . . .
C5 C 0.33658(14) 0.8726(2) 0.4154(2) 0.0482(5) Uani 1 1 d . . . . .
C6 C 0.39039(17) 0.7758(3) 0.4691(3) 0.0667(7) Uani 1 1 d . . . . .
H6 H 0.387019 0.697880 0.429009 0.080 Uiso 1 1 calc R U . . .
C7 C 0.44831(18) 0.7955(3) 0.5808(3) 0.0748(8) Uani 1 1 d . . . . .
H7 H 0.483569 0.730235 0.615493 0.090 Uiso 1 1 calc R U . . .
C8 C 0.27151(14) 0.8523(2) 0.2975(2) 0.0471(5) Uani 1 1 d . . . . .
C9 C 0.24446(15) 0.7382(2) 0.2559(2) 0.0514(6) Uani 1 1 d . . . . .
C10 C 0.18215(14) 0.7174(2) 0.1415(2) 0.0489(5) Uani 1 1 d . . . . .
C11 C 0.15773(16) 0.5961(2) 0.0971(3) 0.0599(6) Uani 1 1 d . . . . .
H11 H 0.181392 0.527559 0.144757 0.072 Uiso 1 1 calc R U . . .
C12 C 0.10048(17) 0.5770(3) -0.0134(3) 0.0651(7) Uani 1 1 d . . . . .
H12 H 0.086330 0.495917 -0.040655 0.078 Uiso 1 1 calc R U . . .
C13 C 0.06280(17) 0.6769(3) -0.0863(3) 0.0630(7) Uani 1 1 d . . . . .
H13 H 0.023937 0.662674 -0.161958 0.076 Uiso 1 1 calc R U . . .
C14 C 0.08317(15) 0.7969(2) -0.0461(2) 0.0550(6) Uani 1 1 d . . . . .
H14 H 0.057702 0.864320 -0.093702 0.066 Uiso 1 1 calc R U . . .
C15 C 0.14243(14) 0.8166(2) 0.0667(2) 0.0464(5) Uani 1 1 d . . . . .
C16 C 0.19629(15) 1.0598(2) 0.0019(2) 0.0467(5) Uani 1 1 d . . . . .
C17 C 0.28152(16) 1.0571(2) -0.0188(2) 0.0558(6) Uani 1 1 d . . . . .
H17 H 0.321098 1.005709 0.031668 0.067 Uiso 1 1 calc R U . . .
C18 C 0.30766(19) 1.1319(3) -0.1160(3) 0.0703(8) Uani 1 1 d . . . . .
H18 H 0.365124 1.130887 -0.130722 0.084 Uiso 1 1 calc R U . . .
C19 C 0.2491(2) 1.2074(3) -0.1904(3) 0.0738(8) Uani 1 1 d . . . . .
H19 H 0.266967 1.257230 -0.255537 0.089 Uiso 1 1 calc R U . . .
C20 C 0.1642(2) 1.2097(3) -0.1693(3) 0.0757(8) Uani 1 1 d . . . . .
H20 H 0.124848 1.261256 -0.220062 0.091 Uiso 1 1 calc R U . . .
C21 C 0.13687(17) 1.1358(2) -0.0730(3) 0.0627(7) Uani 1 1 d . . . . .
H21 H 0.079335 1.137169 -0.058602 0.075 Uiso 1 1 calc R U . . .
N1 N 0.24303(14) 0.96210(18) 0.23357(19) 0.0543(5) Uani 1 1 d . . . . .
.
O1 O 0.52148(18) 1.0136(3) 0.8342(3) 0.1136(9) Uani 1 1 d . . . . .
O2 O 0.08423(11) 1.02178(16) 0.16006(16) 0.0580(5) Uani 1 1 d . . . . .
.
S1 S 0.16313(4) 0.96653(5) 0.12772(5) 0.0467(2) Uani 1 1 d . . . . .
H9A H 0.2678(16) 0.664(3) 0.305(2) 0.064(7) Uiso 1 1 d . . . . .

loop_
_atom_site_aniso_label
_atom_site_aniso_U_11
_atom_site_aniso_U_22
_atom_site_aniso_U_33

```

```

_atom_site_aniso_U_23
_atom_site_aniso_U_13
_atom_site_aniso_U_12
C1 0.074(2) 0.093(2) 0.076(2) -0.0013(18) -0.0051(16) 0.0016(18)
C2 0.0490(14) 0.0769(18) 0.0558(14) 0.0095(13) 0.0005(11) 0.0041(13)
C3 0.0652(16) 0.0643(16) 0.0559(15) -0.0011(12) 0.0018(12) 0.0052(13)
C4 0.0571(15) 0.0562(15) 0.0542(14) 0.0068(11) 0.0008(11) 0.0119(11)
C5 0.0462(12) 0.0539(13) 0.0457(11) 0.0073(10) 0.0104(9) 0.0070(10)
C6 0.0605(16) 0.0577(16) 0.0781(18) 0.0022(13) -0.0036(13) 0.0148(13)
C7 0.0631(17) 0.0731(19) 0.0815(19) 0.0108(16) -0.0136(14) 0.0194(14)
C8 0.0451(12) 0.0507(13) 0.0464(12) 0.0078(10) 0.0092(9) 0.0103(10)
C9 0.0523(13) 0.0454(13) 0.0566(14) 0.0096(11) 0.0081(11) 0.0067(11)
C10 0.0466(12) 0.0450(12) 0.0575(13) 0.0049(10) 0.0161(10) 0.0028(10)
C11 0.0612(15) 0.0450(13) 0.0747(17) 0.0031(12) 0.0140(13) -0.0012(11)
C12 0.0629(16) 0.0529(15) 0.0815(19) -0.0109(14) 0.0171(14) -
0.0107(12)
C13 0.0523(14) 0.0706(17) 0.0654(16) -0.0109(13) 0.0058(12) -
0.0042(13)
C14 0.0505(13) 0.0593(15) 0.0543(13) -0.0009(11) 0.0043(10) 0.0052(11)
C15 0.0442(11) 0.0462(12) 0.0499(12) -0.0012(10) 0.0106(9) 0.0016(9)
C16 0.0549(13) 0.0399(11) 0.0439(12) 0.0012(9) 0.0012(10) 0.0000(10)
C17 0.0548(14) 0.0551(14) 0.0556(14) 0.0020(11) 0.0004(11) -0.0017(11)
C18 0.0635(16) 0.078(2) 0.0701(17) 0.0000(15) 0.0113(13) -0.0193(15)
C19 0.093(2) 0.0625(18) 0.0650(17) 0.0142(14) 0.0087(15) -0.0214(16)
C20 0.088(2) 0.0620(17) 0.0720(18) 0.0233(14) -0.0054(15) 0.0013(15)
C21 0.0616(15) 0.0582(15) 0.0662(16) 0.0156(13) 0.0018(12) 0.0057(12)
N1 0.0656(13) 0.0450(11) 0.0487(11) 0.0042(8) -0.0047(9) 0.0061(9)
O1 0.109(2) 0.124(2) 0.0977(19) -0.0123(17) -0.0236(15) 0.0081(17)
O2 0.0599(11) 0.0588(11) 0.0568(10) 0.0018(8) 0.0126(8) 0.0171(8)
S1 0.0520(4) 0.0430(3) 0.0446(3) 0.0034(2) 0.0043(2) 0.0085(2)

```

```
_geom_special_details
```

```
;
```

All esds (except the esd in the dihedral angle between two l.s. planes)

are estimated using the full covariance matrix. The cell esds are taken

into account individually in the estimation of esds in distances, angles

and torsion angles; correlations between esds in cell parameters are only

used when they are defined by crystal symmetry. An approximate (isotropic)

treatment of cell esds is used for estimating esds involving l.s. planes.

```
;
```

```
loop_
```

```
_geom_bond_atom_site_label_1
```

```
_geom_bond_atom_site_label_2
```

```
_geom_bond_distance
```

```
_geom_bond_site_symmetry_2
```

geom_bond_publ_flag

C1 O1 1.204(4) . ?
 C1 C2 1.475(4) . ?
 C2 C7 1.370(4) . ?
 C2 C3 1.388(4) . ?
 C3 C4 1.382(3) . ?
 C4 C5 1.385(3) . ?
 C5 C6 1.398(3) . ?
 C5 C8 1.485(3) . ?
 C6 C7 1.376(4) . ?
 C8 C9 1.345(3) . ?
 C8 N1 1.390(3) . ?
 C9 C10 1.436(3) . ?
 C10 C15 1.405(3) . ?
 C10 C11 1.413(3) . ?
 C11 C12 1.360(4) . ?
 C12 C13 1.390(4) . ?
 C13 C14 1.375(4) . ?
 C14 C15 1.395(3) . ?
 C15 S1 1.739(2) . ?
 C16 C17 1.376(3) . ?
 C16 C21 1.385(3) . ?
 C16 S1 1.769(2) . ?
 C17 C18 1.386(4) . ?
 C18 C19 1.371(4) . ?
 C19 C20 1.372(4) . ?
 C20 C21 1.381(4) . ?
 N1 S1 1.537(2) . ?
 O2 S1 1.4460(17) . ?

loop_

geom_angle_atom_site_label_1
geom_angle_atom_site_label_2
geom_angle_atom_site_label_3
geom_angle
geom_angle_site_symmetry_1
geom_angle_site_symmetry_3
geom_angle_publ_flag
 O1 C1 C2 124.7(3) . . ?
 C7 C2 C3 118.9(2) . . ?
 C7 C2 C1 118.9(3) . . ?
 C3 C2 C1 122.2(3) . . ?
 C4 C3 C2 120.1(3) . . ?
 C3 C4 C5 121.1(2) . . ?
 C4 C5 C6 118.1(2) . . ?
 C4 C5 C8 120.7(2) . . ?
 C6 C5 C8 121.2(2) . . ?
 C7 C6 C5 120.3(3) . . ?
 C2 C7 C6 121.4(2) . . ?
 C9 C8 N1 123.7(2) . . ?
 C9 C8 C5 122.7(2) . . ?
 N1 C8 C5 113.5(2) . . ?

C8 C9 C10 123.2(2) . . ?
 C15 C10 C11 116.2(2) . . ?
 C15 C10 C9 121.9(2) . . ?
 C11 C10 C9 121.9(2) . . ?
 C12 C11 C10 121.6(2) . . ?
 C11 C12 C13 120.9(3) . . ?
 C14 C13 C12 119.8(2) . . ?
 C13 C14 C15 119.4(2) . . ?
 C14 C15 C10 122.1(2) . . ?
 C14 C15 S1 120.54(18) . . ?
 C10 C15 S1 117.19(17) . . ?
 C17 C16 C21 120.8(2) . . ?
 C17 C16 S1 119.32(17) . . ?
 C21 C16 S1 119.88(19) . . ?
 C16 C17 C18 119.2(2) . . ?
 C19 C18 C17 120.2(3) . . ?
 C18 C19 C20 120.4(3) . . ?
 C19 C20 C21 120.3(3) . . ?
 C20 C21 C16 119.1(3) . . ?
 C8 N1 S1 122.35(17) . . ?
 O2 S1 N1 118.81(11) . . ?
 O2 S1 C15 109.90(11) . . ?
 N1 S1 C15 108.56(11) . . ?
 O2 S1 C16 106.40(10) . . ?
 N1 S1 C16 104.15(11) . . ?
 C15 S1 C16 108.47(11) . . ?

_refine_diff_density_max 0.730
 _refine_diff_density_min -0.251
 _refine_diff_density_rms 0.044

_shelx_res_file

;

TITL RED1 in P2(1)/c

shelx.res

created by SHELXL-2016/6 at 14:43:55 on 13-Apr-2018

CELL 0.71073 15.6015 10.7198 10.2858 90.000 98.036 90.000

ZERR 4.00 0.0005 0.0004 0.0004 0.000 0.004 0.000

LATT 1

SYMM - X, 1/2 + Y, 1/2 - Z

SFAC C H N O S

UNIT 84 60 4 8 4

MERG 2

FMAP 2

PLAN 20

ACTA

L.S. 10

WGHT 0.073600 0.566900

FVAR 5.69392

C1 1 0.517433 0.923969 0.763080 11.00000 0.07361

0.09288 =

0.07566 -0.00126 -0.00511 0.00156

```

AFIX 43
H1 2 0.556381 0.859328 0.785991 11.00000 -1.20000
AFIX 0
C2 1 0.455172 0.909250 0.642253 11.00000 0.04901
0.07691 =
0.05583 0.00950 0.00054 0.00414
C3 1 0.403084 1.006603 0.588979 11.00000 0.06523
0.06431 =
0.05595 -0.00113 0.00182 0.00518
AFIX 43
H3 2 0.407379 1.084559 0.629040 11.00000 -1.20000
AFIX 0
C4 1 0.344826 0.987975 0.476504 11.00000 0.05711
0.05620 =
0.05421 0.00678 0.00079 0.01193
AFIX 43
H4 2 0.310566 1.054054 0.441227 11.00000 -1.20000
AFIX 0
C5 1 0.336585 0.872561 0.415404 11.00000 0.04619
0.05388 =
0.04568 0.00730 0.01037 0.00697
C6 1 0.390391 0.775846 0.469054 11.00000 0.06052
0.05770 =
0.07805 0.00224 -0.00364 0.01484
AFIX 43
H6 2 0.387019 0.697880 0.429009 11.00000 -1.20000
AFIX 0
C7 1 0.448306 0.795537 0.580843 11.00000 0.06310
0.07311 =
0.08146 0.01081 -0.01360 0.01941
AFIX 43
H7 2 0.483569 0.730235 0.615493 11.00000 -1.20000
AFIX 0
C8 1 0.271509 0.852328 0.297452 11.00000 0.04514
0.05066 =
0.04636 0.00778 0.00921 0.01027
C9 1 0.244461 0.738151 0.255926 11.00000 0.05232
0.04539 =
0.05657 0.00963 0.00810 0.00673
C10 1 0.182152 0.717414 0.141455 11.00000 0.04659
0.04502 =
0.05755 0.00490 0.01608 0.00282
C11 1 0.157726 0.596059 0.097136 11.00000 0.06123
0.04503 =
0.07468 0.00313 0.01404 -0.00116
AFIX 43
H11 2 0.181392 0.527559 0.144757 11.00000 -1.20000
AFIX 0
C12 1 0.100478 0.576971 -0.013412 11.00000 0.06287
0.05291 =
0.08149 -0.01092 0.01706 -0.01072
AFIX 43

```

```

H12    2    0.086330    0.495917   -0.040655    11.00000    -1.20000
AFIX    0
C13    1    0.062799    0.676934   -0.086283    11.00000     0.05228
0.07062 =
          0.06539   -0.01093    0.00577   -0.00421
AFIX   43
H13    2    0.023937    0.662674   -0.161958    11.00000    -1.20000
AFIX    0
C14    1    0.083173    0.796933   -0.046120    11.00000     0.05050
0.05934 =
          0.05427   -0.00094    0.00425    0.00523
AFIX   43
H14    2    0.057702    0.864320   -0.093702    11.00000    -1.20000
AFIX    0
C15    1    0.142435    0.816645    0.066722    11.00000     0.04418
0.04624 =
          0.04989   -0.00115    0.01060    0.00164
C16    1    0.196293    1.059769    0.001937    11.00000     0.05486
0.03985 =
          0.04390    0.00117    0.00116    0.00005
C17    1    0.281520    1.057088   -0.018847    11.00000     0.05477
0.05509 =
          0.05555    0.00203    0.00039   -0.00169
AFIX   43
H17    2    0.321098    1.005709    0.031668    11.00000    -1.20000
AFIX    0
C18    1    0.307659    1.131887   -0.115976    11.00000     0.06350
0.07773 =
          0.07012   -0.00002    0.01126   -0.01925
AFIX   43
H18    2    0.365124    1.130887   -0.130722    11.00000    -1.20000
AFIX    0
C19    1    0.249062    1.207366   -0.190405    11.00000     0.09339
0.06247 =
          0.06495    0.01421    0.00875   -0.02140
AFIX   43
H19    2    0.266967    1.257230   -0.255537    11.00000    -1.20000
AFIX    0
C20    1    0.164180    1.209711   -0.169299    11.00000     0.08822
0.06204 =
          0.07200    0.02325   -0.00537    0.00130
AFIX   43
H20    2    0.124848    1.261256   -0.220062    11.00000    -1.20000
AFIX    0
C21    1    0.136871    1.135839   -0.072969    11.00000     0.06160
0.05823 =
          0.06617    0.01556    0.00180    0.00568
AFIX   43
H21    2    0.079335    1.137169   -0.058602    11.00000    -1.20000
AFIX    0
N1     3    0.243033    0.962097    0.233573    11.00000     0.06562
0.04500 =

```

```

      0.04869    0.00420   -0.00468    0.00607
O1      4      0.521483    1.013589    0.834178    11.00000    0.10860
0.12375 =
      0.09770   -0.01226   -0.02359    0.00812
O2      4      0.084229    1.021776    0.160060    11.00000    0.05988
0.05876 =
      0.05677    0.00176    0.01260    0.01707
S1      5      0.163125    0.966534    0.127721    11.00000    0.05195
0.04302 =
      0.04458    0.00337    0.00434    0.00846
H9A     2      0.267797    0.663728    0.304756    11.00000    0.06359
HKLF      4

```

```

REM RED1 in P2(1)/c
REM R1 = 0.0549 for 2934 Fo > 4sig(Fo) and 0.0746 for all
3905 data
REM 230 parameters refined using 0 restraints

```

END

```

WGHT      0.0736      0.5669

```

```

REM Highest difference peak 0.730, deepest hole -0.251, 1-sigma
level 0.044

```

```

Q1      1      0.5633    0.8309    0.8153    11.00000    0.05    0.73
Q2      1      0.1801    1.0201    0.0635    11.00000    0.05    0.22
Q3      1      0.1730    0.7783    0.0925    11.00000    0.05    0.21
Q4      1      0.1407    0.8764    0.1036    11.00000    0.05    0.20
Q5      1      0.2030    0.9526    0.2010    11.00000    0.05    0.17
Q6      1      0.4409    0.9628    0.5866    11.00000    0.05    0.16
Q7      1      0.2326    0.7981    0.3098    11.00000    0.05    0.15
Q8      1      0.1003    0.6375   -0.0570    11.00000    0.05    0.15
Q9      1      0.1877    0.6628    0.0998    11.00000    0.05    0.15
Q10     1      0.3171    0.9158    0.4625    11.00000    0.05    0.15
Q11     1      0.2472    1.0160    0.2641    11.00000    0.05    0.14
Q12     1      0.2635    1.1391   -0.1640    11.00000    0.05    0.14
Q13     1      0.3370    0.8297    0.4632    11.00000    0.05    0.14
Q14     1      0.2637    0.9150    0.2551    11.00000    0.05    0.14
Q15     1      0.4057    0.7135    0.3741    11.00000    0.05    0.13
Q16     1      0.4753    0.9235    0.6735    11.00000    0.05    0.13
Q17     1      0.2783    0.9422    0.2105    11.00000    0.05    0.13
Q18     1      0.0994    0.7991    0.0425    11.00000    0.05    0.13
Q19     1      0.0817    1.1009   -0.0885    11.00000    0.05    0.13
Q20     1      0.1093    1.1182    0.1818    11.00000    0.05    0.12

```

;

```

_shelx_res_checksum 18849

```


^1H and ^{13}C NMR spectra for sulfoximines

SM-1

8.05
8.04
8.03
7.52
7.51
7.50
7.49
7.49
7.47
7.47
7.46
7.45
7.45
7.28

— 2.95

— 0.00

SM-1

SM-2

SM-2

143.34
140.81129.84
127.9277.48
77.16
76.84

21.53

SM-4

SM-8

SM-8

SM-3

SM-3

— 162.83

— 135.58

— 129.84

— 114.36

77.48
77.16
76.84

— 55.68

SM-5

SM-5

166.60
164.06

139.39

130.77
130.67116.65
116.4377.48
77.16
76.84

SM-6

SM-6

SM-7

7.88
7.86
7.63
7.61
7.27

2.44

0.00

SM-7

132.69
129.62
128.28

77.48
77.16
76.84

SM-15

SM-15

^1H and ^{13}C NMR spectra for sulfoximine derivatives

VH-02-019

VH-02-019

VH-02-204

VH-02-204

VH-01-258

VH-02-060

VH-02-060

VH-01-364

VH-01-364

VH-01-360

VH-01-360

VH-02-046

VH-02-046

VH-02-022

VH-02-022

VH-02-022

VH-02-035

VH-02-035

VH-01-369-1

7.993
7.979
7.910
7.895
7.612
7.601
7.555
7.455
7.440
7.418
7.322
7.305
7.207
6.780

— 2.376

— 0.000

VH-01-369

VH-01-370

VH-02-051

VH-02-TMSOme

VH-02-029

VH-02-059

VH-02-059

VH-01-376

VH-01-376

VH-01-376

— -113.15

VH-02-061

VH-02-061

VH-01-375

VH-01-375

VH-01-373-1

VH-01-373

VH-01-371

VH-01-371

VH-02-007

VH-02-007

VH-02-037

VH-02-037