SUPPORTING INFORMATION

- Atomic coordinates, MO diagrams and CIF files.

Table S1. DFT optimized cartesian coordinates (in solvent THF)
PBE1PBE/LANL2DZ + polarisation + diffuse on Au

$[Au_2\{Se_2P(OEth_2)_2\}_2]$ ***(S = 0)*** ***C_2***
Energy = -938.367581707 a. u.

Atom	X	Y	Z (Angstrom)
Au	0.000000	0.000000	1.612371
Au	0.000000	0.000000	-1.436014
Se	0.695637	2.353012	1.797892
Se	-1.334500	2.065694	-1.441703
P	0.000000	3.232989	-0.115237
O	1.268219	3.849927	-0.918586
O	-0.715184	4.657599	0.180373
C	2.329221	2.990577	-1.403416
H	1.902581	2.277485	-2.127636
H	2.747910	2.429562	-0.552560
C	3.373758	3.874101	-2.051491
H	4.188722	3.241349	-2.431531
H	3.793565	4.584083	-1.325689
H	2.946266	4.434844	-2.894027
C	-1.968192	4.711461	0.911124
H	-1.865506	4.132170	1.842901
H	-2.755502	4.255205	0.290166
C	-2.266228	6.167458	1.198474
H	-3.218895	6.235529	1.742976
H	-2.356387	6.741674	0.266210
H	-1.477265	6.614213	1.818757
Se	-0.695637	-2.353012	1.797892
Se	1.334500	-2.065694	-1.441703
P	0.000000	-3.232989	-0.115237
O	-1.268219	-3.849927	-0.918586
O	0.715184	-4.657599	0.180373
C	-2.329221	-2.990577	-1.403416
H	-1.902581	-2.277485	-2.127636
H	-2.747910	-2.429562	-0.552560
C	-3.373758	-3.874101	-2.051491
H	-4.188722	-3.241349	-2.431531
H	-3.793565	-4.584083	-1.325689
H	-2.946266	-4.434844	-2.894027
C	1.968192	-4.711461	0.911124
H	1.865506	-4.132170	1.842901
H	2.755502	-4.255205	0.290166
C	2.266228	-6.167458	1.198474
H	3.218895	-6.235529	1.742976

H	2.356387	-6.741674	0.266210
H	1.477265	-6.614213	1.818757

$[Au_4\{Se_2P(OEth_2)_2\}_4]$ ***(S = 0)*** ***C_1***

Energy = -1876.74963881 a. u.

Atom	X	Y	Z (Angstrom)
Au	-1.601470	-0.000033	-0.000017
Au	-4.707688	0.000034	-0.000017
Se	-1.633812	-1.291866	2.100566
Se	-4.997100	-2.354590	0.660274
P	-2.981859	-2.900285	1.393937
O	-3.139933	-3.982690	2.591311
O	-2.250824	-3.906001	0.351401
C	-3.702383	-3.588135	3.870121
H	-4.632117	-3.022600	3.695901
H	-2.977065	-2.938018	4.384820
C	-3.968433	-4.851379	4.660739
H	-4.379343	-4.577858	5.643100
H	-3.040899	-5.419105	4.817167
H	-4.696352	-5.491196	4.143493
C	-2.056654	-3.545097	-1.039138
H	-1.384690	-2.672325	-1.087812
H	-3.031822	-3.272103	-1.472729
C	-1.453916	-4.741164	-1.744172
H	-1.298737	-4.485915	-2.802468
H	-2.125398	-5.609134	-1.688859
H	-0.482418	-5.008800	-1.306781
Se	-1.633800	1.291808	-2.100594
Se	-4.997055	2.354659	-0.660323
P	-2.981784	2.900278	-1.393955
O	-3.139791	3.982704	-2.591319
O	-2.250719	3.905948	-0.351396
C	-3.702263	3.588197	-3.870134
H	-4.632051	3.022749	-3.695921
H	-2.977001	2.938010	-4.384824
C	-3.968186	4.851463	-4.660760
H	-4.379115	4.577976	-5.643123
H	-3.040596	5.419099	-4.817184
H	-4.696048	5.491353	-4.143523
C	-2.056600	3.545028	1.039147
H	-1.384646	2.672250	1.087833
H	-3.031786	3.272038	1.472703
C	-1.453879	4.741084	1.744214
H	-1.298731	4.485820	2.802511
H	-2.125357	5.609056	1.688894
H	-0.482368	5.008724	1.306854
H	4.379330	-4.577874	-5.643095
H	4.632116	-3.022617	-3.695898
C	3.968417	-4.851390	-4.660735
H	4.696330	-5.491214	-4.143488
C	3.702377	-3.588143	-3.870118
H	2.977066	-2.938020	-4.384818
H	3.040878	-5.419108	-4.817163

Se	4.997056	2.354656	0.660322
Se	4.997102	-2.354591	-0.660282
Au	4.707688	0.000032	0.000013
O	3.139923	-3.982692	-2.591308
H	3.031789	3.272038	-1.472703
P	2.981857	-2.900284	-1.393936
H	4.632044	3.022738	3.695928
C	2.056603	3.545028	-1.039147
Se	1.633810	-1.291864	-2.100564
P	2.981786	2.900278	1.393955
O	2.250721	3.905947	0.351395
H	2.125359	5.609056	-1.688893
C	3.702260	3.588195	3.870136
H	4.696062	5.491342	4.143526
O	3.139797	3.982705	2.591318
C	1.453881	4.741083	-1.744214
H	1.384649	2.672250	-1.087834
H	1.298734	4.485820	-2.802511
O	2.250823	-3.905995	-0.351394
C	3.968191	4.851460	4.660761
Au	1.601469	-0.000031	0.000018
H	4.379113	4.577971	5.643126
H	2.976989	2.938016	4.384824
H	3.031822	-3.272082	1.472731
H	0.482370	5.008723	-1.306854
C	2.056655	-3.545086	1.039143
Se	1.633802	1.291810	2.100596
H	3.040606	5.419105	4.817179
H	1.384684	-2.672320	1.087815
C	1.453929	-4.741155	1.744185
H	2.125418	-5.609119	1.688874
H	0.482433	-5.008802	1.306798
H	1.298752	-4.485902	2.802480

$[AuSe_2\{P(CH_2)_2Ph)_2\}]_2$ ***(S = 0)*** ***C_i***

Energy = -1560.88917365 a. u.

Atom	X	Y	Z (Angstrom)
Au	0.190205	-1.657706	-0.146881
Se	2.101673	2.178915	-0.583964
Se	2.520348	-1.567664	-0.930297
P	3.190263	0.330357	0.028372
C	3.306137	0.176792	1.868222
H	3.958834	-0.691203	2.049751
H	3.843272	1.082339	2.194536
C	1.984533	0.022253	2.626859
H	1.341799	0.897480	2.424303
H	1.452593	-0.873155	2.258095
C	2.237543	-0.101166	4.112295
C	2.331421	1.043921	4.920453
H	2.190514	2.032139	4.470985
C	2.408746	-1.360957	4.708807
H	2.329353	-2.262502	4.093014
C	2.669517	-1.475907	6.079912
H	2.794513	-2.464926	6.528687
C	2.592284	0.934602	6.291792
H	2.656536	1.836206	6.906755
C	2.763766	-0.327220	6.876693
H	2.963666	-0.414929	7.947714
C	4.920381	0.626003	-0.554219
H	4.851976	0.791215	-1.639949
H	5.233416	1.576200	-0.092735
C	5.919160	-0.498714	-0.232014
H	5.973618	-0.652203	0.859956
H	5.567778	-1.442583	-0.686417
C	7.291409	-0.150799	-0.765064
C	7.635633	-0.438934	-2.096155
H	6.911582	-0.945827	-2.741726
C	8.235726	0.493347	0.050290
H	7.983849	0.719233	1.090984
C	9.496117	0.842704	-0.450881
H	10.221255	1.339724	0.198947
C	8.894063	-0.091701	-2.601701
H	9.147552	-0.327864	-3.638586
C	9.829421	0.551775	-1.780104
H	10.813461	0.820904	-2.172516
Au	-0.190205	1.657706	0.146881
Se	-2.101673	-2.178915	0.583964
Se	-2.520348	1.567664	0.930297
P	-3.190263	-0.330357	-0.028372
C	-3.306137	-0.176792	-1.868222
H	-3.958834	0.691203	-2.049751
H	-3.843272	-1.082339	-2.194536
C	-1.984533	-0.022253	-2.626859
H	-1.341799	-0.897480	-2.424303

H	-1.452593	0.873155	-2.258095
C	-2.237543	0.101166	-4.112295
C	-2.331421	-1.043921	-4.920453
H	-2.190514	-2.032139	-4.470985
C	-2.408746	1.360957	-4.708807
H	-2.329353	2.262502	-4.093014
C	-2.669517	1.475907	-6.079912
H	-2.794513	2.464926	-6.528687
C	-2.592284	-0.934602	-6.291792
H	-2.656536	-1.836206	-6.906755
C	-2.763766	0.327220	-6.876693
H	-2.963666	0.414929	-7.947714
C	-4.920381	-0.626003	0.554219
H	-4.851976	-0.791215	1.639949
H	-5.233416	-1.576200	0.092735
C	-5.919160	0.498714	0.232014
H	-5.973618	0.652203	-0.859956
H	-5.567778	1.442583	0.686417
C	-7.291409	0.150799	0.765064
C	-7.635633	0.438934	2.096155
H	-6.911582	0.945827	2.741726
C	-8.235726	-0.493347	-0.050290
H	-7.983849	-0.719233	-1.090984
C	-9.496117	-0.842704	0.450881
H	-10.221255	-1.339724	-0.198947
C	-8.894063	0.091701	2.601701
H	-9.147552	0.327864	3.638586
C	-9.829421	-0.551775	1.780104
H	-10.813461	-0.820904	2.172516

Table S2. MP2 optimized cartesian coordinates (in solvent THF)
MP2/LANL2DZ + polarisation + diffuse on Au

$[Au_2\{Se_2P(OEth_2)_2\}_2]$ ***(S = 0)*** ***C_2***
Energy = -935.3867203 a. u.

Atom	X	Y	Z (Angstrom)
Au	0.000000	0.000000	9.068472
Au	0.000000	0.000000	6.181952
Se	2.010716	1.389791	9.307707
Se	0.146007	2.446807	6.167571
P	2.015948	2.346177	7.328305
O	3.267011	1.791318	6.435135
O	2.601739	3.863982	7.487376
C	3.330434	0.375476	6.091672
H	2.587188	0.175891	5.303158
H	3.094358	-0.227613	6.982908
C	4.746060	0.106453	5.598404
H	4.830409	-0.950307	5.299516
H	5.476125	0.309243	6.395067
H	4.977148	0.739460	4.729597
C	1.779630	4.845791	8.188591
H	1.453694	4.425001	9.152794
H	0.895174	5.070763	7.571689
C	2.647437	6.082646	8.387320
H	2.059169	6.860452	8.898594
H	2.986014	6.474676	7.417782
H	3.525883	5.840763	9.002105
Se	-2.010716	-1.389791	9.307707
Se	-0.146007	-2.446807	6.167571
P	-2.015948	-2.346177	7.328305
O	-3.267011	-1.791318	6.435135
O	-2.601739	-3.863982	7.487376
C	-3.330434	-0.375476	6.091672
H	-2.587188	-0.175891	5.303158
H	-3.094358	0.227613	6.982908
C	-4.746060	-0.106453	5.598404
H	-4.830409	0.950307	5.299516
H	-5.476125	-0.309243	6.395067
H	-4.977148	-0.739460	4.729597
C	-1.779630	-4.845791	8.188591
H	-1.453694	-4.425001	9.152794
H	-0.895174	-5.070763	7.571689
C	-2.647437	-6.082646	8.387320
H	-2.059169	-6.860452	8.898594
H	-2.986014	-6.474676	7.417782
H	-3.525883	-5.840763	9.002105

Table S3. Cartesian coordinates from the **[Au_2{$Se_2P(OEth_2)_2$}$_2$]** RX model PBE1PBE/LANL2DZ + polarisation + diffuse on Au

[Au_2{$Se_2P(OEth_2)_2$}$_2$] ***(S = 0)*** ***C_2***
Energy = -938.028097743 a.u.

Atom	**X**	**Y**	**Z (Angstrom)**
Au	0.000	0.000	9.040
Au	0.000	0.000	6.097
Se	2.034	1.270	9.266
Se	0.589	2.344	6.019
P	2.277	2.312	7.381
O	3.569	1.840	6.682
O	2.763	3.758	7.664
C	3.831	0.495	6.214
H	3.023	0.121	5.831
H	4.095	-0.064	6.962
C	4.903	0.496	5.194
H	5.044	-0.398	4.875
H	5.716	0.827	5.585
H	4.647	1.061	4.462
C	2.021	4.724	8.477
H	1.966	4.413	9.394
H	1.120	4.827	8.133
C	2.736	6.018	8.424
H	2.262	6.667	8.951
H	2.786	6.319	7.514
H	3.623	5.908	8.774
Se	-2.034	-1.270	9.266
Se	-0.589	-2.344	6.019
P	-2.277	-2.312	7.381
O	-3.569	-1.840	6.682
O	-2.763	-3.758	7.664
C	-3.831	-0.495	6.214
H	-3.023	-0.121	5.831
H	-4.095	0.064	6.962
C	-4.903	-0.496	5.194
H	-5.044	0.398	4.875
H	-5.716	0.827	5.585
H	-4.647	-1.061	4.462
C	-2.021	-4.724	8.477
H	-1.966	-4.413	9.394
H	-1.120	-4.827	8.133
C	-2.736	-6.018	8.424
H	-2.262	-6.667	8.951
H	-2.786	-6.319	7.514
H	-3.623	-5.908	8.774

Table S4. Distances benchmark in function of the functional

Distances(Å)|Functional	X-ray[a]	PBE0	MP2	BP86	B3LYP	LC-ωPBE	Cam-B3LYP
Au1a-Au1b	2.943	3.044	2.886	3.062	3.170	3.005	3.091
Au1a-Se1a	2.409	2.459	2.453	2.474	2.486	2.44	2.47
Se1b-P	2.177	2.216	2.200	2.251	2.240	2.19	2.21

Table S5. Computed emission wavelength in function of the basis set (a =LANL2DZ + pol + diff, b= Def2TZPVP)

Compound |Basis set	Basis set a	Basis set b
Compound 4	495 nm	484 nm

Figure S1: TD-DFT benchmark

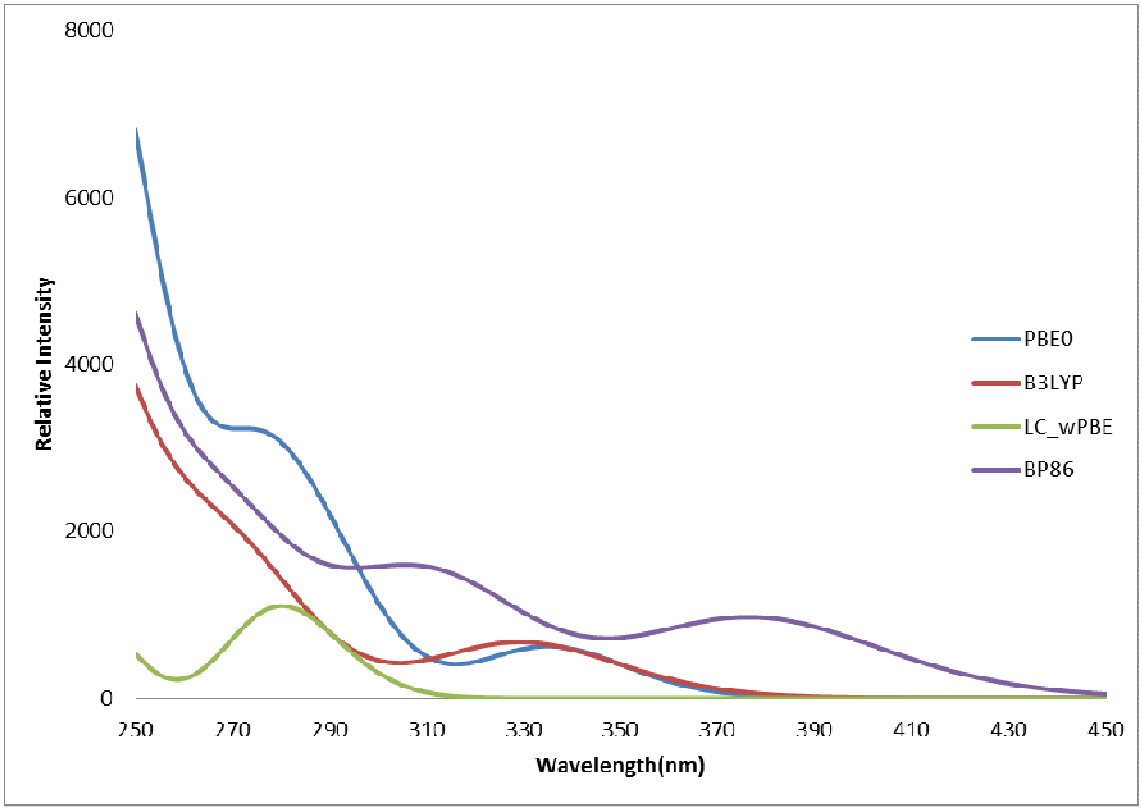


Figure S2 : Frontier MO diagram of $[Au]_2$
(X-ray geometry, cut-off equal to 0.035 au)

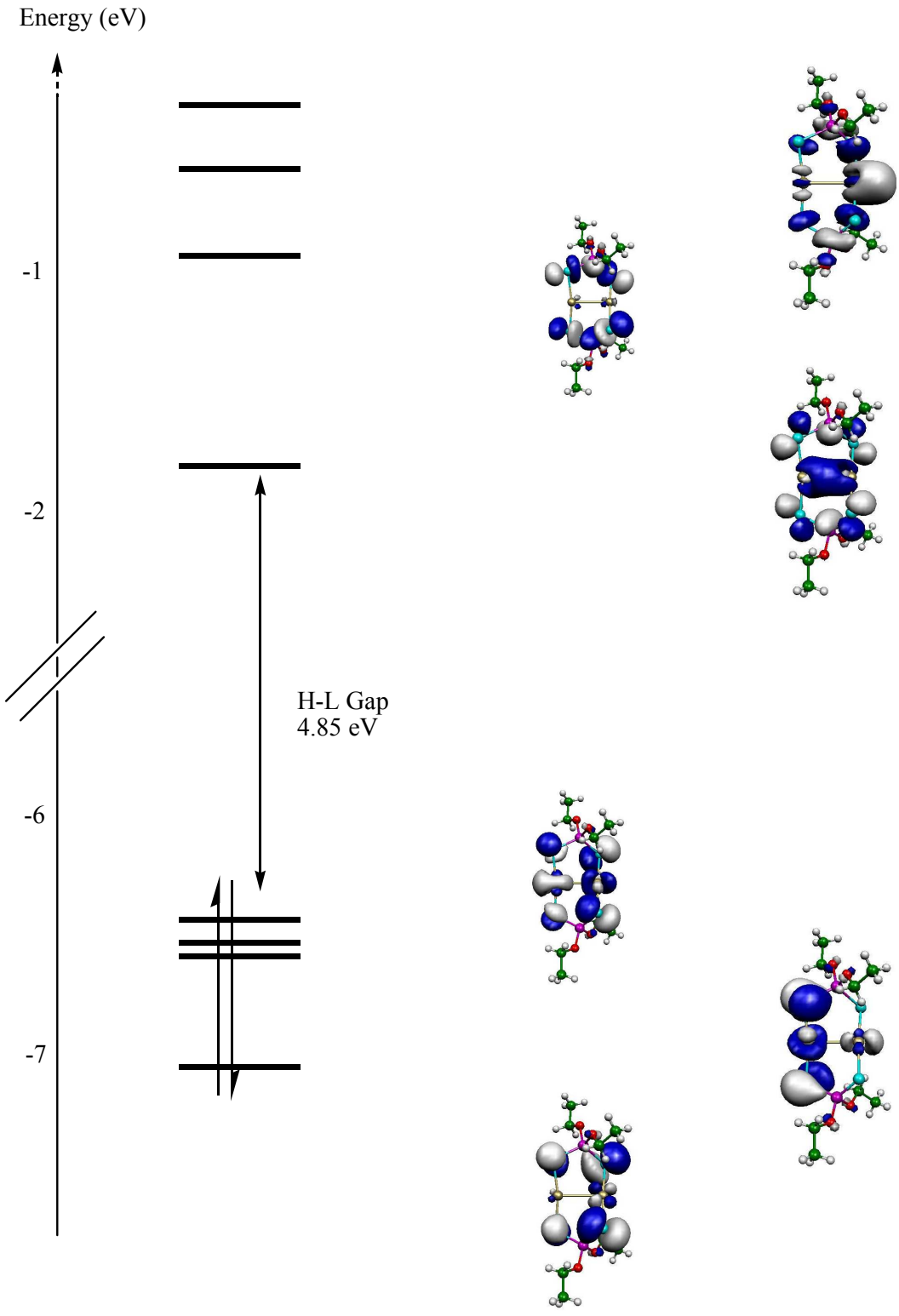


Figure S3 : Frontier MO diagram of $[Au]_4$ (X-ray geometry, cut-off equal to 0.035 au)

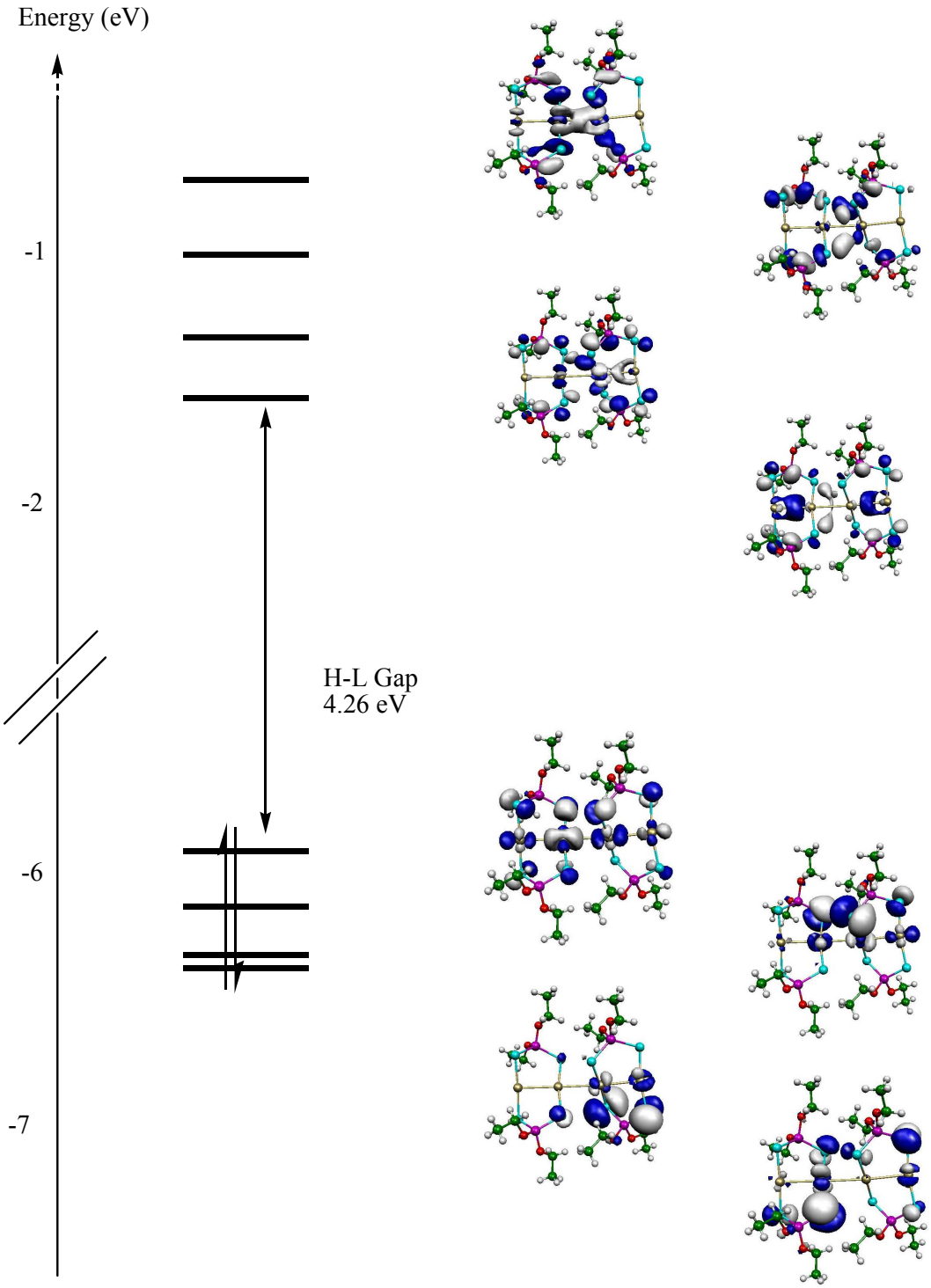


Figure S4 : Frontier MO diagram of $[Au]_6$
(X-ray geometry, cut-off equal to 0.035 au)

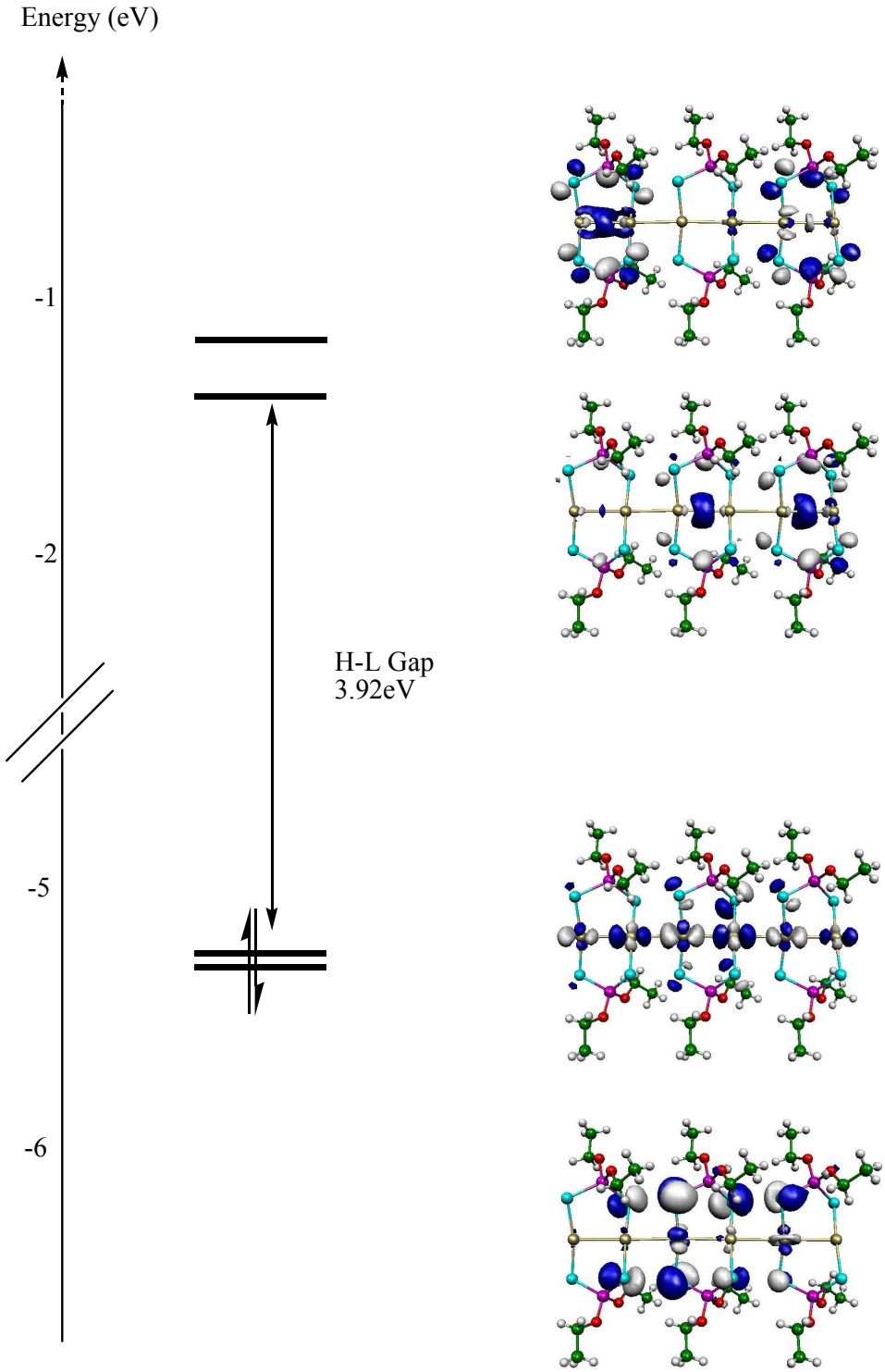
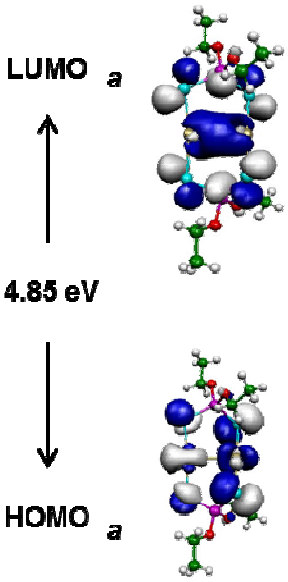


Figure S5. Plots (cut-off equal to 0.035 au) of the HOMO and LUMO of $[Au]_2$ model.



CIF Files of 3 and 4

```
data_3

_audit_creation_method            SHELXL-97
_chemical_name_systematic
;
 ?
;
_chemical_name_common             ?
_chemical_melting_point           ?
_chemical_formula_moiety          ?
_chemical_formula_sum
 'C12 H28 Au2 O4 P2 Se4'
_chemical_formula_weight          1008.06

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'
 'P'  'P'   0.1023   0.0942
 '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'
 'Au'  'Au'  -2.0133   8.8022
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

_symmetry_cell_setting            Orthorhombic
_symmetry_space_group_name_H-M    Pccn

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

_cell_length_a                    8.8851(11)
_cell_length_b                    23.393(3)
_cell_length_c                    12.0871(15)
_cell_angle_alpha                 90.00
_cell_angle_beta                  90.00
_cell_angle_gamma                 90.00
_cell_volume                      2512.3(6)
```

```
_cell_formula_units_Z            4
_cell_measurement_temperature    296(2)
_cell_measurement_reflns_used    4639
_cell_measurement_theta_min      2.45
_cell_measurement_theta_max      24.37

_exptl_crystal_description       column
_exptl_crystal_colour            yellow
_exptl_crystal_size_max          0.28
_exptl_crystal_size_mid          0.25
_exptl_crystal_size_min          0.15
_exptl_crystal_density_meas      ?
_exptl_crystal_density_diffrn    2.665
_exptl_crystal_density_method    'not measured'
_exptl_crystal_F_000             1824
_exptl_absorpt_coefficient_mu    17.601
_exptl_absorpt_correction_type   multi-scan
_exptl_absorpt_correction_T_min  0.0836
_exptl_absorpt_correction_T_max  0.1777
_exptl_absorpt_process_details   SADABS

_exptl_special_details
;
 ?
;

_diffrn_ambient_temperature      296(2)
_diffrn_radiation_wavelength     0.71073
_diffrn_radiation_type           MoK\a
_diffrn_radiation_source         'fine-focus sealed tube'
_diffrn_radiation_monochromator  graphite
_diffrn_measurement_device_type  'Bruker APEX-II CCD'
_diffrn_measurement_method       '\f and \w scans'
_diffrn_detector_area_resol_mean ?
_diffrn_reflns_number            20746
_diffrn_reflns_av_R_equivalents  0.0406
_diffrn_reflns_av_sigmaI/netI    0.0257
_diffrn_reflns_limit_h_min       -10
_diffrn_reflns_limit_h_max       10
_diffrn_reflns_limit_k_min       -28
_diffrn_reflns_limit_k_max       27
_diffrn_reflns_limit_l_min       -14
_diffrn_reflns_limit_l_max       13
_diffrn_reflns_theta_min         1.74
_diffrn_reflns_theta_max         25.99
_reflns_number_total             2399
_reflns_number_gt                1592
_reflns_threshold_expression     >2sigma(I)

_computing_data_collection       'Bruker APEX2'
_computing_cell_refinement       'Bruker SAINT'
_computing_data_reduction        'Bruker SAINT'
_computing_structure_solution    'SHELXS-97 (Sheldrick, 2008)'
_computing_structure_refinement  'SHELXL-97 (Sheldrick, 2008)'
_computing_molecular_graphics    'Bruker SHELXTL'
_computing_publication_material  'Bruker SHELXTL'

_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^)+(0.0568P)^2^+7.8512P] 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          2399
_refine_ls_number_parameters      110
_refine_ls_number_restraints      0
_refine_ls_R_factor_all           0.0554
_refine_ls_R_factor_gt            0.0347
_refine_ls_wR_factor_ref          0.1133
_refine_ls_wR_factor_gt           0.0998
_refine_ls_goodness_of_fit_ref    1.016
_refine_ls_restrained_S_all       1.016
_refine_ls_shift/su_max           0.001
_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
Au1 Au 1.2500 0.2500 0.65927(4) 0.06409(19) Uani 1 2 d S . .
Au2 Au 1.2500 0.2500 0.41181(3) 0.05928(18) Uani 1 2 d S . .
C1 C 0.7228(12) 0.3383(6) 0.5793(12) 0.109(4) Uani 1 1 d . . .
H1A H 0.7093 0.3068 0.5281 0.131 Uiso 1 1 calc R . .
H1B H 0.7503 0.3226 0.6508 0.131 Uiso 1 1 calc R . .
C2 C 0.5828(14) 0.3700(7) 0.5892(13) 0.127(5) Uani 1 1 d . . .
H2A H 0.5054 0.3441 0.6154 0.153 Uiso 1 1 calc R . .
H2B H 0.5960 0.3993 0.6453 0.153 Uiso 1 1 calc R . .
C3 C 0.5314(18) 0.3960(9) 0.4933(14) 0.174(8) Uani 1 1 d . . .
H3A H 0.5803 0.4324 0.4844 0.261 Uiso 1 1 calc R . .
H3B H 0.4246 0.4016 0.4982 0.261 Uiso 1 1 calc R . .
H3C H 0.5539 0.3722 0.4309 0.261 Uiso 1 1 calc R . .
C4 C 1.0712(15) 0.4304(6) 0.3769(10) 0.117(4) Uani 1 1 d . . .
H4A H 0.9675 0.4431 0.3722 0.140 Uiso 1 1 calc R . .
H4B H 1.0863 0.4015 0.3203 0.140 Uiso 1 1 calc R . .
C5 C 1.1681(16) 0.4779(5) 0.3544(10) 0.115(4) Uani 1 1 d . . .
H5A H 1.2715 0.4646 0.3568 0.138 Uiso 1 1 calc R . .
```

```
H5B H 1.1557 0.5058 0.4130 0.138 Uiso 1 1 calc R . .
C6 C 1.1428(17) 0.5063(6) 0.2481(11) 0.135(5) Uani 1 1 d . . .
H6A H 1.1612 0.4799 0.1890 0.202 Uiso 1 1 calc R . .
H6B H 1.2100 0.5383 0.2414 0.202 Uiso 1 1 calc R . .
H6C H 1.0406 0.5196 0.2443 0.202 Uiso 1 1 calc R . .
O1 O 0.8429(7) 0.3758(3) 0.5395(5) 0.0789(17) Uani 1 1 d . . .
O2 O 1.0955(8) 0.4051(3) 0.4825(5) 0.0844(18) Uani 1 1 d . . .
P1 P 1.0081(3) 0.35166(10) 0.52399(19) 0.0649(6) Uani 1 1 d . . .
Se1 Se 0.99434(11) 0.28360(4) 0.40185(7) 0.0747(3) Uani 1 1 d . . .
Se2 Se 1.10275(15) 0.33438(5) 0.68515(8) 0.0982(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
Au1 0.0770(4) 0.0700(4) 0.0453(3) 0.000 0.000 0.0067(2)
Au2 0.0733(3) 0.0610(3) 0.0435(3) 0.000 0.000 0.0076(2)
C1 0.080(8) 0.104(10) 0.143(11) 0.019(8) 0.027(7) -0.007(6)
C2 0.076(8) 0.147(13) 0.159(14) -0.022(10) 0.006(8) 0.001(8)
C3 0.124(12) 0.24(2) 0.159(15) 0.037(15) -0.065(11) 0.012(13)
C4 0.135(10) 0.124(10) 0.091(8) 0.035(8) -0.023(7) -0.033(8)
C5 0.138(10) 0.087(8) 0.121(10) 0.018(7) 0.011(8) -0.035(8)
C6 0.161(13) 0.113(10) 0.130(10) 0.046(9) -0.012(10) -0.032(10)
O1 0.070(4) 0.068(4) 0.099(4) 0.004(3) 0.009(3) 0.013(3)
O2 0.095(5) 0.084(4) 0.074(4) 0.011(3) -0.004(3) -0.013(4)
P1 0.0683(14) 0.0636(13) 0.0629(13) 0.0040(10) 0.0043(12) 0.0074(11)
Se1 0.0764(6) 0.0804(6) 0.0673(5) -0.0055(5) -0.0096(5) 0.0120(5)
Se2 0.1368(11) 0.0981(8) 0.0596(5) -0.0150(5) -0.0094(6) 0.0440(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
Au1 Se2 2.3887(11) . ?
Au1 Se2 2.3887(11) 2_755 ?
Au1 Au2 2.9910(7) . ?
Au1 Au2 3.0525(7) 7_566 ?
Au2 Se1 2.4067(10) . ?
Au2 Se1 2.4067(10) 2_755 ?
Au2 Au1 3.0526(7) 7_565 ?
C1 C2 1.453(16) . ?
C1 O1 1.463(12) . ?
C1 H1A 0.9700 . ?
C1 H1B 0.9700 . ?
```

```
C2 C3 1.387(19) . ?
C2 H2A 0.9700 . ?
C2 H2B 0.9700 . ?
C3 H3A 0.9600 . ?
C3 H3B 0.9600 . ?
C3 H3C 0.9600 . ?
C4 O2 1.424(12) . ?
C4 C5 1.432(15) . ?
C4 H4A 0.9700 . ?
C4 H4B 0.9700 . ?
C5 C6 1.464(16) . ?
C5 H5A 0.9700 . ?
C5 H5B 0.9700 . ?
C6 H6A 0.9600 . ?
C6 H6B 0.9600 . ?
C6 H6C 0.9600 . ?
O1 P1 1.584(6) . ?
O2 P1 1.555(7) . ?
P1 Se2 2.160(3) . ?
P1 Se1 2.175(3) . ?

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
Se2 Au1 Se2 164.95(5) . 2_755 ?
Se2 Au1 Au2 97.53(3) . . ?
Se2 Au1 Au2 97.53(3) 2_755 . ?
Se2 Au1 Au2 82.47(3) . 7_566 ?
Se2 Au1 Au2 82.47(3) 2_755 7_566 ?
Au2 Au1 Au2 180.0 . 7_566 ?
Se1 Au2 Se1 174.26(5) . 2_755 ?
Se1 Au2 Au1 92.87(2) . . ?
Se1 Au2 Au1 92.87(2) 2_755 . ?
Se1 Au2 Au1 87.13(2) . 7_565 ?
Se1 Au2 Au1 87.13(2) 2_755 7_565 ?
Au1 Au2 Au1 180.0 . 7_565 ?
C2 C1 O1 110.2(11) . . ?
C2 C1 H1A 109.6 . . ?
O1 C1 H1A 109.6 . . ?
C2 C1 H1B 109.6 . . ?
O1 C1 H1B 109.6 . . ?
H1A C1 H1B 108.1 . . ?
C3 C2 C1 115.9(14) . . ?
C3 C2 H2A 108.3 . . ?
C1 C2 H2A 108.3 . . ?
C3 C2 H2B 108.3 . . ?
C1 C2 H2B 108.3 . . ?
H2A C2 H2B 107.4 . . ?
C2 C3 H3A 109.5 . . ?
C2 C3 H3B 109.5 . . ?
H3A C3 H3B 109.5 . . ?
C2 C3 H3C 109.5 . . ?
H3A C3 H3C 109.5 . . ?
H3B C3 H3C 109.5 . . ?
O2 C4 C5 113.7(10) . . ?
O2 C4 H4A 108.8 . . ?
```

```
C5 C4 H4A 108.8 . . ?
O2 C4 H4B 108.8 . . ?
C5 C4 H4B 108.8 . . ?
H4A C4 H4B 107.7 . . ?
C4 C5 C6 115.3(12) . . ?
C4 C5 H5A 108.4 . . ?
C6 C5 H5A 108.4 . . ?
C4 C5 H5B 108.4 . . ?
C6 C5 H5B 108.4 . . ?
H5A C5 H5B 107.5 . . ?
C5 C6 H6A 109.5 . . ?
C5 C6 H6B 109.5 . . ?
H6A C6 H6B 109.5 . . ?
C5 C6 H6C 109.5 . . ?
H6A C6 H6C 109.5 . . ?
H6B C6 H6C 109.5 . . ?
C1 O1 P1 120.1(7) . . ?
C4 O2 P1 123.2(7) . . ?
O2 P1 O1 102.4(4) . . ?
O2 P1 Se2 104.3(3) . . ?
O1 P1 Se2 108.7(3) . . ?
O2 P1 Se1 113.4(3) . . ?
O1 P1 Se1 106.8(3) . . ?
Se2 P1 Se1 119.80(11) . . ?
P1 Se1 Au2 98.76(7) . . ?
P1 Se2 Au1 104.47(7) . . ?

_diffrn_measured_fraction_theta_max    0.972
_diffrn_reflns_theta_full              25.99
_diffrn_measured_fraction_theta_full   0.972
_refine_diff_density_max    1.246
_refine_diff_density_min   -0.966
_refine_diff_density_rms    0.200


#===END



data_4

_audit_creation_method            SHELXL-97
_chemical_name_systematic
;
 ?
;
_chemical_name_common             ?
_chemical_melting_point           ?
_chemical_formula_moiety          ?
_chemical_formula_sum
 'C32 H36 Au2 P2 Se4'
_chemical_formula_weight          1192.32

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'
 'P'  'P'   0.1023   0.0942
 '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'
 'Au'  'Au'  -2.0133   8.8022
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

_symmetry_cell_setting            Triclinic
_symmetry_space_group_name_H-M    P-1

loop_
 _symmetry_equiv_pos_as_xyz
 'x, y, z'
 '-x, -y, -z'

_cell_length_a                    9.7733(8)
_cell_length_b                    13.1376(11)
_cell_length_c                    14.1643(12)
_cell_angle_alpha                 79.489(2)
_cell_angle_beta                  84.857(2)
_cell_angle_gamma                 72.986(2)
_cell_volume                      1708.6(2)
_cell_formula_units_Z             2
_cell_measurement_temperature     296(2)
_cell_measurement_reflns_used     6834
_cell_measurement_theta_min       2.18
_cell_measurement_theta_max       24.96

_exptl_crystal_description        prism
_exptl_crystal_colour             colourless
_exptl_crystal_size_max           0.42
_exptl_crystal_size_mid           0.10
_exptl_crystal_size_min           0.05
_exptl_crystal_density_meas       ?
_exptl_crystal_density_diffrn     2.318
_exptl_crystal_density_method     'not measured'
_exptl_crystal_F_000              1104
_exptl_absorpt_coefficient_mu     12.952
_exptl_absorpt_correction_type    multi-scan
_exptl_absorpt_correction_T_min   0.0739
_exptl_absorpt_correction_T_max   0.5636
_exptl_absorpt_process_details    SADABS

_exptl_special_details
;
 ?
;

_diffrn_ambient_temperature       296(2)
_diffrn_radiation_wavelength      0.71073
_diffrn_radiation_type            MoK\a
_diffrn_radiation_source          'fine-focus sealed tube'
_diffrn_radiation_monochromator   graphite
_diffrn_measurement_device_type   'Bruker APEX-II CCD'
_diffrn_measurement_method        '\f and \w scans'
_diffrn_detector_area_resol_mean  ?
_diffrn_standards_number          0
_diffrn_standards_interval_count  ?
_diffrn_standards_interval_time   ?
```

```
_diffrn_standards_decay_%         ?
_diffrn_reflns_number             19833
_diffrn_reflns_av_R_equivalents   0.0379
_diffrn_reflns_av_sigmaI/netI     0.0382
_diffrn_reflns_limit_h_min        -11
_diffrn_reflns_limit_h_max        11
_diffrn_reflns_limit_k_min        -15
_diffrn_reflns_limit_k_max        15
_diffrn_reflns_limit_l_min        -16
_diffrn_reflns_limit_l_max        16
_diffrn_reflns_theta_min          1.46
_diffrn_reflns_theta_max          25.05
_reflns_number_total              6044
_reflns_number_gt                 4892
_reflns_threshold_expression      >2sigma(I)

_computing_data_collection        'Bruker APEX2'
_computing_cell_refinement        'Bruker SAINT'
_computing_data_reduction         'Bruker SAINT'
_computing_structure_solution     'SHELXS-97 (Sheldrick, 1990)'
_computing_structure_refinement   'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics     'Bruker SHELXTL'
_computing_publication_material   'Bruker SHELXTL'

_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^)+(0.0244P)^2^+0.8907P] 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          6044
_refine_ls_number_parameters      361
_refine_ls_number_restraints      0
_refine_ls_R_factor_all           0.0379
_refine_ls_R_factor_gt            0.0260
_refine_ls_wR_factor_ref          0.0630
_refine_ls_wR_factor_gt           0.0581
_refine_ls_goodness_of_fit_ref    1.026
_refine_ls_restrained_S_all       1.026
_refine_ls_shift/su_max           0.002
_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
Au1 Au 0.48424(2) 0.397669(17) 0.944241(17) 0.04934(8) Uani 1 1 d . . .
Au2 Au 0.50755(2) 0.126327(17) -0.047498(16) 0.04698(8) Uani 1 1 d . . .
Se1 Se 0.31119(7) 0.35214(5) 1.06142(5) 0.06480(19) Uani 1 1 d . . .
Se2 Se 0.64827(7) 0.43075(5) 0.81408(5) 0.05834(17) Uani 1 1 d . . .
Se3 Se 0.27948(6) 0.17853(4) -0.11961(5) 0.05167(15) Uani 1 1 d . . .
Se4 Se 0.74074(6) 0.09624(5) 0.01054(4) 0.05356(16) Uani 1 1 d . . .
P1 P 0.78393(15) 0.49658(11) 0.88456(10) 0.0424(3) Uani 1 1 d . . .
P2 P 0.73358(14) -0.02090(11) 0.13995(10) 0.0393(3) Uani 1 1 d . . .
C1 C 0.8873(6) 0.3926(5) 0.9741(4) 0.0578(16) Uani 1 1 d . . .
H1A H 0.9344 0.3310 0.9428 0.069 Uiso 1 1 calc R . .
H1B H 0.9620 0.4194 0.9923 0.069 Uiso 1 1 calc R . .
C2 C 0.8159(7) 0.3517(5) 1.0649(5) 0.0657(18) Uani 1 1 d . . .
H2A H 0.7626 0.4128 1.0951 0.079 Uiso 1 1 calc R . .
H2B H 0.7473 0.3178 1.0484 0.079 Uiso 1 1 calc R . .
C3 C 0.9132(6) 0.2733(4) 1.1359(4) 0.0460(13) Uani 1 1 d . . .
C4 C 0.8830(8) 0.2774(5) 1.2341(6) 0.075(2) Uani 1 1 d . . .
H4 H 0.8005 0.3263 1.2540 0.091 Uiso 1 1 calc R . .
C5 C 1.0358(7) 0.1994(5) 1.1119(5) 0.0566(15) Uani 1 1 d . . .
H5 H 1.0587 0.1943 1.0474 0.068 Uiso 1 1 calc R . .
C6 C 1.1266(8) 0.1320(6) 1.1808(6) 0.078(2) Uani 1 1 d . . .
H6 H 1.2097 0.0825 1.1625 0.094 Uiso 1 1 calc R . .
C7 C 0.9774(12) 0.2079(7) 1.3017(5) 0.093(3) Uani 1 1 d . . .
H7 H 0.9579 0.2104 1.3669 0.112 Uiso 1 1 calc R . .
C8 C 1.0956(11) 0.1377(7) 1.2726(7) 0.094(3) Uani 1 1 d . . .
H8 H 1.1577 0.0917 1.3182 0.113 Uiso 1 1 calc R . .
C9 C 0.9127(6) 0.5310(4) 0.7936(4) 0.0482(13) Uani 1 1 d . . .
H9A H 0.8618 0.5911 0.7474 0.058 Uiso 1 1 calc R . .
H9B H 0.9789 0.5559 0.8242 0.058 Uiso 1 1 calc R . .
C10 C 1.0003(7) 0.4419(5) 0.7385(5) 0.0607(16) Uani 1 1 d . . .
H10A H 1.0485 0.3795 0.7837 0.073 Uiso 1 1 calc R . .
H10B H 0.9365 0.4203 0.7026 0.073 Uiso 1 1 calc R . .
C11 C 1.1101(6) 0.4792(4) 0.6700(4) 0.0509(14) Uani 1 1 d . . .
C12 C 1.0704(7) 0.5486(5) 0.5862(5) 0.0590(16) Uani 1 1 d . . .
H12 H 0.9752 0.5700 0.5693 0.071 Uiso 1 1 calc R . .
C13 C 1.2528(7) 0.4487(5) 0.6918(5) 0.0600(16) Uani 1 1 d . . .
H13 H 1.2830 0.4009 0.7479 0.072 Uiso 1 1 calc R . .
C14 C 1.3501(7) 0.4875(6) 0.6325(5) 0.0718(19) Uani 1 1 d . . .
H14 H 1.4456 0.4660 0.6489 0.086 Uiso 1 1 calc R . .
C15 C 1.1696(8) 0.5876(5) 0.5262(5) 0.0695(19) Uani 1 1 d . . .
H15 H 1.1408 0.6348 0.4695 0.083 Uiso 1 1 calc R . .
C16 C 1.3096(8) 0.5569(5) 0.5499(5) 0.0678(18) Uani 1 1 d . . .
H16 H 1.3766 0.5833 0.5099 0.081 Uiso 1 1 calc R . .
C17 C 0.5906(6) 0.0327(4) 0.2239(4) 0.0499(14) Uani 1 1 d . . .
H17A H 0.4996 0.0472 0.1943 0.060 Uiso 1 1 calc R . .
H17B H 0.5927 -0.0220 0.2804 0.060 Uiso 1 1 calc R . .
C18 C 0.5981(7) 0.1341(5) 0.2554(5) 0.0610(16) Uani 1 1 d . . .
H18A H 0.5864 0.1907 0.1997 0.073 Uiso 1 1 calc R . .
H18B H 0.6929 0.1216 0.2788 0.073 Uiso 1 1 calc R . .
C19 C 0.4878(6) 0.1742(4) 0.3333(4) 0.0488(14) Uani 1 1 d . . .
C20 C 0.4250(7) 0.1088(5) 0.3973(5) 0.0649(17) Uani 1 1 d . . .
```

```
H20 H 0.4457 0.0362 0.3926 0.078 Uiso 1 1 calc R . .
C21 C 0.4546(7) 0.2804(5) 0.3438(5) 0.0694(18) Uani 1 1 d . . .
H21 H 0.4955 0.3272 0.3013 0.083 Uiso 1 1 calc R . .
C22 C 0.3617(8) 0.3188(6) 0.4162(6) 0.083(2) Uani 1 1 d . . .
H22 H 0.3405 0.3913 0.4216 0.100 Uiso 1 1 calc R . .
C23 C 0.3311(7) 0.1493(6) 0.4690(5) 0.077(2) Uani 1 1 d . . .
H23 H 0.2879 0.1036 0.5110 0.092 Uiso 1 1 calc R . .
C24 C 0.3006(7) 0.2537(7) 0.4797(5) 0.079(2) Uani 1 1 d . . .
H24 H 0.2393 0.2800 0.5294 0.095 Uiso 1 1 calc R . .
C25 C 0.9033(5) -0.0427(4) 0.1947(4) 0.0437(13) Uani 1 1 d . . .
H25A H 0.9801 -0.0674 0.1486 0.052 Uiso 1 1 calc R . .
H25B H 0.9092 0.0260 0.2072 0.052 Uiso 1 1 calc R . .
C26 C 0.9280(6) -0.1227(5) 0.2871(4) 0.0569(16) Uani 1 1 d . . .
H26A H 0.9232 -0.1919 0.2751 0.068 Uiso 1 1 calc R . .
H26B H 0.8523 -0.0983 0.3338 0.068 Uiso 1 1 calc R . .
C27 C 1.0711(6) -0.1371(4) 0.3286(4) 0.0477(14) Uani 1 1 d . . .
C28 C 1.0760(7) -0.1146(5) 0.4190(4) 0.0622(17) Uani 1 1 d . . .
H28 H 0.9913 -0.0907 0.4543 0.075 Uiso 1 1 calc R . .
C29 C 1.1973(7) -0.1735(5) 0.2788(5) 0.0670(18) Uani 1 1 d . . .
H29 H 1.1959 -0.1905 0.2180 0.080 Uiso 1 1 calc R . .
C30 C 1.2062(9) -0.1273(6) 0.4580(5) 0.078(2) Uani 1 1 d . . .
H30 H 1.2082 -0.1112 0.5191 0.093 Uiso 1 1 calc R . .
C31 C 1.3271(7) -0.1854(6) 0.3178(6) 0.082(2) Uani 1 1 d . . .
H31 H 1.4122 -0.2087 0.2827 0.098 Uiso 1 1 calc R . .
C32 C 1.3302(9) -0.1630(6) 0.4080(7) 0.082(2) Uani 1 1 d . . .
H32 H 1.4173 -0.1723 0.4348 0.098 Uiso 1 1 calc R . .

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
Au1 0.04200(13) 0.05060(14) 0.06022(16) -0.01660(11) -0.00045(10) -
0.01634(10)
Au2 0.04869(14) 0.04866(13) 0.04288(13) -0.00836(10) -0.00889(10) -
0.01001(10)
Se1 0.0700(4) 0.0499(3) 0.0854(5) -0.0281(3) 0.0231(4) -0.0311(3)
Se2 0.0637(4) 0.0729(4) 0.0528(4) -0.0174(3) -0.0010(3) -0.0375(3)
Se3 0.0483(3) 0.0413(3) 0.0645(4) -0.0122(3) -0.0127(3) -0.0059(3)
Se4 0.0520(4) 0.0619(4) 0.0470(3) 0.0050(3) -0.0113(3) -0.0222(3)
P1 0.0429(8) 0.0420(7) 0.0466(8) -0.0090(6) -0.0002(6) -0.0180(6)
P2 0.0375(7) 0.0415(7) 0.0380(8) -0.0078(6) -0.0039(6) -0.0082(6)
C1 0.053(4) 0.066(4) 0.051(4) 0.003(3) -0.010(3) -0.017(3)
C2 0.055(4) 0.062(4) 0.079(5) 0.002(3) 0.005(3) -0.025(3)
C3 0.056(4) 0.040(3) 0.048(3) -0.002(3) -0.004(3) -0.025(3)
C4 0.097(6) 0.061(4) 0.083(5) -0.026(4) 0.027(4) -0.044(4)
C5 0.062(4) 0.060(4) 0.053(4) -0.008(3) 0.000(3) -0.025(3)
C6 0.070(5) 0.073(5) 0.092(6) 0.013(4) -0.031(4) -0.027(4)
C7 0.173(10) 0.094(6) 0.032(4) -0.002(4) -0.004(5) -0.074(6)
C8 0.125(8) 0.088(6) 0.089(7) 0.011(5) -0.046(6) -0.062(6)
C9 0.053(3) 0.047(3) 0.050(3) -0.011(3) 0.001(3) -0.022(3)
C10 0.059(4) 0.052(3) 0.074(4) -0.016(3) 0.018(3) -0.022(3)
C11 0.050(4) 0.044(3) 0.058(4) -0.015(3) 0.009(3) -0.011(3)
C12 0.056(4) 0.062(4) 0.058(4) -0.012(3) -0.006(3) -0.012(3)
C13 0.057(4) 0.064(4) 0.053(4) 0.001(3) -0.004(3) -0.014(3)
C14 0.049(4) 0.091(5) 0.074(5) -0.016(4) 0.002(3) -0.019(4)
C15 0.088(5) 0.061(4) 0.049(4) -0.004(3) 0.007(4) -0.011(4)
C16 0.071(5) 0.072(4) 0.067(5) -0.022(4) 0.024(4) -0.032(4)
```

```
C17 0.048(3) 0.055(3) 0.050(3) -0.014(3) 0.002(3) -0.017(3)
C18 0.067(4) 0.055(4) 0.066(4) -0.026(3) 0.014(3) -0.020(3)
C19 0.047(3) 0.050(3) 0.047(3) -0.016(3) -0.002(3) -0.006(3)
C20 0.068(4) 0.059(4) 0.072(5) -0.023(3) 0.013(4) -0.021(3)
C21 0.076(5) 0.057(4) 0.074(5) -0.018(3) 0.007(4) -0.015(3)
C22 0.079(5) 0.066(5) 0.095(6) -0.042(4) -0.011(5) 0.013(4)
C23 0.067(5) 0.096(6) 0.066(5) -0.019(4) 0.012(4) -0.020(4)
C24 0.057(4) 0.111(6) 0.060(5) -0.037(5) -0.002(4) 0.005(4)
C25 0.040(3) 0.050(3) 0.040(3) -0.004(2) -0.009(2) -0.012(2)
C26 0.054(4) 0.059(4) 0.057(4) 0.007(3) -0.017(3) -0.019(3)
C27 0.061(4) 0.037(3) 0.045(3) 0.005(2) -0.019(3) -0.015(3)
C28 0.068(4) 0.071(4) 0.046(4) -0.001(3) -0.012(3) -0.019(3)
C29 0.066(4) 0.066(4) 0.060(4) -0.015(3) -0.010(4) -0.001(3)
C30 0.105(6) 0.084(5) 0.056(4) -0.002(4) -0.027(4) -0.042(5)
C31 0.047(4) 0.085(5) 0.098(6) -0.001(4) -0.011(4) 0.002(4)
C32 0.073(5) 0.070(5) 0.103(7) 0.019(4) -0.051(5) -0.029(4)

_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
Au1 Se1 2.3873(7) . ?
Au1 Se2 2.3966(7) . ?
Au2 Se4 2.3909(6) . ?
Au2 Se3 2.3959(6) . ?
Se1 P1 2.1785(15) 2_667 ?
Se2 P1 2.1739(15) . ?
Se3 P2 2.1833(14) 2_655 ?
Se4 P2 2.1780(15) . ?
P1 C9 1.810(6) . ?
P1 C1 1.812(6) . ?
P1 Se1 2.1785(15) 2_667 ?
P2 C17 1.816(6) . ?
P2 C25 1.818(5) . ?
P2 Se3 2.1833(14) 2_655 ?
C1 C2 1.496(8) . ?
C2 C3 1.482(8) . ?
C3 C5 1.364(8) . ?
C3 C4 1.402(9) . ?
C4 C7 1.396(11) . ?
C5 C6 1.380(9) . ?
C6 C8 1.319(12) . ?
C7 C8 1.336(12) . ?
C9 C10 1.530(8) . ?
C10 C11 1.510(8) . ?
C11 C12 1.369(8) . ?
C11 C13 1.380(8) . ?
C12 C15 1.381(9) . ?
```

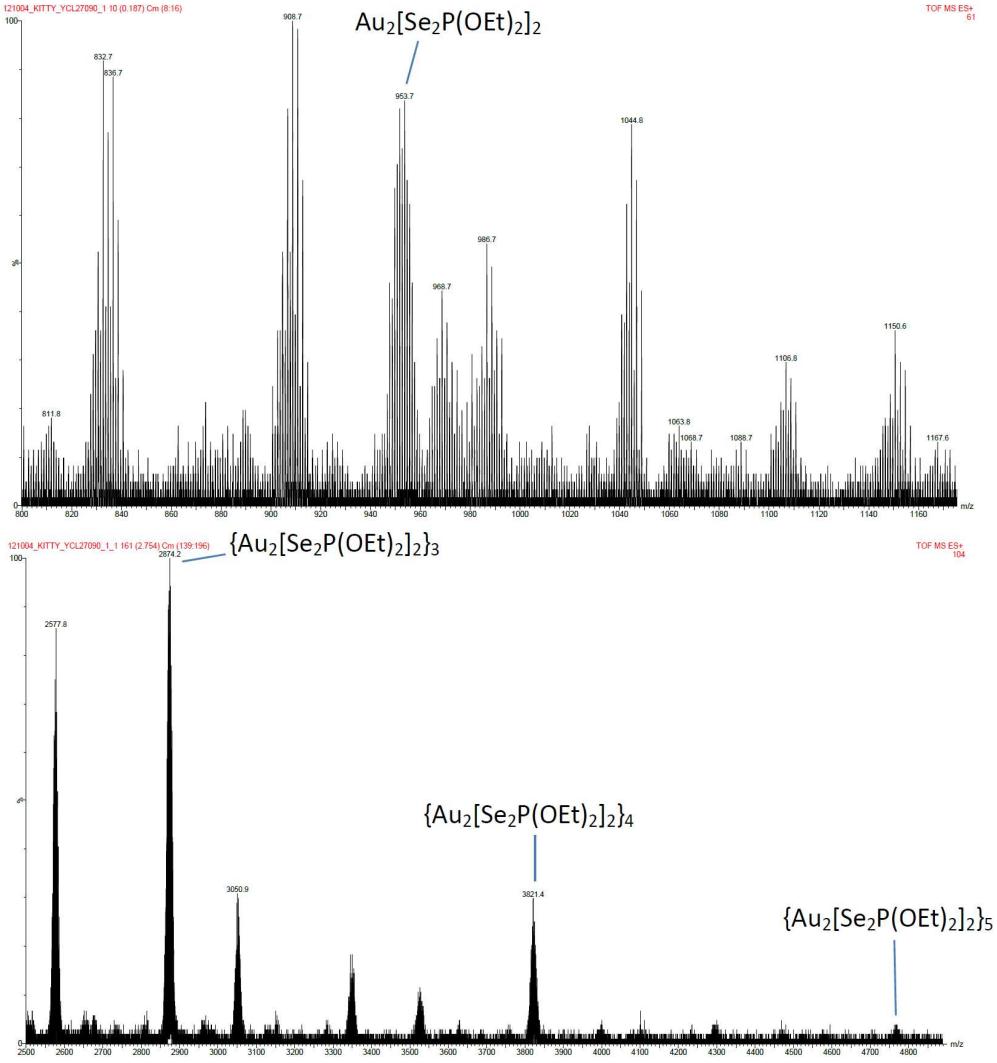
```
C13 C14 1.361(9) . ?
C14 C16 1.357(9) . ?
C15 C16 1.363(9) . ?
C17 C18 1.503(7) . ?
C18 C19 1.524(8) . ?
C19 C20 1.365(8) . ?
C19 C21 1.370(8) . ?
C20 C23 1.378(9) . ?
C21 C22 1.373(9) . ?
C22 C24 1.349(10) . ?
C23 C24 1.350(10) . ?
C25 C26 1.511(7) . ?
C26 C27 1.512(7) . ?
C27 C29 1.367(8) . ?
C27 C28 1.374(8) . ?
C28 C30 1.385(9) . ?
C29 C31 1.385(9) . ?
C30 C32 1.351(10) . ?
C31 C32 1.367(11) . ?

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
Se1 Au1 Se2 172.79(2) . . ?
Se4 Au2 Se3 171.97(2) . . ?
P1 Se1 Au1 102.17(4) 2_667 . ?
P1 Se2 Au1 100.48(5) . . ?
P2 Se3 Au2 99.94(4) 2_655 . ?
P2 Se4 Au2 100.44(4) . . ?
C9 P1 C1 105.9(3) . . ?
C9 P1 Se2 106.32(19) . . ?
C1 P1 Se2 109.9(2) . . ?
C9 P1 Se1 102.58(17) . 2_667 ?
C1 P1 Se1 112.2(2) . 2_667 ?
Se2 P1 Se1 118.73(7) . 2_667 ?
C17 P2 C25 108.0(3) . . ?
C17 P2 Se4 111.88(19) . . ?
C25 P2 Se4 104.02(17) . . ?
C17 P2 Se3 108.63(18) . 2_655 ?
C25 P2 Se3 107.06(18) . 2_655 ?
Se4 P2 Se3 116.70(6) . 2_655 ?
C2 C1 P1 120.4(4) . . ?
C3 C2 C1 115.4(5) . . ?
C5 C3 C4 117.0(6) . . ?
C5 C3 C2 124.0(6) . . ?
C4 C3 C2 119.0(6) . . ?
C7 C4 C3 119.7(7) . . ?
C3 C5 C6 121.6(7) . . ?
C8 C6 C5 120.1(8) . . ?
C8 C7 C4 119.8(8) . . ?
C6 C8 C7 121.7(8) . . ?
C10 C9 P1 117.1(4) . . ?
C11 C10 C9 111.5(4) . . ?
C12 C11 C13 117.6(6) . . ?
C12 C11 C10 121.0(6) . . ?
C13 C11 C10 121.3(6) . . ?
```

```
C11 C12 C15 121.0(6) . . ?
C14 C13 C11 121.1(6) . . ?
C16 C14 C13 120.9(6) . . ?
C16 C15 C12 120.1(6) . . ?
C14 C16 C15 119.2(6) . . ?
C18 C17 P2 114.6(4) . . ?
C17 C18 C19 115.4(5) . . ?
C20 C19 C21 117.4(6) . . ?
C20 C19 C18 123.6(5) . . ?
C21 C19 C18 118.9(6) . . ?
C19 C20 C23 120.7(6) . . ?
C19 C21 C22 120.9(7) . . ?
C24 C22 C21 121.5(7) . . ?
C24 C23 C20 121.5(7) . . ?
C22 C24 C23 118.0(7) . . ?
C26 C25 P2 115.5(4) . . ?
C25 C26 C27 112.7(5) . . ?
C29 C27 C28 118.5(6) . . ?
C29 C27 C26 121.7(5) . . ?
C28 C27 C26 119.8(6) . . ?
C27 C28 C30 120.5(7) . . ?
C27 C29 C31 120.8(7) . . ?
C32 C30 C28 120.4(7) . . ?
C32 C31 C29 120.0(7) . . ?
C30 C32 C31 119.8(7) . . ?

_diffrn_measured_fraction_theta_max    0.999
_diffrn_reflns_theta_full              25.05
_diffrn_measured_fraction_theta_full   0.999
_refine_diff_density_max    1.332
_refine_diff_density_min   -0.750
_refine_diff_density_rms    0.111
```

Figure S6. ESI_MS_data: ESI-mass spectra were recorded on a Fison Quattro Bio-Q (Fisons Instruments, VG Biotech, UK)



2.09 x 10^{-4} M (in CH_2Cl_2) of $Au_2[Se_2P(OEt)_2]_2$.