Supplementary Material only for review purpose

Oligomeric Allylpalladium(II) Complexes of β-Substituted Ethylselenolates: Syntheses, structures and thermal decomposition

Liladhar B. Kumbhare, Amey Wadawale, Sanjio S. Zade, Vimal K. Jain

Supplementary Figure S-1. Variable temperature ^{1}H NMR spectra of **1b** in CD_2Cl_2

Supplementary Figure S-2. Variable temperature ^{1}H NMR spectra of **2b** in CD_2Cl_2

Supplementary Figure S-3. Mass spectrum of **1a**

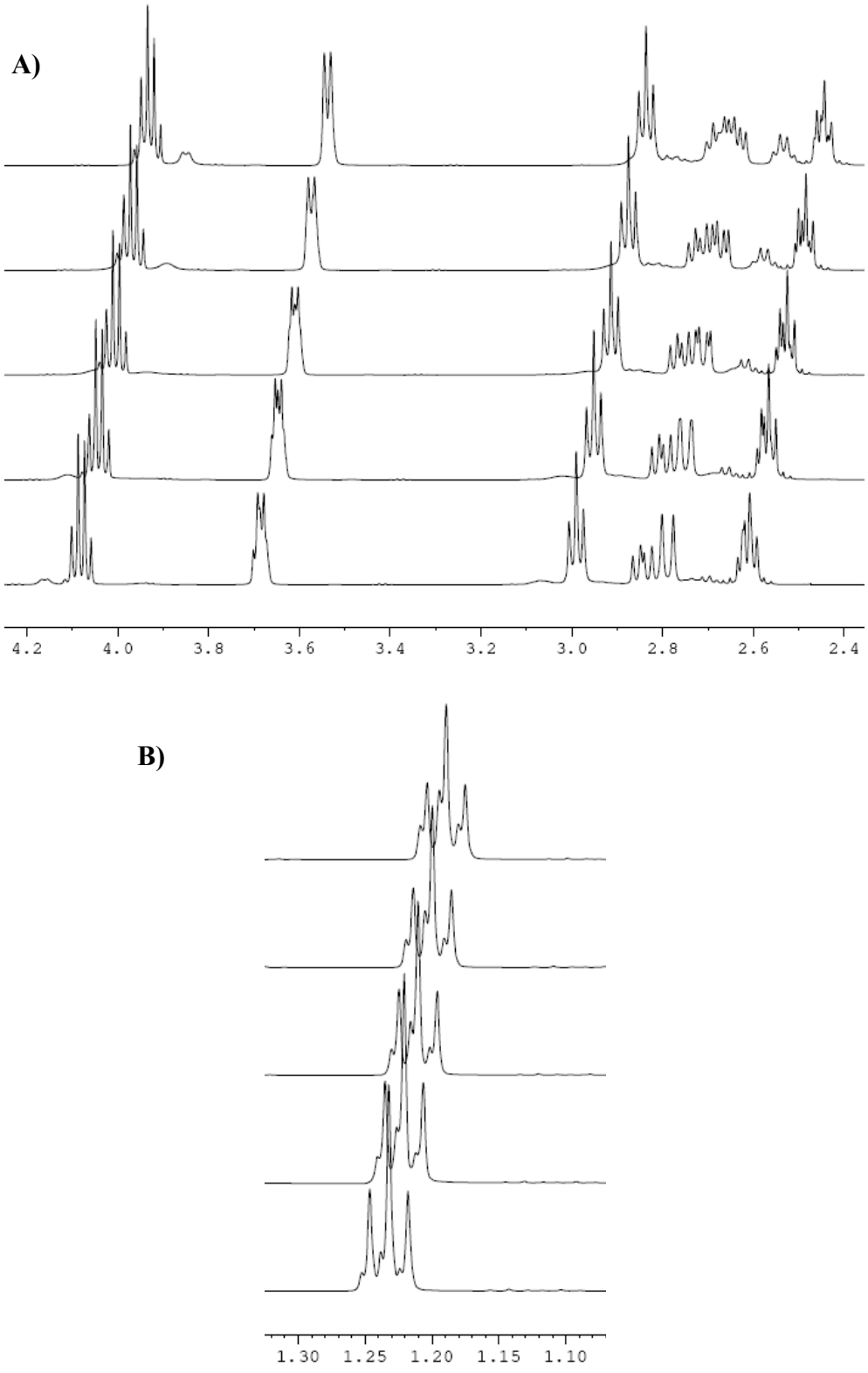
Supplementary Figure S-4. XRD pattern for Pd_7Se_2 (JCPDS 44-0877) obtained by decomposition of **1b** in furnace at 180° C under argon atmosphere for 2 h.

Supplementary Figure S-5. XRD spectra of Pd_7Se_4 obtained by heating **1b** phenyl ether at 140° C for 2h

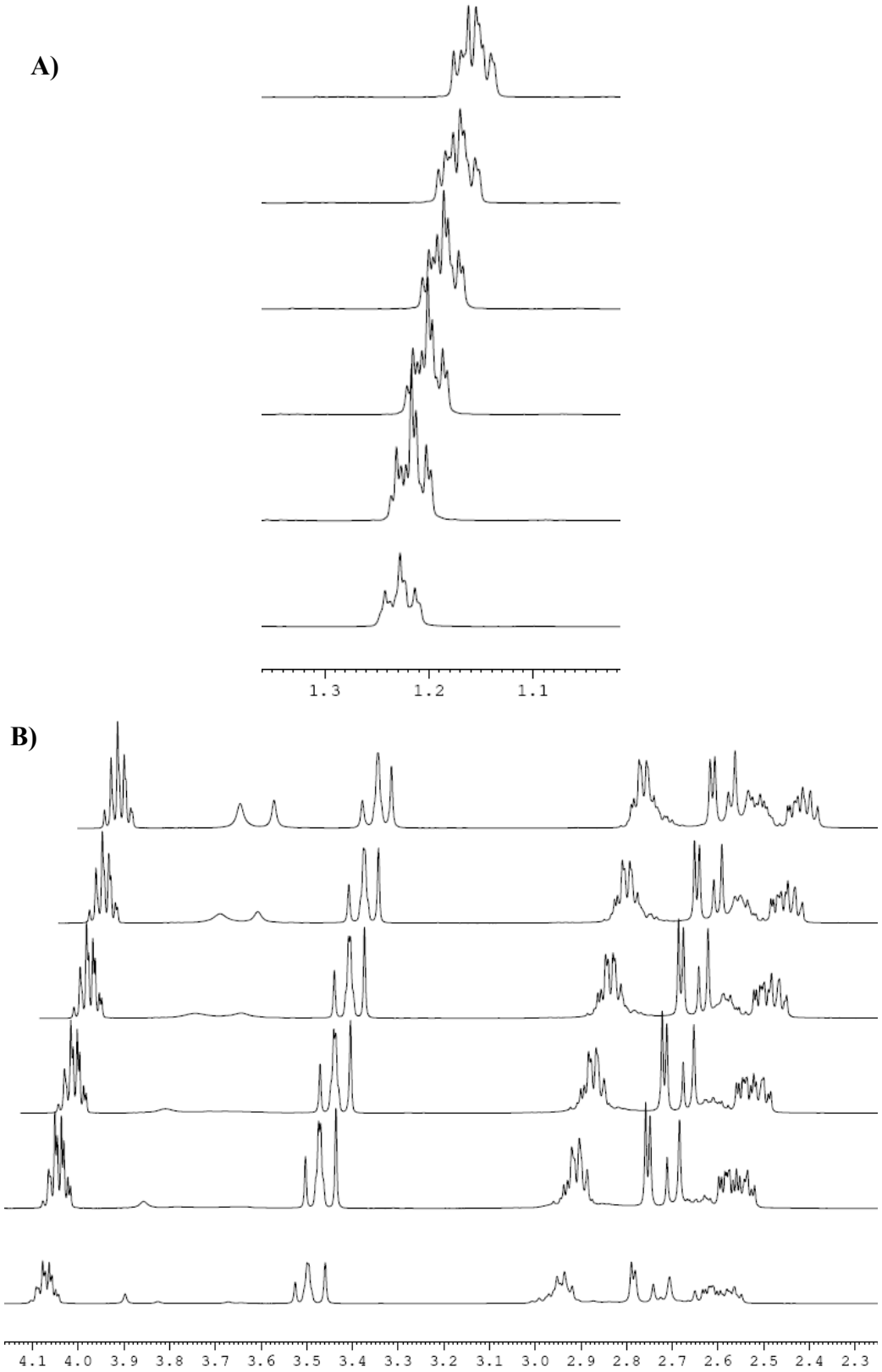
Supplementary Table S-1. Calculated absolute energies at B3LYP/6-31G*/sdd (all values are in Hartrees).

CIF Data for $[Pd(\mu\text{–}SeCH_2CH_2COOEt)(\eta^3\text{–}C_3H_5)]_3$ (**1b**)

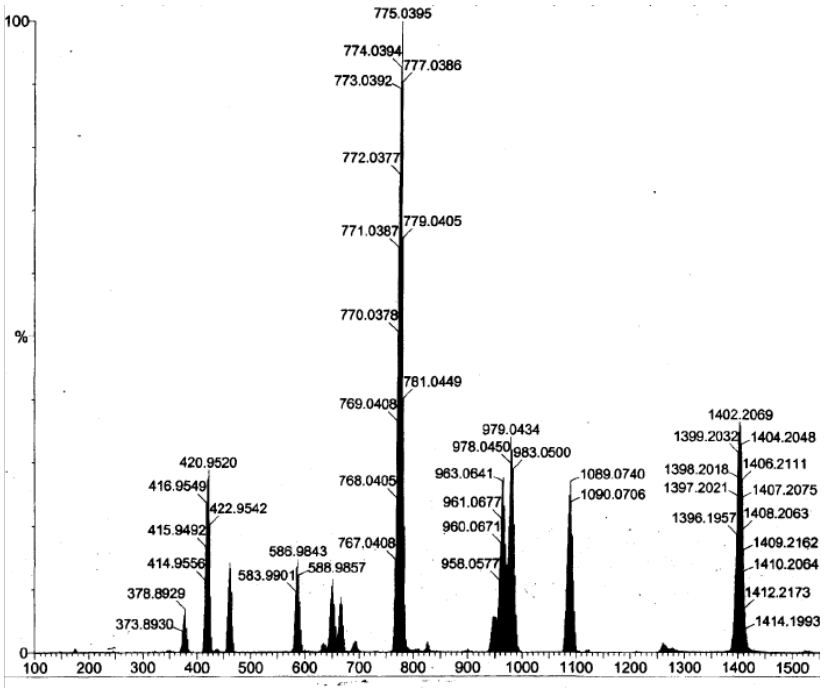
Data for optimized Geometries at B3LYP/G-31G*/sdd for oligomers



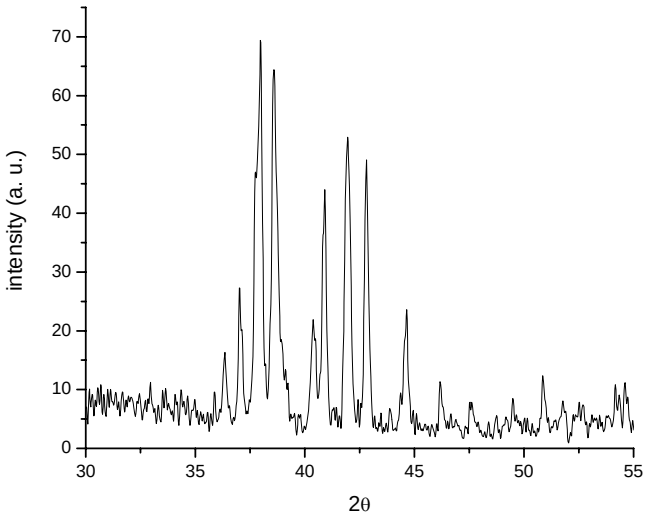
Supplementary Figure S-1. Variable temperature ^{1}H NMR spectra of **1b** in CD_2Cl_2



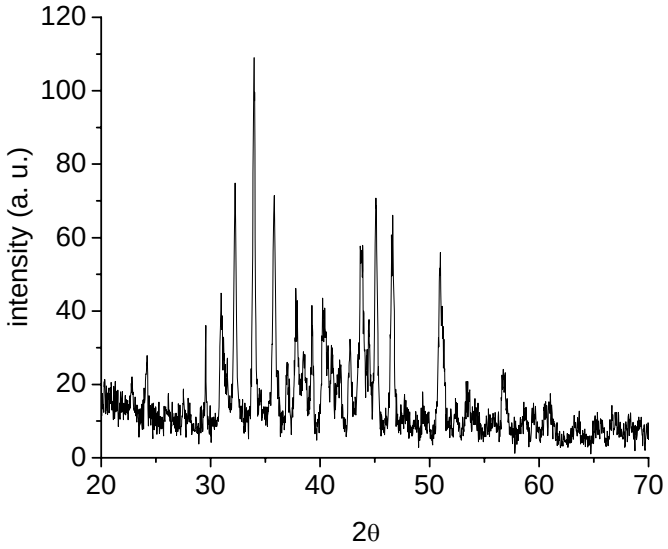
Supplementary Figure S-2. Variable temperature ^{1}H NMR spectra of **2b** in CD_2Cl_2



Supplementary Figure S-1. Mass spectrum of **1a**



Supplementary Figure S-2. XRD pattern for Pd_7Se_2 (JCPDS 44-0877) obtained by decomposition of **1b** in furnace at 180° C under argon atmosphere for 2 h.



Supplementary Figure S-3. XRD spectra of Pd_7Se_4 obtained by heating **1b** phenyl ether at 140° C for 2h

Table S1. Calculated absolute energies at B3LYP/6-31G*/sdd (all values are in Hartrees).

Compound	ΔE	ZPVE	ΔG°	Single point (CH_2Cl_2 solvent)	Single point (CH_3OH solvent)
M2$_x$	-5368.2955831	0.219382	-5368.126838	-5368.3043004	-5368.3063940
M2$_{1a}$	-5902.6619890	0.365034	-5902.366493	-5902.6770183	-5902.6799365
M2$_{2a}$	-5446.9337383	0.275205	-5446.712732	-5446.9414507	-5446.9433322
M3$_x$	-8052.4474098	0.330701	-8052.180501	-8052.4615090	-8052.4651998
M3$_{1a}$	-8853.9935413	0.547320	-8853.538789	-8854.0167128	-8854.0259639
M3$_{2a}$	-8170.4021681	0.414110	-8170.057607	-8170.4146129	-8170.4180069
M4$_x$	-10736.5909805	0.440052	-10736.230841	-10736.6063672	-10736.6108244
M4$_{1a}$	-11805.3301495	0.731088	-11804.716478	-11805.3543632	-11805.3596018

CIF for [Pd(μ–SeCH$_2$CH$_2$COOEt)(η^3–C$_3$H$_5$)]$_3$ (1b)

```
data_lbk-19

_audit_creation_method            SHELXL-97
_chemical_name_systematic
;
 ?
;
_chemical_name_common             ?
_chemical_melting_point           ?
_chemical_formula_moiety          ?
_chemical_formula_sum
 'C24 H42 O6 Pd3 Se3'
_chemical_formula_weight          982.66

loop_
 _atom_type_symbol
 _atom_type_description
 _atom_type_scat_dispersion_real
 _atom_type_scat_dispersion_imag
 _atom_type_scat_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'
 'O'  'O'   0.0106   0.0060
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Se'  'Se'  -0.0929   2.2259
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Pd'  'Pd'  -0.9988   1.0072
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

_symmetry_cell_setting                monoclinic
_symmetry_space_group_name_H-M        'P 1 21/a 1'
_symmetry_space_group_name_Hall       '-P 2yab'
_symmetry_Int_Tables_number           14

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

_cell_length_a                    30.966(7)
_cell_length_b                    6.795(3)
_cell_length_c                    15.901(8)
_cell_angle_alpha                 90.00
_cell_angle_beta                  102.15(3)
_cell_angle_gamma                 90.00
_cell_volume                      3271(2)
```

```
_cell_formula_units_Z            4
_cell_measurement_temperature    298(2)
_cell_measurement_reflns_used         24
_cell_measurement_theta_min           9.4
_cell_measurement_theta_max           12.2

_exptl_crystal_description          'block'
_exptl_crystal_colour               'colorless'
_exptl_crystal_size_max          0.20
_exptl_crystal_size_mid          0.20
_exptl_crystal_size_min          0.20
_exptl_crystal_density_meas      ?
_exptl_crystal_density_diffrn    1.996
_exptl_crystal_density_method    'not measured'
_exptl_crystal_F_000             1896
_exptl_absorpt_coefficient_mu    5.003
_exptl_absorpt_correction_type        psi-scan
_exptl_absorpt_process_details        '(North, Phillips & Mathews,
1968)'
_exptl_absorpt_correction_T_min  0.4344
_exptl_absorpt_correction_T_max  0.4344


_exptl_special_details
;
 ?
;

_diffrn_ambient_temperature      298(2)
_diffrn_radiation_wavelength     0.71069
_diffrn_radiation_type           MoK\a
_diffrn_radiation_source         'fine-focus sealed tube'
_diffrn_radiation_monochromator  graphite
_diffrn_measurement_device_type      'Rigaku AFC7S'
_diffrn_measurement_method           \w
_diffrn_detector_area_resol_mean ?
_diffrn_standards_number             3
_diffrn_standards_interval_count     150
_diffrn_standards_decay_%            -1.59
_diffrn_reflns_number            9911
_diffrn_reflns_av_R_equivalents  0.0754
_diffrn_reflns_av_sigmaI/netI    0.2532
_diffrn_reflns_limit_h_min       -22
_diffrn_reflns_limit_h_max       40
_diffrn_reflns_limit_k_min       -8
_diffrn_reflns_limit_k_max       4
_diffrn_reflns_limit_l_min       -20
_diffrn_reflns_limit_l_max       20
_diffrn_reflns_theta_min         2.62
_diffrn_reflns_theta_max         27.50
_reflns_number_total             7428
_reflns_number_gt                2287
_reflns_threshold_expression     >2sigma(I)
```

```
_computing_data_collection            'WinAFC'
_computing_cell_refinement            'WinAFC'
_computing_data_reduction             'CrystalStructure'
_computing_structure_solution         'SIR92'
_computing_structure_refinement   'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics     'Ortep 3 for Windows'
_computing_publication_material   'WinGX 1.70.01'

_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            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0701P)^2^+0.0000P] where
P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      direct
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     constr
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_number_reflns          7428
_refine_ls_number_parameters      306
_refine_ls_number_restraints      0
_refine_ls_R_factor_all           0.2853
_refine_ls_R_factor_gt            0.0730
_refine_ls_wR_factor_ref          0.2185
_refine_ls_wR_factor_gt           0.1533
_refine_ls_goodness_of_fit_ref    0.986
_refine_ls_restrained_S_all       0.986
_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_symmetry_multiplicity
 _atom_site_calc_flag
 _atom_site_refinement_flags
 _atom_site_disorder_assembly
 _atom_site_disorder_group
C1 C 0.5507(7) 0.194(2) 1.0197(11) 0.086(6) Uani 1 1 d . . .
H1A H 0.5771 0.1145 1.0381 0.103 Uiso 1 1 calc R . .
H1B H 0.5361 0.2292 1.0659 0.103 Uiso 1 1 calc R . .
C2 C 0.5260(7) 0.151(3) 0.9474(15) 0.102 Uani 1 1 d . . .
H2 H 0.5397 0.0448 0.9203 0.123 Uiso 1 1 calc R . .
C3 C 0.4957(6) 0.229(3) 0.8921(12) 0.087(5) Uani 1 1 d . . .
H3A H 0.4695 0.2715 0.9116 0.104 Uiso 1 1 calc R . .
H3B H 0.4893 0.1698 0.8353 0.104 Uiso 1 1 calc R . .
C4 C 0.4823(4) 0.587(3) 0.7255(10) 0.067(5) Uani 1 1 d . . .
H4A H 0.4768 0.4460 0.7221 0.080 Uiso 1 1 calc R . .
H4B H 0.4598 0.6477 0.7510 0.080 Uiso 1 1 calc R . .
C5 C 0.4798(7) 0.667(2) 0.6374(13) 0.090(7) Uani 1 1 d . . .
H5A H 0.5052 0.6200 0.6167 0.108 Uiso 1 1 calc R . .
H5B H 0.4821 0.8092 0.6416 0.108 Uiso 1 1 calc R . .
C6 C 0.4387(9) 0.617(4) 0.5706(16) 0.109(8) Uani 1 1 d . . .
C7 C 0.3884(9) 0.322(6) 0.5158(16) 0.204(19) Uani 1 1 d . . .
H7A H 0.3787 0.2297 0.5546 0.244 Uiso 1 1 calc R . .
H7B H 0.3648 0.4120 0.4914 0.244 Uiso 1 1 calc R . .
C8 C 0.4042(12) 0.246(7) 0.4649(19) 0.25(2) Uani 1 1 d . . .
H8A H 0.4259 0.3327 0.4495 0.370 Uiso 1 1 calc R . .
H8B H 0.3819 0.2176 0.4148 0.370 Uiso 1 1 calc R . .
H8C H 0.4183 0.1264 0.4881 0.370 Uiso 1 1 calc R . .
C9 C 0.5443(9) 0.197(3) 0.6785(16) 0.117(10) Uani 1 1 d . . .
H9A H 0.5214 0.1540 0.7076 0.140 Uiso 1 1 calc R . .
H9B H 0.5336 0.2220 0.6176 0.140 Uiso 1 1 calc R . .
C10 C 0.5833(11) 0.106(3) 0.7005(16) 0.116(9) Uani 1 1 d . . .
H10 H 0.5855 0.0032 0.7446 0.139 Uiso 1 1 calc R . .
C11 C 0.6212(7) 0.176(3) 0.6863(14) 0.091(7) Uani 1 1 d . . .
H11A H 0.6227 0.1965 0.6267 0.109 Uiso 1 1 calc R . .
H11B H 0.6480 0.1189 0.7206 0.109 Uiso 1 1 calc R . .
C12 C 0.6975(5) 0.539(2) 0.7273(8) 0.051 Uani 1 1 d . . .
H12A H 0.6996 0.3970 0.7242 0.062 Uiso 1 1 calc R . .
H12B H 0.6864 0.5885 0.6696 0.062 Uiso 1 1 calc R . .
C13 C 0.7428(5) 0.624(2) 0.7624(11) 0.068(5) Uani 1 1 d . . .
H13A H 0.7556 0.5627 0.8169 0.082 Uiso 1 1 calc R . .
H13B H 0.7403 0.7645 0.7722 0.082 Uiso 1 1 calc R . .
C14 C 0.7732(7) 0.589(2) 0.6969(14) 0.070(5) Uani 1 1 d . . .
C15 C 0.8471(6) 0.569(2) 0.6853(12) 0.072(5) Uani 1 1 d . . .
H15A H 0.8479 0.6838 0.6496 0.086 Uiso 1 1 calc R . .
H15B H 0.8388 0.4556 0.6480 0.086 Uiso 1 1 calc R . .
C16 C 0.8919(6) 0.535(3) 0.7436(12) 0.097(7) Uani 1 1 d . . .
H16A H 0.8975 0.6365 0.7866 0.146 Uiso 1 1 calc R . .
H16B H 0.9143 0.5384 0.7102 0.146 Uiso 1 1 calc R . .
H16C H 0.8922 0.4091 0.7711 0.146 Uiso 1 1 calc R . .
C17 C 0.7114(7) 0.175(3) 0.8963(11) 0.097(7) Uani 1 1 d . . .
```

```
H17A H 0.6983 0.0777 0.8536 0.117 Uiso 1 1 calc R . .
H17B H 0.7401 0.2202 0.8896 0.117 Uiso 1 1 calc R . .
C18 C 0.7070(9) 0.143(3) 0.9724(16) 0.112 Uani 1 1 d . . .
H18 H 0.7338 0.2058 1.0056 0.134 Uiso 1 1 calc R . .
C19 C 0.6818(7) 0.161(3) 1.0214(14) 0.103(7) Uani 1 1 d . . .
H19A H 0.6949 0.2007 1.0798 0.124 Uiso 1 1 calc R . .
H19B H 0.6594 0.0600 1.0181 0.124 Uiso 1 1 calc R . .
C20 C 0.6294(6) 0.533(3) 1.1151(10) 0.076(5) Uani 1 1 d . . .
H20A H 0.6060 0.5871 1.1399 0.091 Uiso 1 1 calc R . .
H20B H 0.6287 0.3905 1.1209 0.091 Uiso 1 1 calc R . .
C21 C 0.6729(5) 0.608(2) 1.1635(9) 0.054(4) Uani 1 1 d . . .
H21A H 0.6755 0.7466 1.1501 0.064 Uiso 1 1 calc R . .
H21B H 0.6965 0.5384 1.1446 0.064 Uiso 1 1 calc R . .
C22 C 0.6788(6) 0.585(2) 1.2606(13) 0.061(5) Uani 1 1 d . . .
C23 C 0.7304(5) 0.584(2) 1.3946(9) 0.060(5) Uani 1 1 d . . .
H23A H 0.7175 0.4643 1.4120 0.072 Uiso 1 1 calc R . .
H23B H 0.7183 0.6958 1.4196 0.072 Uiso 1 1 calc R . .
C24 C 0.7795(5) 0.579(3) 1.4228(10) 0.088(6) Uani 1 1 d . . .
H24A H 0.7915 0.7029 1.4099 0.132 Uiso 1 1 calc R . .
H24B H 0.7912 0.4756 1.3930 0.132 Uiso 1 1 calc R . .
H24C H 0.7874 0.5555 1.4837 0.132 Uiso 1 1 calc R . .
O1 O 0.4085(6) 0.726(3) 0.5479(11) 0.135(7) Uani 1 1 d . . .
O2 O 0.4353(6) 0.433(3) 0.5583(13) 0.177(10) Uani 1 1 d . . .
O3 O 0.7606(4) 0.5773(19) 0.6231(8) 0.083(4) Uani 1 1 d . . .
O4 O 0.8148(4) 0.5976(15) 0.7412(7) 0.070(3) Uani 1 1 d . . .
O5 O 0.6493(4) 0.5524(17) 1.2949(7) 0.075(4) Uani 1 1 d . . .
O6 O 0.7213(4) 0.6001(15) 1.2993(7) 0.069(3) Uani 1 1 d . . .
Se1 Se 0.54092(5) 0.6375(2) 0.79803(12) 0.0591(5) Uani 1 1 d . . .
Se2 Se 0.65588(6) 0.6105(2) 0.80157(11) 0.0547(5) Uani 1 1 d . . .
Se3 Se 0.61898(5) 0.6023(2) 0.99209(10) 0.0516(5) Uani 1 1 d . . .
Pd1 Pd 0.55274(4) 0.41616(17) 0.92279(8) 0.0542(4) Uani 1 1 d . . .
Pd2 Pd 0.59065(4) 0.40384(17) 0.74600(8) 0.0547(4) Uani 1 1 d . . .
Pd3 Pd 0.66802(4) 0.39158(17) 0.92761(8) 0.0526(4) Uani 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 0.097(15) 0.088(14) 0.064(13) 0.022(11) -0.004(12) -0.048(12)
C2 0.090 0.094 0.108 0.023 -0.013 -0.030
C3 0.059(11) 0.105(15) 0.081 0.019(12) -0.017(11) -0.031
C4 0.024(8) 0.107(14) 0.064(12) 0.016(11) -0.003(8) 0.018(10)
C5 0.105(17) 0.050(11) 0.095(16) 0.003(11) -0.021(14) 0.009(11)
C6 0.12(2) 0.10(2) 0.094(18) 0.007(17) -0.014(16) 0.008(19)
C7 0.075(19) 0.45(6) 0.07(2) -0.07(3) -0.022(16) 0.03(3)
C8 0.19(4) 0.45(6) 0.10(3) -0.10(3) 0.02(2) 0.05(4)
C9 0.13(2) 0.046(13) 0.16(2) -0.036(13) -0.006(18) 0.023(14)
C10 0.17(3) 0.067(16) 0.13(2) -0.041(15) 0.07(2) -0.043(18)
C11 0.082(16) 0.061(13) 0.128(19) -0.017(12) 0.018(15) 0.000(12)
C12 0.067 0.046 0.027 -0.004 -0.020 -0.021
```

```
C13 0.050(11) 0.082(13) 0.063(12) -0.010(10) -0.009(10) -0.005(10)
C14 0.078(15) 0.052(11) 0.077(15) 0.006(12) 0.009(13) -0.025(11)
C15 0.068(13) 0.068(12) 0.090(14) -0.007(10) 0.041(12) -0.002(10)
C16 0.057(13) 0.135(19) 0.095(16) -0.032(14) 0.006(12) -0.014(13)
C17 0.133(19) 0.102(15) 0.051(12) 0.006(11) 0.006(12) 0.075(14)
C18 0.147 0.095 0.104 0.038 0.050 0.087
C19 0.115(19) 0.083(15) 0.128(19) 0.031(13) 0.064(16) 0.029(13)
C20 0.061(11) 0.090(13) 0.084 -0.028(10) 0.034(10) -0.025
C21 0.051(10) 0.055(10) 0.052(11) 0.006(9) 0.005(8) 0.002(9)
C22 0.039(10) 0.035(9) 0.105(16) 0.014(10) 0.008(11) -0.005(9)
C23 0.085(14) 0.058(11) 0.040(10) 0.010(9) 0.019(9) 0.013(10)
C24 0.059(12) 0.17(2) 0.045(11) -0.002(12) 0.026(10) 0.019(13)
O1 0.117(14) 0.140(15) 0.121(14) 0.021(11) -0.036(11) 0.030(12)
O2 0.137(16) 0.119(15) 0.22(2) -0.038(14) -0.086(15) -0.012(13)
O3 0.081(9) 0.118(11) 0.053(8) 0.001(9) 0.018(7) -0.008(8)
O4 0.070(8) 0.065(8) 0.080(9) -0.004(7) 0.024(8) -0.028(7)
O5 0.069(9) 0.093(10) 0.063(8) -0.005(7) 0.012(7) -0.027(8)
O6 0.069(8) 0.080(8) 0.061(8) -0.004(7) 0.020(7) 0.001(7)
Se1 0.0539(11) 0.0475(11) 0.0717(12) 0.0042(9) 0.0034(9) -0.0010(8)
Se2 0.0563(10) 0.0510(10) 0.0569(11) 0.0026(9) 0.0125(9) -0.0064(9)
Se3 0.0516(10) 0.0487(10) 0.0545(10) -0.0018(9) 0.0112(8) -0.0077(8)
Pd1 0.0525(8) 0.0478(8) 0.0617(9) 0.0000(7) 0.0110(7) -0.0095(7)
Pd2 0.0560(8) 0.0435(7) 0.0646(9) 0.0024(7) 0.0127(7) -0.0080(7)
Pd3 0.0531(8) 0.0438(7) 0.0593(8) 0.0022(7) 0.0085(6) -0.0011(7)

_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 C2 1.27(2) . ?
C1 Pd1 2.169(15) . ?
C1 H1A 0.9700 . ?
C1 H1B 0.9700 . ?
C2 C3 1.26(2) . ?
C2 Pd1 2.057(19) . ?
C2 H2 0.9800 . ?
```

```
C3 Pd1 2.150(16) . ?
C3 H3A 0.9700 . ?
C3 H3B 0.9700 . ?
C4 C5 1.49(2) . ?
C4 Se1 1.966(13) . ?
C4 H4A 0.9700 . ?
C4 H4B 0.9700 . ?
C5 C6 1.51(3) . ?
C5 H5A 0.9700 . ?
C5 H5B 0.9700 . ?
C6 O1 1.19(2) . ?
C6 O2 1.27(2) . ?
C7 C8 1.15(3) . ?
C7 O2 1.65(3) . ?
C7 H7A 0.9700 . ?
C7 H7B 0.9700 . ?
C8 H8A 0.9600 . ?
C8 H8B 0.9600 . ?
C8 H8C 0.9600 . ?
C9 C10 1.34(3) . ?
C9 Pd2 2.13(2) . ?
C9 H9A 0.9700 . ?
C9 H9B 0.9700 . ?
C10 C11 1.33(3) . ?
C10 Pd2 2.15(2) . ?
C10 H10 0.9800 . ?
C11 Pd2 2.141(19) . ?
C11 H11A 0.9700 . ?
C11 H11B 0.9700 . ?
C12 C13 1.512(18) . ?
C12 Se2 1.982(15) . ?
C12 H12A 0.9700 . ?
C12 H12B 0.9700 . ?
C13 C14 1.56(2) . ?
C13 H13A 0.9700 . ?
C13 H13B 0.9700 . ?
C14 O3 1.159(19) . ?
C14 O4 1.33(2) . ?
C15 O4 1.484(18) . ?
C15 C16 1.52(2) . ?
C15 H15A 0.9700 . ?
C15 H15B 0.9700 . ?
C16 H16A 0.9600 . ?
C16 H16B 0.9600 . ?
C16 H16C 0.9600 . ?
C17 C18 1.26(2) . ?
C17 Pd3 2.123(17) . ?
C17 H17A 0.9700 . ?
C17 H17B 0.9700 . ?
C18 C19 1.22(2) . ?
C18 Pd3 2.109(17) . ?
C18 H18 0.9800 . ?
C19 Pd3 2.143(18) . ?
C19 H19A 0.9700 . ?
```

```
C19 H19B 0.9700 . ?
C20 C21 1.50(2) . ?
C20 Se3 1.972(17) . ?
C20 H20A 0.9700 . ?
C20 H20B 0.9700 . ?
C21 C22 1.52(2) . ?
C21 H21A 0.9700 . ?
C21 H21B 0.9700 . ?
C22 O5 1.181(19) . ?
C22 O6 1.334(18) . ?
C23 O6 1.486(16) . ?
C23 C24 1.49(2) . ?
C23 H23A 0.9700 . ?
C23 H23B 0.9700 . ?
C24 H24A 0.9600 . ?
C24 H24B 0.9600 . ?
C24 H24C 0.9600 . ?
Se1 Pd1 2.455(2) . ?
Se1 Pd2 2.472(2) . ?
Se2 Pd3 2.460(2) . ?
Se2 Pd2 2.466(2) . ?
Se3 Pd3 2.462(2) . ?
Se3 Pd1 2.464(2) . ?

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
C2 C1 Pd1 67.7(11) . . ?
C2 C1 H1A 116.9 . . ?
Pd1 C1 H1A 116.9 . . ?
C2 C1 H1B 116.9 . . ?
Pd1 C1 H1B 116.9 . . ?
H1A C1 H1B 113.9 . . ?
C3 C2 C1 139(3) . . ?
C3 C2 Pd1 76.7(12) . . ?
C1 C2 Pd1 77.3(12) . . ?
C3 C2 H2 109.3 . . ?
C1 C2 H2 109.3 . . ?
Pd1 C2 H2 109.3 . . ?
C2 C3 Pd1 68.6(11) . . ?
C2 C3 H3A 116.8 . . ?
Pd1 C3 H3A 116.8 . . ?
C2 C3 H3B 116.8 . . ?
Pd1 C3 H3B 116.8 . . ?
H3A C3 H3B 113.8 . . ?
C5 C4 Se1 110.2(12) . . ?
C5 C4 H4A 109.6 . . ?
Se1 C4 H4A 109.6 . . ?
C5 C4 H4B 109.6 . . ?
```

```
Se1 C4 H4B 109.6 . . ?
H4A C4 H4B 108.1 . . ?
C4 C5 C6 116.6(18) . . ?
C4 C5 H5A 108.2 . . ?
C6 C5 H5A 108.2 . . ?
C4 C5 H5B 108.2 . . ?
C6 C5 H5B 108.2 . . ?
H5A C5 H5B 107.3 . . ?
O1 C6 O2 122(3) . . ?
O1 C6 C5 124(2) . . ?
O2 C6 C5 111(2) . . ?
C8 C7 O2 91(3) . . ?
C8 C7 H7A 113.4 . . ?
O2 C7 H7A 113.4 . . ?
C8 C7 H7B 113.4 . . ?
O2 C7 H7B 113.4 . . ?
H7A C7 H7B 110.7 . . ?
C7 C8 H8A 109.5 . . ?
C7 C8 H8B 109.5 . . ?
H8A C8 H8B 109.5 . . ?
C7 C8 H8C 109.5 . . ?
H8A C8 H8C 109.5 . . ?
H8B C8 H8C 109.5 . . ?
C10 C9 Pd2 72.6(14) . . ?
C10 C9 H9A 116.3 . . ?
Pd2 C9 H9A 116.3 . . ?
C10 C9 H9B 116.3 . . ?
Pd2 C9 H9B 116.3 . . ?
H9A C9 H9B 113.3 . . ?
C11 C10 C9 125(3) . . ?
C11 C10 Pd2 71.6(12) . . ?
C9 C10 Pd2 71.0(14) . . ?
C11 C10 H10 116.3 . . ?
C9 C10 H10 116.3 . . ?
Pd2 C10 H10 116.3 . . ?
C10 C11 Pd2 72.2(13) . . ?
C10 C11 H11A 116.4 . . ?
Pd2 C11 H11A 116.4 . . ?
C10 C11 H11B 116.4 . . ?
Pd2 C11 H11B 116.4 . . ?
H11A C11 H11B 113.3 . . ?
C13 C12 Se2 110.8(10) . . ?
C13 C12 H12A 109.5 . . ?
Se2 C12 H12A 109.5 . . ?
C13 C12 H12B 109.5 . . ?
Se2 C12 H12B 109.5 . . ?
H12A C12 H12B 108.1 . . ?
C12 C13 C14 109.8(14) . . ?
C12 C13 H13A 109.7 . . ?
C14 C13 H13A 109.7 . . ?
C12 C13 H13B 109.7 . . ?
C14 C13 H13B 109.7 . . ?
H13A C13 H13B 108.2 . . ?
O3 C14 O4 128(2) . . ?
```

```
O3 C14 C13 124.2(19) . . ?
O4 C14 C13 107.1(16) . . ?
O4 C15 C16 107.4(15) . . ?
O4 C15 H15A 110.2 . . ?
C16 C15 H15A 110.2 . . ?
O4 C15 H15B 110.2 . . ?
C16 C15 H15B 110.2 . . ?
H15A C15 H15B 108.5 . . ?
C15 C16 H16A 109.5 . . ?
C15 C16 H16B 109.5 . . ?
H16A C16 H16B 109.5 . . ?
C15 C16 H16C 109.5 . . ?
H16A C16 H16C 109.5 . . ?
H16B C16 H16C 109.5 . . ?
C18 C17 Pd3 72.0(12) . . ?
C18 C17 H17A 116.4 . . ?
Pd3 C17 H17A 116.4 . . ?
C18 C17 H17B 116.4 . . ?
Pd3 C17 H17B 116.4 . . ?
H17A C17 H17B 113.4 . . ?
C19 C18 C17 144(3) . . ?
C19 C18 Pd3 74.9(13) . . ?
C17 C18 Pd3 73.2(12) . . ?
C19 C18 H18 101.3 . . ?
C17 C18 H18 101.3 . . ?
Pd3 C18 H18 101.3 . . ?
C18 C19 Pd3 71.8(13) . . ?
C18 C19 H19A 116.4 . . ?
Pd3 C19 H19A 116.4 . . ?
C18 C19 H19B 116.4 . . ?
Pd3 C19 H19B 116.4 . . ?
H19A C19 H19B 113.4 . . ?
C21 C20 Se3 111.7(11) . . ?
C21 C20 H20A 109.3 . . ?
Se3 C20 H20A 109.3 . . ?
C21 C20 H20B 109.3 . . ?
Se3 C20 H20B 109.3 . . ?
H20A C20 H20B 107.9 . . ?
C20 C21 C22 112.8(14) . . ?
C20 C21 H21A 109.0 . . ?
C22 C21 H21A 109.0 . . ?
C20 C21 H21B 109.0 . . ?
C22 C21 H21B 109.0 . . ?
H21A C21 H21B 107.8 . . ?
O5 C22 O6 125.9(18) . . ?
O5 C22 C21 123.3(16) . . ?
O6 C22 C21 110.8(16) . . ?
O6 C23 C24 105.7(13) . . ?
O6 C23 H23A 110.6 . . ?
C24 C23 H23A 110.6 . . ?
O6 C23 H23B 110.6 . . ?
C24 C23 H23B 110.6 . . ?
H23A C23 H23B 108.7 . . ?
C23 C24 H24A 109.5 . . ?
```

```
C23 C24 H24B 109.5 . . ?
H24A C24 H24B 109.5 . . ?
C23 C24 H24C 109.5 . . ?
H24A C24 H24C 109.5 . . ?
H24B C24 H24C 109.5 . . ?
C6 O2 C7 124(2) . . ?
C14 O4 C15 112.1(15) . . ?
C22 O6 C23 114.9(14) . . ?
C4 Se1 Pd1 109.2(5) . . ?
C4 Se1 Pd2 104.7(5) . . ?
Pd1 Se1 Pd2 83.08(7) . . ?
C12 Se2 Pd3 109.3(4) . . ?
C12 Se2 Pd2 103.5(4) . . ?
Pd3 Se2 Pd2 85.46(7) . . ?
C20 Se3 Pd3 106.7(5) . . ?
C20 Se3 Pd1 105.5(5) . . ?
Pd3 Se3 Pd1 92.50(7) . . ?
C2 Pd1 C3 34.8(6) . . ?
C2 Pd1 C1 35.0(6) . . ?
C3 Pd1 C1 66.6(6) . . ?
C2 Pd1 Se1 133.9(6) . . ?
C3 Pd1 Se1 101.8(5) . . ?
C1 Pd1 Se1 168.4(5) . . ?
C2 Pd1 Se3 134.1(6) . . ?
C3 Pd1 Se3 166.7(5) . . ?
C1 Pd1 Se3 100.7(5) . . ?
Se1 Pd1 Se3 90.88(7) . . ?
C9 Pd2 C11 67.2(8) . . ?
C9 Pd2 C10 36.5(8) . . ?
C11 Pd2 C10 36.1(7) . . ?
C9 Pd2 Se2 166.0(7) . . ?
C11 Pd2 Se2 99.5(6) . . ?
C10 Pd2 Se2 132.8(9) . . ?
C9 Pd2 Se1 101.0(7) . . ?
C11 Pd2 Se1 168.1(5) . . ?
C10 Pd2 Se1 133.6(8) . . ?
Se2 Pd2 Se1 92.02(7) . . ?
C18 Pd3 C17 34.7(7) . . ?
C18 Pd3 C19 33.3(7) . . ?
C17 Pd3 C19 67.1(7) . . ?
C18 Pd3 Se2 137.5(7) . . ?
C17 Pd3 Se2 103.0(5) . . ?
C19 Pd3 Se2 169.3(6) . . ?
C18 Pd3 Se3 133.1(7) . . ?
C17 Pd3 Se3 167.8(5) . . ?
C19 Pd3 Se3 100.7(6) . . ?
Se2 Pd3 Se3 89.19(8) . . ?

loop_
 _geom_torsion_atom_site_label_1
 _geom_torsion_atom_site_label_2
 _geom_torsion_atom_site_label_3
 _geom_torsion_atom_site_label_4
 _geom_torsion
```

```
 _geom_torsion_site_symmetry_1
 _geom_torsion_site_symmetry_2
 _geom_torsion_site_symmetry_3
 _geom_torsion_site_symmetry_4
 _geom_torsion_publ_flag
Pd1 C1 C2 C3 -52(3) . . . . ?
C1 C2 C3 Pd1 52(3) . . . . ?
Se1 C4 C5 C6 172.5(16) . . . . ?
C4 C5 C6 O1 101(3) . . . . ?
C4 C5 C6 O2 -62(3) . . . . ?
Pd2 C9 C10 C11 -50(2) . . . . ?
C9 C10 C11 Pd2 50(2) . . . . ?
Se2 C12 C13 C14 -172.9(11) . . . . ?
C12 C13 C14 O3 29(2) . . . . ?
C12 C13 C14 O4 -157.5(13) . . . . ?
Pd3 C17 C18 C19 29(4) . . . . ?
C17 C18 C19 Pd3 -29(4) . . . . ?
Se3 C20 C21 C22 171.0(10) . . . . ?
C20 C21 C22 O5 -16(2) . . . . ?
C20 C21 C22 O6 162.2(13) . . . . ?
O1 C6 O2 C7 -4(5) . . . . ?
C5 C6 O2 C7 159(2) . . . . ?
C8 C7 O2 C6 127(4) . . . . ?
O3 C14 O4 C15 -6(3) . . . . ?
C13 C14 O4 C15 -179.2(12) . . . . ?
C16 C15 O4 C14 -167.5(14) . . . . ?
O5 C22 O6 C23 -3(2) . . . . ?
C21 C22 O6 C23 178.7(11) . . . . ?
C24 C23 O6 C22 173.0(14) . . . . ?
C5 C4 Se1 Pd1 -161.4(11) . . . . ?
C5 C4 Se1 Pd2 -73.8(13) . . . . ?
C13 C12 Se2 Pd3 -79.8(11) . . . . ?
C13 C12 Se2 Pd2 -169.6(10) . . . . ?
C21 C20 Se3 Pd3 73.1(12) . . . . ?
C21 C20 Se3 Pd1 170.6(10) . . . . ?
C1 C2 Pd1 C3 -148(3) . . . . ?
C3 C2 Pd1 C1 148(3) . . . . ?
C3 C2 Pd1 Se1 -27(2) . . . . ?
C1 C2 Pd1 Se1 -174.7(11) . . . . ?
C3 C2 Pd1 Se3 168.5(11) . . . . ?
C1 C2 Pd1 Se3 20.9(19) . . . . ?
C2 C3 Pd1 C1 -19.5(16) . . . . ?
C2 C3 Pd1 Se1 160.4(15) . . . . ?
C2 C3 Pd1 Se3 -38(4) . . . . ?
C2 C1 Pd1 C3 19.4(15) . . . . ?
C2 C1 Pd1 Se1 19(4) . . . . ?
C2 C1 Pd1 Se3 -164.9(14) . . . . ?
C4 Se1 Pd1 C2 22.2(11) . . . . ?
Pd2 Se1 Pd1 C2 -81.0(10) . . . . ?
C4 Se1 Pd1 C3 6.8(8) . . . . ?
Pd2 Se1 Pd1 C3 -96.4(6) . . . . ?
C4 Se1 Pd1 C1 7(3) . . . . ?
Pd2 Se1 Pd1 C1 -96(3) . . . . ?
C4 Se1 Pd1 Se3 -168.9(5) . . . . ?
```

```
Pd2 Se1 Pd1 Se3 87.85(7) . . . . ?
C20 Se3 Pd1 C2 -30.3(12) . . . . ?
Pd3 Se3 Pd1 C2 77.7(10) . . . . ?
C20 Se3 Pd1 C3 -1(3) . . . . ?
Pd3 Se3 Pd1 C3 107(2) . . . . ?
C20 Se3 Pd1 C1 -18.3(8) . . . . ?
Pd3 Se3 Pd1 C1 89.7(6) . . . . ?
C20 Se3 Pd1 Se1 160.8(6) . . . . ?
Pd3 Se3 Pd1 Se1 -91.10(8) . . . . ?
C10 C9 Pd2 C11 25.1(16) . . . . ?
C10 C9 Pd2 Se2 45(4) . . . . ?
C10 C9 Pd2 Se1 -156.7(16) . . . . ?
C10 C11 Pd2 C9 -25.3(17) . . . . ?
C10 C11 Pd2 Se2 159.5(16) . . . . ?
C10 C11 Pd2 Se1 -34(4) . . . . ?
C11 C10 Pd2 C9 139(3) . . . . ?
C9 C10 Pd2 C11 -139(3) . . . . ?
C11 C10 Pd2 Se2 -28(2) . . . . ?
C9 C10 Pd2 Se2 -166.6(14) . . . . ?
C11 C10 Pd2 Se1 170.9(11) . . . . ?
C9 C10 Pd2 Se1 32(2) . . . . ?
C12 Se2 Pd2 C9 4(3) . . . . ?
Pd3 Se2 Pd2 C9 -104(3) . . . . ?
C12 Se2 Pd2 C11 22.9(7) . . . . ?
Pd3 Se2 Pd2 C11 -85.9(6) . . . . ?
C12 Se2 Pd2 C10 39.2(10) . . . . ?
Pd3 Se2 Pd2 C10 -69.6(9) . . . . ?
C12 Se2 Pd2 Se1 -154.4(4) . . . . ?
Pd3 Se2 Pd2 Se1 96.78(7) . . . . ?
C4 Se1 Pd2 C9 -18.3(9) . . . . ?
Pd1 Se1 Pd2 C9 89.8(7) . . . . ?
C4 Se1 Pd2 C11 -10(3) . . . . ?
Pd1 Se1 Pd2 C11 98(3) . . . . ?
C4 Se1 Pd2 C10 -37.2(12) . . . . ?
Pd1 Se1 Pd2 C10 70.9(10) . . . . ?
C4 Se1 Pd2 Se2 156.6(5) . . . . ?
Pd1 Se1 Pd2 Se2 -95.32(7) . . . . ?
C19 C18 Pd3 C17 -163(3) . . . . ?
C17 C18 Pd3 C19 163(3) . . . . ?
C19 C18 Pd3 Se2 -171.2(12) . . . . ?
C17 C18 Pd3 Se2 -9(2) . . . . ?
C19 C18 Pd3 Se3 16(2) . . . . ?
C17 C18 Pd3 Se3 178.2(12) . . . . ?
C18 C17 Pd3 C19 -10.2(18) . . . . ?
C18 C17 Pd3 Se2 174.1(17) . . . . ?
C18 C17 Pd3 Se3 -6(4) . . . . ?
C18 C19 Pd3 C17 10.6(19) . . . . ?
C18 C19 Pd3 Se2 34(5) . . . . ?
C18 C19 Pd3 Se3 -168.5(17) . . . . ?
C12 Se2 Pd3 C18 -4.9(12) . . . . ?
Pd2 Se2 Pd3 C18 97.9(11) . . . . ?
C12 Se2 Pd3 C17 -9.8(7) . . . . ?
Pd2 Se2 Pd3 C17 92.9(6) . . . . ?
C12 Se2 Pd3 C19 -32(3) . . . . ?
```

```
Pd2 Se2 Pd3 C19 71(3) . . . . ?
C12 Se2 Pd3 Se3 170.2(4) . . . . ?
Pd2 Se2 Pd3 Se3 -87.05(7) . . . . ?
C20 Se3 Pd3 C18 11.1(12) . . . . ?
Pd1 Se3 Pd3 C18 -95.9(11) . . . . ?
C20 Se3 Pd3 C17 16(3) . . . . ?
Pd1 Se3 Pd3 C17 -91(3) . . . . ?
C20 Se3 Pd3 C19 19.7(8) . . . . ?
Pd1 Se3 Pd3 C19 -87.3(6) . . . . ?
C20 Se3 Pd3 Se2 -164.3(5) . . . . ?
Pd1 Se3 Pd3 Se2 88.66(7) . . . . ?

_diffrn_measured_fraction_theta_max    0.989
_diffrn_reflns_theta_full              27.50
_diffrn_measured_fraction_theta_full   0.989
_refine_diff_density_max    1.098
_refine_diff_density_min   -1.190
_refine_diff_density_rms    0.207
```

Data for optimized Geometries at B3LYP/G-31G*/sdd for oligomers

$M2_x$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.348305	1.223799	0.740933
2	1	0	-3.922617	1.318878	-0.178861
3	6	0	-3.323396	-0.000046	1.446048
4	6	0	-3.348306	-1.223842	0.740847
5	1	0	-3.164235	-2.151148	1.275621
6	1	0	-3.164234	2.151067	1.275773
7	1	0	-3.922616	-1.318857	-0.178955
8	1	0	-3.012255	-0.000084	2.489986
9	1	0	3.164237	2.151065	1.275764
10	6	0	3.348306	1.223793	0.740930

11	1	0	3.922620	1.318865	-0.178864
12	6	0	3.323394	-0.000048	1.446054
13	6	0	3.348302	-1.223848	0.740860
14	1	0	3.012251	-0.000077	2.489991
15	1	0	3.922614	-1.318870	-0.178940
16	1	0	3.164228	-2.151150	1.275640
17	46	0	-1.663358	0.000003	0.038241
18	46	0	1.663358	-0.000003	0.038244
19	34	0	-0.000002	-1.653239	-0.835206
20	34	0	0.000003	1.653289	-0.835108
21	6	0	0.000007	3.195669	0.415964
22	1	0	0.892237	3.794163	0.220741
23	1	0	-0.892222	3.794165	0.220744
24	1	0	0.000008	2.848214	1.449173
25	6	0	-0.000008	-3.195690	0.415778
26	1	0	-0.000010	-2.848296	1.449008
27	1	0	-0.892238	-3.794173	0.220520
28	1	0	0.892221	-3.794175	0.220525

$M2_{1a}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.158117	2.752112	0.553796
2	1	0	2.432681	3.339761	-0.320876
3	6	0	0.967645	3.040239	1.255569
4	6	0	-0.178297	3.480433	0.555307
5	1	0	-1.128807	3.546386	1.077011
6	1	0	2.977130	2.260418	1.071941
7	1	0	-0.077706	4.121556	-0.318853
8	1	0	0.854531	2.669172	2.273371
9	1	0	1.128749	-3.546274	1.077147
10	6	0	0.178298	-3.480348	0.555330
11	1	0	0.077807	-4.121538	-0.318792
12	6	0	-0.967724	-3.040145	1.255466
13	6	0	-2.158120	-2.752046	0.553565
14	1	0	-0.854717	-2.669051	2.273271
15	1	0	-2.432572	-3.339689	-0.321145
16	1	0	-2.977190	-2.260356	1.071621
17	46	0	0.491749	1.560151	-0.267072
18	46	0	-0.491681	-1.560090	-0.267161
19	34	0	-1.579673	0.504604	-1.196756
20	34	0	1.579685	-0.504488	-1.196897
21	6	0	3.064774	-0.889846	0.076925
22	1	0	3.184733	-1.975491	0.118698
23	1	0	2.766185	-0.527421	1.059849
24	6	0	-3.064697	0.889830	0.077175
25	1	0	-2.766172	0.527153	1.060022
26	1	0	-3.184545	1.975477	0.119192
27	6	0	4.361952	-0.209771	-0.379160
28	1	0	4.136939	0.806089	-0.727187
29	1	0	4.826689	-0.747929	-1.208629
30	6	0	-4.361944	0.209999	-0.379041

31	1	0	-4.137045	-0.805804	-0.727330
32	1	0	-4.826664	0.748362	-1.208386
33	6	0	-5.337799	0.058590	0.773790
34	6	0	5.337789	-0.058546	0.773699
35	8	0	5.065396	0.462350	1.837526
36	8	0	-5.065263	-0.461917	1.837769
37	8	0	-6.556139	0.555509	0.480360
38	8	0	6.555916	-0.556143	0.480525
39	6	0	-7.544213	0.421020	1.516609
40	1	0	-7.223952	0.944016	2.421600
41	1	0	-8.452588	0.869742	1.113914
42	1	0	-7.708120	-0.633140	1.755527
43	6	0	7.543910	-0.421988	1.516896
44	1	0	8.452039	-0.871482	1.114508
45	1	0	7.708517	0.632143	1.755465
46	1	0	7.223131	-0.944437	2.422017

$M2_{2a}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.113561	1.209480	1.149103
2	1	0	2.657878	1.277797	2.135602
3	6	0	3.722253	0.000155	0.722978
4	6	0	3.113510	-1.209205	1.148873
5	1	0	3.452412	-2.151351	0.726021
6	1	0	3.452697	2.151675	0.726513
7	1	0	2.657425	-1.277588	2.135178
8	1	0	-3.452230	2.151250	0.726196
9	6	0	-3.113398	1.208990	1.148857
10	1	0	-2.657331	1.277134	2.135185
11	6	0	-3.722341	-0.000196	0.722798
12	6	0	-3.113870	-1.209651	1.148777
13	1	0	-2.657716	-1.277955	2.135053
14	1	0	-3.453018	-2.151795	0.726116
15	46	0	1.637469	0.000427	0.088315
16	46	0	-1.637405	-0.000405	0.088119
17	34	0	-0.000348	1.657688	-0.832434
18	34	0	0.000394	-1.657607	-0.832862
19	6	0	0.001016	-3.214880	0.399555
20	1	0	-0.891011	-3.811874	0.198402
21	1	0	0.893834	-3.810811	0.198768
22	1	0	0.000609	-2.880947	1.437042
23	6	0	-0.001084	3.215017	0.399897
24	1	0	-0.000951	2.881162	1.437411
25	1	0	0.891057	3.811894	0.198902
26	1	0	-0.893786	3.811038	0.198856
27	6	0	-4.799682	-0.000139	-0.337792
28	1	0	-4.738954	0.889339	-0.972632
29	1	0	-4.737490	-0.888452	-0.974145
30	1	0	-5.785669	-0.001423	0.145395
31	6	0	4.799445	-0.000007	-0.337777
32	1	0	5.785495	-0.000642	0.145302

33	1	0	4.737451	-0.888719	-0.973569
34	1	0	4.738353	0.889094	-0.973110

M3$_x$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.597888	2.125105	0.193146
2	46	0	-2.164096	-0.553414	0.171067
3	46	0	1.574334	-1.569867	0.187772
4	34	0	1.974735	0.514978	-1.143849
5	34	0	-1.448908	1.479096	-1.101454
6	34	0	-0.538735	-1.978663	-1.093078
7	6	0	2.164761	3.120076	1.371120
8	1	0	2.970595	2.533626	1.801542
9	1	0	2.471469	3.908902	0.686767
10	6	0	-1.048663	-3.860512	-0.717411
11	1	0	-0.305799	-4.511403	-1.183485
12	1	0	-1.091437	-4.053992	0.354115
13	6	0	-3.622688	0.326685	1.561994
14	1	0	-2.973240	0.603167	2.390534
15	1	0	-4.300500	1.101966	1.217963
16	6	0	1.705519	-3.414633	1.378768
17	1	0	0.815752	-3.820687	1.850679
18	1	0	2.210962	-4.080274	0.681399
19	6	0	3.448135	-1.700109	1.339195
20	1	0	4.087374	-2.230849	0.636011
21	1	0	3.878662	-0.805365	1.779020
22	6	0	3.872884	1.010167	-0.839320
23	1	0	4.103805	1.066677	0.224145
24	1	0	4.499543	0.253664	-1.316498
25	6	0	-2.990413	-2.032924	1.576371
26	1	0	-3.186654	-3.046603	1.240938
27	1	0	-2.290887	-1.937711	2.404768
28	6	0	-2.806662	2.876573	-0.716967
29	1	0	-2.938601	3.020398	0.355198
30	1	0	-2.472998	3.808297	-1.178860
31	6	0	-3.949357	-1.027228	1.329983
32	1	0	-4.815075	-1.263057	0.713148
33	6	0	2.416870	-2.378858	2.023139
34	1	0	1.996541	-1.930806	2.922326
35	6	0	0.930732	3.201397	2.051957
36	1	0	0.776600	2.588651	2.938988
37	6	0	-0.189764	3.776227	1.413796
38	1	0	-0.066365	4.617044	0.733599
39	1	0	-1.167683	3.689311	1.877643
40	1	0	-2.025935	-4.043257	-1.169878
41	1	0	4.050610	1.978938	-1.311187
42	1	0	-3.749780	2.564328	-1.170994

$M3_{1a}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.528264	-2.186907	-1.063567
2	46	0	-1.643381	1.512483	-1.049289
3	46	0	2.125072	0.613408	-1.111222
4	34	0	1.479092	-1.409514	0.216425
5	34	0	-1.962094	-0.604086	0.243132
6	34	0	0.478439	1.971314	0.197928
7	6	0	0.314418	-3.824880	-2.265256
8	1	0	1.287325	-3.707506	-2.732928
9	1	0	0.217275	-4.668259	-1.584168
10	6	0	0.897433	3.892337	-0.148766
11	1	0	1.015287	4.046413	-1.222188
12	1	0	0.029995	4.455002	0.201326
13	6	0	-3.339970	1.439944	-2.446866
14	1	0	-2.900263	0.881146	-3.271283
15	1	0	-4.312739	1.092179	-2.112258
16	6	0	3.111758	2.149630	-2.337867
17	1	0	2.520675	2.933833	-2.802040
18	1	0	3.901386	2.489270	-1.670107
19	6	0	3.802793	-0.193743	-2.292943
20	1	0	4.633927	-0.029252	-1.609329
21	1	0	3.735535	-1.190096	-2.719398
22	6	0	2.934951	-2.741463	-0.082996
23	1	0	3.862071	-2.242471	0.203403
24	6	0	-1.646337	3.198584	-2.467151
25	1	0	-1.327534	4.183152	-2.139767
26	1	0	-1.077352	2.766547	-3.288572
27	6	0	-3.844903	-1.194314	-0.064596
28	1	0	-3.895690	-2.227061	0.284675
29	6	0	-2.972394	2.784723	-2.221018
30	1	0	-3.618414	3.415377	-1.612055
31	6	0	3.211463	0.891677	-2.973162
32	1	0	2.604872	0.695715	-3.856258
33	6	0	-0.826727	-3.295819	-2.907759
34	1	0	-0.696098	-2.686890	-3.801190
35	6	0	-2.061540	-3.256632	-2.225764
36	1	0	-2.333725	-4.049332	-1.531051
37	1	0	-2.891298	-2.707619	-2.660196
38	1	0	2.979691	-2.994431	-1.143091
39	1	0	-4.061539	-1.169964	-1.133939
40	6	0	2.158568	4.331001	0.598280
41	1	0	3.034301	3.773309	0.257713
42	1	0	2.340151	5.396458	0.391182
43	6	0	-4.835932	-0.316118	0.702690
44	1	0	-4.793441	0.720791	0.359299
45	1	0	-5.855142	-0.687820	0.517858
46	6	0	2.718443	-3.999137	0.760762
47	1	0	1.790373	-4.506190	0.485286
48	1	0	3.547694	-4.698502	0.574309
49	6	0	-4.625256	-0.287312	2.208133
50	6	0	2.090386	4.162257	2.107352
51	6	0	2.657752	-3.753338	2.259955

52	8	0	1.849258	-4.250538	3.012850
53	8	0	2.975168	3.701674	2.795050
54	8	0	-4.626485	0.714621	2.889470
55	8	0	3.653031	-2.934428	2.664920
56	8	0	-4.472874	-1.532675	2.708077
57	8	0	0.922925	4.628573	2.602506
58	6	0	-4.225123	-1.604456	4.121823
59	1	0	-5.059743	-1.171947	4.680324
60	1	0	-4.119346	-2.666041	4.346884
61	1	0	-3.307625	-1.066297	4.373184
62	6	0	0.749240	4.477046	4.020805
63	1	0	1.533871	5.011344	4.563400
64	1	0	-0.230473	4.901068	4.242615
65	1	0	0.779726	3.419380	4.294965
66	6	0	3.656711	-2.611942	4.065269
67	1	0	3.763013	-3.518135	4.667798
68	1	0	4.510382	-1.949448	4.210749
69	1	0	2.727807	-2.105318	4.339410

$M3_{2a}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.198067	1.937290	-0.051709
2	46	0	-2.195027	-0.002963	0.140225
3	46	0	1.204339	-1.934054	-0.052025
4	34	0	2.035596	0.003065	-1.408086
5	34	0	-1.038900	1.789496	-1.175532
6	34	0	-1.033282	-1.792081	-1.175195
7	6	0	3.034713	2.562629	0.960346
8	1	0	3.726275	1.819449	1.347176
9	1	0	3.450196	3.244186	0.220166
10	6	0	-1.966040	-3.489345	-0.733728
11	1	0	-1.430168	-4.306950	-1.220744
12	1	0	-2.000321	-3.658008	0.342749
13	6	0	-3.342456	1.200928	1.561132
14	1	0	-2.631481	1.265368	2.382978
15	1	0	-3.782105	2.144014	1.248405
16	6	0	0.961009	-3.764217	1.121982
17	1	0	0.025203	-3.964280	1.636728
18	1	0	1.259165	-4.512312	0.389520
19	6	0	3.043216	-2.554467	0.958934
20	1	0	3.460366	-3.234515	0.218303
21	1	0	3.732709	-1.809380	1.345764
22	6	0	4.011439	0.006420	-1.208885
23	1	0	4.307420	0.006316	-0.159733
24	1	0	4.403315	-0.884019	-1.705285
25	6	0	-3.339146	-1.210111	1.561105
26	1	0	-3.776180	-2.154385	1.248296
27	1	0	-2.627999	-1.272610	2.382944
28	6	0	-1.976444	3.484027	-0.733768

29	1	0	-2.010521	3.652837	0.342693
30	1	0	-1.443379	4.303141	-1.221330
31	6	0	-4.046165	-0.005560	1.319102
32	6	0	1.934061	-2.946872	1.748927
33	6	0	1.924047	2.951414	1.749990
34	6	0	0.948872	3.766193	1.122995
35	1	0	1.245096	4.515588	0.391079
36	1	0	0.012223	3.963145	1.637412
37	1	0	-2.980641	-3.431639	-1.134462
38	1	0	4.400151	0.898844	-1.704202
39	1	0	-2.991122	3.423121	-1.133819
40	6	0	1.670915	-2.316600	3.097350
41	1	0	2.090616	-2.954170	3.886987
42	1	0	2.139994	-1.331171	3.178266
43	1	0	0.598522	-2.209223	3.288033
44	6	0	1.662083	2.319538	3.097894
45	1	0	0.589898	2.209925	3.288429
46	1	0	2.133028	1.334938	3.177947
47	1	0	2.080507	2.957250	3.888097
48	6	0	-5.372268	-0.007415	0.593605
49	1	0	-6.189722	-0.008983	1.326706
50	1	0	-5.488231	0.881327	-0.034679
51	1	0	-5.485378	-0.896099	-0.035283

$M4_x$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.648086	2.090568	-0.505688
2	1	0	-4.955369	2.097619	-1.550095
3	6	0	-5.163230	1.120907	0.384425
4	6	0	-5.416915	-0.190313	-0.066914
5	1	0	-5.655971	-0.965559	0.654502
6	1	0	-4.307765	3.044066	-0.113145
7	1	0	-5.765936	-0.368378	-1.082526
8	1	0	-5.108495	1.306724	1.456532
9	1	0	-2.251926	1.841981	2.247607
10	6	0	-1.366133	2.468694	2.228756
11	1	0	-1.532634	3.518601	1.992619
12	6	0	-0.208170	2.066143	2.924369
13	6	0	1.019237	2.734114	2.711206
14	1	0	-0.197241	1.086830	3.400486
15	1	0	1.035012	3.807826	2.530345
16	1	0	1.932930	2.316893	3.124736
17	46	0	-3.310108	0.353128	-0.467998
18	46	0	0.240014	1.998910	0.792790
19	34	0	-2.309682	-1.949817	-0.613412
20	34	0	-1.175999	1.417165	-1.215030
21	6	0	-1.635499	3.253021	-1.819403
22	1	0	-0.710008	3.732732	-2.145442
23	1	0	-2.325768	3.176708	-2.662200
24	1	0	-2.090160	3.833176	-1.015284
25	6	0	-3.598361	-3.133261	0.330715

26	1	0	-3.151142	-4.126521	0.413865
27	1	0	-3.833449	-2.747627	1.323506
28	1	0	-4.509293	-3.196491	-0.268329
29	1	0	-1.908725	-3.033498	2.933923
30	6	0	-1.089655	-2.331804	2.808101
31	6	0	0.235867	-2.817889	2.752735
32	1	0	-1.292250	-1.313478	3.134324
33	46	0	-0.250449	-1.956590	0.807508
34	6	0	1.290924	-1.959094	2.380404
35	1	0	0.397187	-3.894860	2.720887
36	34	0	1.197130	-1.467332	-1.202057
37	34	0	2.307077	1.930086	-0.609396
38	1	0	1.278095	-0.906492	2.653946
39	1	0	2.270807	-2.371249	2.160798
40	46	0	3.316503	-0.369677	-0.460876
41	6	0	1.664033	-3.337521	-1.681834
42	6	0	3.591829	3.122615	0.328155
43	6	0	5.421387	0.194737	-0.069333
44	6	0	5.180953	-1.118350	0.382633
45	6	0	4.670139	-2.091512	-0.506653
46	1	0	2.106592	-3.865218	-0.835577
47	1	0	0.741677	-3.836134	-1.987448
48	1	0	2.365025	-3.316986	-2.519206
49	1	0	4.512132	3.167009	-0.257859
50	1	0	3.151378	4.120629	0.384296
51	1	0	3.807348	2.756469	1.332941
52	1	0	5.655437	0.971994	0.651498
53	1	0	5.763581	0.376500	-1.086595
54	1	0	5.131730	-1.304844	1.454776
55	1	0	4.973130	-2.094904	-1.552397
56	1	0	4.340142	-3.048792	-0.114561

$M4_{1a}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-2.891162	-1.534091	-0.642075
2	46	0	2.855409	1.383124	1.294708
3	46	0	-1.266121	1.454969	1.385634
4	34	0	-2.639313	0.977667	-0.663850
5	34	0	2.825616	-1.043028	0.596313
6	34	0	0.794996	1.961699	0.003783
7	6	0	-4.862198	-1.713755	-1.626601
8	1	0	-5.677577	-1.051156	-1.350631
9	1	0	-4.566053	-1.684051	-2.674025
10	6	0	0.695198	3.956315	0.037033
11	1	0	-0.311504	4.226317	-0.293018
12	1	0	0.831135	4.293880	1.064407
13	6	0	4.569660	1.215346	2.673841
14	1	0	4.045846	0.910503	3.578058
15	1	0	5.430862	0.608928	2.408177

16	6	0	-2.743788	1.000950	2.953060
17	1	0	-3.776601	1.317079	2.837614
18	1	0	-2.585852	-0.071667	3.042902
19	6	0	-0.417563	1.591756	3.409485
20	1	0	-0.080793	0.563785	3.528093
21	1	0	0.318256	2.357513	3.633637
22	6	0	-4.475767	1.647296	-0.243029
23	1	0	-4.358779	2.533991	0.384044
24	6	0	3.275121	3.265540	2.361315
25	1	0	3.151340	4.225753	1.868676
26	1	0	2.671378	3.118028	3.255800
27	6	0	4.621769	-1.206166	-0.258198
28	1	0	5.364792	-0.944285	0.499004
29	6	0	4.476521	2.540150	2.200105
30	1	0	5.217273	2.898039	1.486024
31	6	0	-1.790706	1.911983	3.457993
32	1	0	-2.085564	2.948289	3.618607
33	6	0	-4.609781	-2.865390	-0.850636
34	1	0	-5.165654	-3.011460	0.074744
35	6	0	-3.441721	-3.625153	-1.074111
36	1	0	-3.041461	-3.718088	-2.082956
37	1	0	-3.173887	-4.428606	-0.394133
38	1	0	-5.001307	0.878894	0.325503
39	1	0	4.678980	-0.481591	-1.071639
40	6	0	1.757810	4.575239	-0.882776
41	1	0	2.714412	4.060493	-0.729821
42	1	0	1.480694	4.466432	-1.934024
43	6	0	4.856515	-2.634259	-0.772159
44	1	0	4.930035	-3.331764	0.066160
45	1	0	4.017384	-2.934501	-1.407973
46	6	0	-5.230946	1.999983	-1.533738
47	1	0	-4.769041	2.865420	-2.015325
48	1	0	-5.196578	1.155064	-2.227834
49	6	0	6.144731	-2.715095	-1.566986
50	6	0	1.992740	6.033014	-0.537734
51	6	0	-6.676996	2.342569	-1.232784
52	8	0	-7.129474	3.457237	-1.091319
53	8	0	2.367286	6.425475	0.550817
54	8	0	7.217212	-3.091148	-1.147705
55	8	0	-7.421765	1.215307	-1.094626
56	8	0	5.960188	-2.264237	-2.835088
57	8	0	1.739961	6.856475	-1.574840
58	6	0	7.137482	-2.246425	-3.658300
59	1	0	7.547747	-3.254469	-3.762311
60	1	0	6.813912	-1.862248	-4.626102
61	1	0	7.901828	-1.597172	-3.222494
62	6	0	1.946370	8.255944	-1.317101
63	1	0	2.985687	8.444635	-1.035224
64	1	0	1.702538	8.763903	-2.250482
65	1	0	1.292524	8.597377	-0.510215
66	6	0	-8.802289	1.428078	-0.757781
67	1	0	-9.298011	2.021963	-1.530272
68	1	0	-9.246180	0.434144	-0.694360
69	1	0	-8.888966	1.950173	0.199113
70	46	0	1.178867	-1.264955	-1.283500
71	6	0	1.318444	-1.519103	-3.451496
72	6	0	-0.011560	-1.175342	-3.134967

73	1	0	-0.806266	-1.897835	-3.293579
74	1	0	-0.324424	-0.134066	-3.089921
75	6	0	2.381101	-0.686113	-3.036466
76	1	0	2.246977	0.393064	-2.993713
77	1	0	3.404548	-1.034878	-3.142279
78	34	0	-0.632877	-1.803933	0.391615
79	6	0	-0.338882	-3.768333	0.594118
80	1	0	0.738295	-3.912994	0.708264
81	1	0	-0.668923	-4.264936	-0.318672
82	6	0	-1.097344	-4.304752	1.818598
83	1	0	-2.116313	-3.901576	1.823102
84	1	0	-0.602594	-3.998218	2.743355
85	6	0	-1.225903	-5.813529	1.750935
86	8	0	-0.487127	-6.437058	2.691011
87	8	0	-1.902811	-6.404581	0.931656
88	6	0	-0.543398	-7.873454	2.668766
89	1	0	-0.180287	-8.256540	1.711330
90	1	0	0.100675	-8.203732	3.484102
91	1	0	-1.568949	-8.219455	2.823087
92	1	0	1.540942	-2.539790	-3.760950