Radical change in the structure of $Au_{25}(SR)_{18}$ thiolate clusters after removal of bridging S*R groups from six (SR)Au(S*R)Au(SR) 'staples'

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Table of Contents

[Au$_{25}$(SMe)$_{18}$]$^{-}$: atomic coordinates, minimum harmonic frequency (ν_1, cm^{-1}) and total energy (E, Hartree)

ν_1 = 16.85

E = -483501.833091

79	-0.182185860	2.808981040	0.397999860
79	2.356890820	3.727384300	2.421674180
79	-4.156028720	-0.655384950	-2.772676500
79	-2.085641420	1.495733790	-1.220006540
79	-2.053719160	0.895928530	1.746763220
79	-3.207733160	3.836038970	0.574249080
79	-1.027887740	4.408797520	-2.231337450
79	0.772569900	1.587219920	-2.208123470
79	0.880683350	0.919067340	2.533145240
79	-1.501540250	0.144170660	4.786349600
79	-3.995976780	-1.406296820	2.714065620
79	2.476699120	1.363610070	0.243051660
79	0.001071890	-0.000098160	0.000033170
16	0.342797920	4.736980340	1.783414880
16	4.467913270	2.954777210	3.080200960
16	-4.086016530	1.678493660	-2.600527120
16	-2.751618760	5.466355590	-1.043281410
16	0.806650590	3.653326660	-3.487056980
16	-3.817261540	2.454510970	2.364605490
16	0.695504520	0.953045600	4.957080400
16	-3.752499100	-0.498719360	4.859972990
16	-4.505899750	-2.377660550	0.647974890
6	0.843341630	6.155667720	0.707270230
1	1.542317330	5.831883960	-0.074049610
1	-0.072007240	6.551965750	0.241608750
6	4.511725020	3.149549190	4.920089200
1	4.447672040	4.223047060	5.152317330
1	3.685367780	2.605695940	5.396125780
6	-3.452473630	2.162194570	-4.268644630
1	-2.649597940	1.482783860	-4.586769290

1	-3.066008270	3.191836930	-4.192110570
6	-4.226071230	5.410322790	-2.156309280
1	-4.001385180	6.002651900	-3.055249070
1	-4.472576150	4.372219930	-2.421980050
6	0.112857630	3.301659110	-5.164342170
1	0.829572760	2.655802280	-5.695327860
1	-0.847502200	2.778123060	-5.093460470
6	-3.170793690	3.420450000	3.803685270
1	-3.135928590	2.741871570	4.670707520
1	-2.167708920	3.813197980	3.587806640
6	0.458718300	2.707715770	5.492877920
1	1.401189730	3.246968950	5.311244330
1	-0.341047730	3.189682200	4.917061280
6	-3.820065560	-1.979284710	5.967165980
1	-3.174393670	-2.783967040	5.591398620
1	-3.503562590	-1.670534660	6.974543220
6	-4.046854960	-4.149521850	0.912441200
1	-3.993095490	-4.622891890	-0.081256890
1	-3.076573970	-4.229882310	1.421802550
79	0.183543920	-2.809028460	-0.398024650
79	-2.354075680	-3.727379990	-2.421913840
79	4.157121170	0.653483950	2.774268830
79	2.086213880	-1.495471060	1.221250440
79	2.054051590	-0.896612710	-1.748022000
79	3.206565990	-3.838981570	-0.573411660
79	1.027457770	-4.409887650	2.233434270
79	-0.771467930	-1.588219300	2.207229090
79	-0.879646430	-0.917585830	-2.533816090
79	1.502685240	-0.142219540	-4.787897560
79	3.997051790	1.406172450	-2.714618700
79	-2.474783710	-1.364115240	-0.243643410
16	-0.339462350	-4.736899890	-1.784774160
16	-4.465725340	-2.956518540	-3.080417380
16	4.085635140	-1.680350860	2.603123830

16	2.750179540	-5.468476110	1.044944080
16	-0.807549690	-3.653133840	3.487552160
16	3.818079770	-2.456081410	-2.361940260
16	-0.694904480	-0.949731070	-4.957825300
16	3.753520850	0.500794010	-4.861582230
16	4.507301850	2.376242100	-0.648308130
6	-0.839531750	-6.156730150	-0.708801050
1	-1.537073610	-5.833103160	0.073855310
1	0.076504370	-6.553784450	-0.245142240
6	-4.509359530	-3.150250530	-4.920414030
1	-4.444881820	-4.223601030	-5.153240250
1	-3.683229260	-2.605794560	-5.396151250
6	3.444858060	-2.163956190	4.268566950
1	2.643076990	-1.482273270	4.584596750
1	3.055290860	-3.192268870	4.189210490
6	4.224679620	-5.412527630	2.157889600
1	3.999062300	-6.002929660	3.057873820
1	4.472644080	-4.374330420	2.421894360
6	-0.116537390	-3.301766870	5.166034050
1	-0.833460710	-2.654780490	5.695282180
1	0.844681080	-2.779581810	5.097031730
6	3.173833180	-3.419800940	-3.803515350
1	3.140548090	-2.739946860	-4.669593650
1	2.170224500	-3.812506140	-3.589916380
6	-0.459087680	-2.704059340	-5.495169540
1	-1.400692260	-3.243938490	-5.310893090
1	0.342578080	-3.185951020	-4.921900090
6	3.819402230	1.983332750	-5.966420270
1	3.172530650	2.786366190	-5.589161270
1	3.503641650	1.675885310	-6.974417560
6	4.048244780	4.148135320	-0.912637860
1	3.994457690	4.621716700	0.080996270
1	3.077807270	4.228344110	-1.421731950
1	-4.832068380	-4.623382250	1.520025300

1	-5.469871140	-2.745068470	-5.272514760
1	-0.214255160	-2.707822460	-6.567828510
1	3.866791960	-4.252145100	-3.997744140
1	5.064741400	-5.864535250	1.610033150
1	-0.012616520	4.257643040	-5.694483200
1	4.863251350	2.330598140	-5.987700830
1	4.833145780	4.622410260	-1.520305340
1	4.275492620	-2.123378130	4.989277280
1	5.472086200	2.744144330	5.272342160
1	1.309291640	6.924136990	1.341859470
1	-4.864335180	-2.325200160	5.989284660
1	0.210736830	2.712043750	6.564807670
1	-4.285507780	2.118040770	-4.986371180
1	0.006481960	-4.257801270	5.696654000
1	-1.306925050	-6.924076470	-1.343654620
1	-5.066615810	5.860182280	-1.607447140
1	-3.863716980	4.252841720	3.997815260

[Au₂₅(SCH₂CH₂Ph)₁₈]⁻: atomic coordinates and total energy (*E*, Hartree)

E = -488365.38534208

79	-0.130422760	2.815170320	0.398567530
79	2.385655530	3.677221290	2.419819470
79	-4.205362820	-0.620436960	-2.713189020
79	-2.053532710	1.534891430	-1.231024160
79	-2.031267860	0.930497260	1.755425360
79	-3.173676450	3.872990440	0.531001550
79	-0.896108780	4.439937680	-2.201981180
79	0.789557240	1.584365930	-2.208327010
79	0.885203130	0.906438880	2.534900190
79	-1.485573220	0.211779850	4.818724010
79	-3.972567730	-1.359147460	2.750773000
79	2.496036660	1.313410120	0.239588700
79	-0.000522620	0.001128790	0.001573530
16	0.357750070	4.704674500	1.847539430
16	4.528013600	2.929222170	2.996958770
16	-4.077534980	1.718102380	-2.577832870
16	-2.631153230	5.517446180	-1.045198320
16	0.897499400	3.647869830	-3.497878440
16	-3.853887880	2.448429600	2.265879070
16	0.746725670	0.907017530	4.958486370
16	-3.739588730	-0.416943850	4.889899250
16	-4.518812560	-2.326857800	0.688921080
6	0.840337420	6.187163160	0.828202940
1	1.743968570	5.949968510	0.249307310
1	0.007613730	6.338523230	0.121150320
6	1.034246310	7.448663440	1.685065020
1	0.117700410	7.626063150	2.273216250
1	1.136997570	8.295524920	0.980665210
6	2.236076490	7.419581250	2.601627510
6	3.523759360	7.647773130	2.092486320
1	3.654581740	7.859777890	1.026026760

6	4.639516330	7.608837460	2.929681160
1	5.634510870	7.789864960	2.513803460
6	4.486034420	7.347058960	4.294366150
1	5.359687720	7.326047780	4.951811380
6	3.209923910	7.119643660	4.814207040
1	3.072359930	6.908619690	5.878445790
6	2.096457660	7.154934540	3.970869110
1	1.100751920	6.964467230	4.383371580
6	4.624598580	3.169612840	4.840167450
1	4.445705550	4.242735090	5.015971080
1	3.819733250	2.592365420	5.317174560
6	5.993327260	2.735110750	5.383068560
1	6.165382970	1.680091130	5.105463250
1	6.785483800	3.332518050	4.900591580
6	6.051588040	2.898978900	6.885042920
6	6.488175000	4.100010970	7.463129320
1	6.833806710	4.910533670	6.813540400
6	6.490484450	4.271278180	8.849046050
1	6.840852870	5.213413610	9.279637040
6	6.051244000	3.240640320	9.683896350
1	6.052738860	3.372414760	10.768945420
6	5.615117450	2.038047020	9.121783510
1	5.273573230	1.221474950	9.763474190
6	5.616079170	1.871103230	7.735496300
1	5.274108560	0.923712700	7.306419080
6	-3.483944050	2.136659220	-4.287407030
1	-2.581350630	1.541053930	-4.489597440
1	-3.205969780	3.204616400	-4.268256420
6	-4.574623780	1.863899390	-5.331557830
1	-5.494787810	2.406580930	-5.055112130
1	-4.814742250	0.784835720	-5.285672170
6	-4.153896840	2.249917390	-6.732101010
6	-4.826270390	3.262324830	-7.432275830
1	-5.668116270	3.772168340	-6.952840790

6	-4.435193630	3.626179780	-8.723462080
1	-4.973210560	4.418437490	-9.251151130
6	-3.356991090	2.984100400	-9.336301710
1	-3.045758550	3.270388220	-10.344333710
6	-2.676821190	1.974409640	-8.648811290
1	-1.829031740	1.466110270	-9.117054780
6	-3.072298860	1.609232700	-7.360643660
1	-2.526607160	0.820300270	-6.830248290
6	-4.029069290	5.470255700	-2.269148650
1	-3.698928780	6.069785430	-3.132645910
1	-4.170748620	4.425702640	-2.584086120
6	-5.330825550	6.017391000	-1.669246280
1	-5.179848840	7.054308690	-1.323720870
1	-5.590427200	5.408800080	-0.784411730
6	-6.443474950	5.961826220	-2.692259340
6	-6.827439160	7.102899390	-3.410421380
1	-6.338693790	8.058559490	-3.195312070
6	-7.823540910	7.035867260	-4.387658750
1	-8.112230770	7.938803950	-4.932803650
6	-8.451356640	5.819635650	-4.665268380
1	-9.233254410	5.764660160	-5.427330510
6	-8.076922110	4.673962050	-3.957097110
1	-8.565181350	3.717171460	-4.162543680
6	-7.082448770	4.745108340	-2.980344050
1	-6.790595990	3.842517520	-2.433122250
6	0.188990790	3.295404980	-5.184487380
1	0.746956520	2.415774200	-5.553069710
1	-0.862667930	2.998423720	-5.075542630
6	0.340813830	4.474333290	-6.159414270
1	1.391452530	4.811797330	-6.167198130
1	0.122939950	4.076886400	-7.168492080
6	-0.578003520	5.642750590	-5.885147980
6	-0.120589570	6.790575610	-5.223605300
1	0.926248360	6.843762170	-4.908760450

6	-0.982004890	7.858020400	-4.960546320
1	-0.606614100	8.744283690	-4.441465480
6	-2.319398980	7.794506080	-5.357190570
1	-2.994505160	8.630256450	-5.154847910
6	-2.786792180	6.657445140	-6.022402690
1	-3.830259860	6.598628790	-6.343793270
6	-1.922021660	5.593792190	-6.285561700
1	-2.296356620	4.714121550	-6.818263090
6	-3.390272340	3.437502150	3.772185120
1	-3.351736490	2.717628770	4.607485450
1	-2.387183190	3.866864360	3.628384900
6	-4.439264930	4.531138540	4.022699890
1	-4.463696910	5.197749650	3.142923850
1	-5.433659090	4.058030770	4.099017300
6	-4.156551900	5.334015160	5.271957680
6	-4.523067370	4.848404880	6.537030210
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1	-4.565853150	5.194716770	8.667883000
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1	-3.450119320	7.419700400	8.506592630
6	-3.262922100	7.326393880	6.351443660
1	-2.771564740	8.299906910	6.269667000
6	-3.515622350	6.579152530	5.198818540
6	0.701600190	2.660965910	5.574208100
1	1.648434130	3.115182990	5.237299660
1	-0.115911870	3.202428300	5.076750280
6	0.573083230	2.711667960	7.104382400
1	-0.446033360	2.395396970	7.387548890
1	1.275032130	1.984584870	7.547887760
6	0.876293790	4.093042210	7.642581170
6	2.150397390	4.393833500	8.147694440
1	2.917174920	3.613226780	8.182341760
6	2.453990020	5.674564670	8.614346950

1	3.453128780	5.879901380	9.008287170
6	1.485663490	6.681028700	8.578071180
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6	0.213722720	6.393784560	8.075575530
1	-0.555339290	7.169653090	8.043774970
6	-0.088546700	5.111400100	7.613537880
1	-1.091967630	4.901165500	7.229545830
6	-3.792510300	-1.889090080	6.027410840
1	-3.090769840	-2.649381350	5.654374500
1	-3.443977390	-1.536396460	7.011797350
6	-5.213878390	-2.462627330	6.116434270
1	-5.901294070	-1.685024630	6.490775720
1	-5.546756820	-2.727777220	5.097070790
6	-5.254235900	-3.676099810	7.017435960
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1	-4.696876960	-5.065621540	5.456286860
6	-4.931390220	-6.066385210	7.354285450
1	-4.685559630	-7.048814250	6.942649100
6	-5.243918950	-5.930415260	8.709280630
1	-5.241861210	-6.805170540	9.364643080
6	-5.563611680	-4.670062450	9.219148470
1	-5.814639040	-4.554350330	10.277082410
6	-5.566876930	-3.554629980	8.379011970
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6	-4.011506250	-4.102971340	0.879575980
1	-4.155653160	-4.552443450	-0.118609460
1	-2.938257900	-4.132193180	1.121119190
6	-4.838198390	-4.835409650	1.944030150
1	-4.624878770	-4.364912750	2.921152080
1	-5.913632740	-4.690927610	1.743050210
6	-4.511478390	-6.311858600	1.982484630
6	-5.426584890	-7.268618840	1.520666470
1	-6.402927270	-6.937988680	1.152382500
6	-5.109455160	-8.629484120	1.525364810

1	-5.839378770	-9.359168500	1.163927360
6	-3.862089210	-9.056687250	1.986482830
1	-3.609776270	-10.120357200	1.986350420
6	-2.939381790	-8.112735110	2.447009670
1	-1.956504200	-8.433392360	2.804525380
6	-3.262218020	-6.754665160	2.448541650
1	-2.532039090	-6.021189310	2.810026910
1	-3.220093770	6.968844430	4.219536180
79	0.130239900	-2.811856160	-0.395397330
79	-2.385475170	-3.672181300	-2.421717780
79	4.203866120	0.625664660	2.719436810
79	2.051963020	-1.531690900	1.236188450
79	2.027710080	-0.929107020	-1.754123430
79	3.171744840	-3.866609300	-0.526048780
79	0.897449190	-4.435104990	2.209130520
79	-0.790606660	-1.581640930	2.212970810
79	-0.889098180	-0.902428680	-2.532384680
79	1.482093290	-0.208571980	-4.816670260
79	3.973497100	1.352585380	-2.747358400
79	-2.496212680	-1.313410250	-0.235510650
16	-0.356347580	-4.698506960	-1.850855240
16	-4.530277890	-2.923890650	-2.993820260
16	4.075103240	-1.712491890	2.585174580
16	2.633096190	-5.510523850	1.052194660
16	-0.896482120	-3.644186730	3.505448790
16	3.843981610	-2.452132320	-2.272033730
16	-0.753185150	-0.893714480	-4.956819810
16	3.738432410	0.411228270	-4.886594960
16	4.521832870	2.319366160	-0.685697290
6	-0.836951520	-6.187032060	-0.839727900
1	-1.743569820	-5.955941410	-0.263111270
1	-0.006358160	-6.338661510	-0.130194950
6	-1.022855790	-7.445226020	-1.703225990
1	-0.102603880	-7.617752030	-2.287068450

1	-1.127337740	-8.295531610	-1.003272200
6	-2.219475800	-7.414716830	-2.626510200
6	-3.509229510	-7.650705790	-2.126307640
1	-3.645236090	-7.870278890	-1.062021780
6	-4.620312060	-7.609822220	-2.969616090
1	-5.617083970	-7.796995610	-2.560765560
6	-4.459929100	-7.338042000	-4.331550520
1	-5.329850810	-7.315478250	-4.993873110
6	-3.181681800	-7.102692310	-4.842588310
1	-3.039134420	-6.883688650	-5.904561720
6	-2.072965120	-7.140168920	-3.993109400
1	-1.075558160	-6.943355140	-4.398505320
6	-4.626245270	-3.160080620	-4.837432640
1	-4.453031470	-4.233841500	-5.015079580
1	-3.816595820	-2.587459860	-5.311853670
6	-5.989902760	-2.716614930	-5.385878170
1	-6.158203900	-1.661414210	-5.106893080
1	-6.788000260	-3.311527490	-4.910170930
6	-6.039059920	-2.876769360	-6.888749330
6	-6.474877110	-4.075292670	-7.472586850
1	-6.824875740	-4.887298550	-6.827203570
6	-6.471208120	-4.242196010	-8.859038450
1	-6.821163940	-5.182406300	-9.294152230
6	-6.026796110	-3.209583790	-9.688706190
1	-6.023818160	-3.337832860	-10.774178990
6	-5.591418960	-2.009423660	-9.120819250
1	-5.246001280	-1.191163490	-9.758281250
6	-5.598284950	-1.846875750	-7.734018990
1	-5.257155110	-0.901143070	-7.300692320
6	3.480191320	-2.130130160	4.294380870
1	2.577172720	-1.534779140	4.495396430
1	3.202664400	-3.198221710	4.275537390
6	4.569709140	-1.856524430	5.339546660
1	5.490172160	-2.399412200	5.064477230

1	4.809789130	-0.777480700	5.293468380
6	4.147149440	-2.242145350	6.739650170
6	4.816759970	-3.256339050	7.439894320
1	5.658062750	-3.767629380	6.961039220
6	4.423674680	-3.620105810	8.730509550
1	4.959509940	-4.413810390	9.258240150
6	3.346224110	-2.976107840	9.342631420
1	3.033452450	-3.262257670	10.350226700
6	2.668904750	-1.964497430	8.655106920
1	1.821932390	-1.454513450	9.122985310
6	3.066342610	-1.599508720	7.367533130
1	2.523100180	-0.808841810	6.837193460
6	4.031699140	-5.463411870	2.275262470
1	3.703063330	-6.065163600	3.137802840
1	4.172137360	-4.419311670	2.592277010
6	5.333516590	-6.007590840	1.672876530
1	5.183015440	-7.043483740	1.324091110
1	5.591960380	-5.396071800	0.789719180
6	6.447355930	-5.954880520	2.694745610
6	6.835021450	-7.099060640	3.405953850
1	6.347725040	-8.054506280	3.186649590
6	7.833155660	-7.035460710	4.381346010
1	8.124670420	-7.940795660	4.920983510
6	8.459452720	-5.819631640	4.664033800
1	9.243037110	-5.767357530	5.424549280
6	8.081309460	-4.670857440	3.962901760
1	8.568367800	-3.714316760	4.172314470
6	7.084651340	-4.738534330	2.988139970
1	6.790121640	-3.833574910	2.446275970
6	-0.185720340	-3.289263630	5.190761700
1	-0.742185250	-2.408407250	5.558737950
1	0.865992580	-2.993487300	5.079516540
6	-0.336502420	-4.465963670	6.168580130
1	-1.388245520	-4.799860680	6.182715670

1	-0.111539340	-4.067621740	7.175727160
6	0.575991730	-5.638508460	5.890680370
6	0.110214840	-6.783444870	5.229991350
1	-0.938080110	-6.831127630	4.919227170
6	0.965022580	-7.855107150	4.962553750
1	0.583047790	-8.739027980	4.444260260
6	2.304238360	-7.798868640	5.353898520
1	2.974235450	-8.637901910	5.148212010
6	2.780030950	-6.664773480	6.018230340
1	3.825020790	-6.611736710	6.335683780
6	1.921853730	-5.596839460	6.285720310
1	2.302868050	-4.719469840	6.817622110
6	3.371433760	-3.452768590	-3.767637590
1	3.342993050	-2.742834770	-4.611845700
1	2.363328530	-3.869316250	-3.620737010
6	4.408972990	-4.560978870	-4.002075760
1	4.427819780	-5.212779240	-3.110948300
1	5.408063780	-4.099840840	-4.087702790
6	4.116137540	-5.382173470	-5.236762610
6	4.545258330	-4.955891490	-6.503196570
1	5.102531780	-4.017457130	-6.590113990
6	4.281136770	-5.714927100	-7.644471110
1	4.629250380	-5.367852090	-8.621248690
6	3.581411530	-6.919992640	-7.538868860
1	3.383777170	-7.520394730	-8.430798480
6	3.139591540	-7.351628180	-6.285767650
1	2.590945620	-8.292856290	-6.191524130
6	3.402050260	-6.586090040	-5.147681190
1	3.057518060	-6.929219370	-4.166953170
6	-0.712243010	-2.644999950	-5.581409630
1	-1.656713880	-3.101531800	-5.241147270
1	0.108594770	-3.188522320	-5.091787950
6	-0.593166690	-2.687161090	-7.112517820
1	0.423311150	-2.366620200	-7.400667190

1	-1.299360580	-1.959149550	-7.547633280
6	-0.896989840	-4.065441180	-7.658326870
6	-2.169314830	-4.360640110	-8.171196390
1	-2.934540820	-3.578500470	-8.203997240
6	-2.473387000	-5.637814870	-8.647152220
1	-3.471405990	-5.838554440	-9.046178690
6	-1.507322310	-6.646426910	-8.612838990
1	-1.741614260	-7.647446870	-8.984746970
6	-0.237315960	-6.364932150	-8.102324540
1	0.530124840	-7.142289730	-8.071266980
6	0.065427030	-5.086206730	-7.630659120
1	1.067317270	-4.881115320	-7.239865280
6	3.798590010	1.882906410	-6.024464450
1	3.100068210	2.646614110	-5.652327160
1	3.449029860	1.531428810	-7.008933400
6	5.222914100	2.449259080	-6.112582680
1	5.906352160	1.668021410	-6.486652150
1	5.556621060	2.712326410	-5.092947810
6	5.270761990	3.662835150	-7.013078620
6	4.962715710	4.937413730	-6.512863070
1	4.724235640	5.055556590	-5.450914920
6	4.965193040	6.055597460	-7.348442070
1	4.726830330	7.039550220	-6.936069500
6	5.275978430	5.918098980	-8.703681490
1	5.280064770	6.793217910	-9.358554570
6	5.585995190	4.655688180	-9.214464650
1	5.835482030	4.538713800	-10.272625480
6	5.581613490	3.539806830	-8.374941860
1	5.829160300	2.553148420	-8.779625400
6	4.021810160	4.097368460	-0.878999890
1	4.169447410	4.548355550	0.117958840
1	2.948381360	4.130545860	-1.119179380
6	4.850270160	4.823328760	-1.946447400
1	4.633849410	4.350485790	-2.921810470

1	5.925351430	4.674491440	-1.746626470
6	4.530150050	6.301069100	-1.990015180
6	5.451043920	7.255448430	-1.534803670
1	6.426622150	6.921692430	-1.167311980
6	5.140716040	8.617843540	-1.545214200
1	5.875073680	9.345556570	-1.188832940
6	3.894514360	9.049102550	-2.005663260
1	3.647521000	10.114007050	-2.010081340
6	2.966028970	8.107582350	-2.459524910
1	1.984076880	8.431610230	-2.816562710
6	3.282043120	6.747899860	-2.455358410
1	2.547465900	6.016448930	-2.812038830

[Au25(SMe)12]− (symmetrical): atomic coordinates, minimum harmonic frequency (v_1, cm−1) and total energy (*E*, Hartree)

$v_1 = 8.7$

E = -480867.1848880453

79	0.217556860	0.096093220	-0.064530120
79	1.006588840	1.081488670	2.570606020
79	0.166919050	2.966633530	0.352479390
79	-1.886759470	1.119494320	1.651562010
79	2.811598920	1.403501860	0.097774090
79	2.345632230	-1.340646060	1.264788280
79	3.800666540	0.988262700	2.696454090
79	-1.512813560	0.166511450	4.236338530
79	2.666800840	3.311060030	2.133369170
79	-3.290635700	-1.076695430	2.738394110
79	-0.566857420	-1.557914300	2.206698090
79	-1.050424250	4.091686600	-1.913388820
79	-2.521540220	3.809062290	0.265964110
16	-0.202640750	-3.652223910	3.523295630
16	4.170727150	-1.357767980	3.009887470
16	4.821616930	2.324999900	-1.111480830
16	0.505715230	1.176083430	5.028045660
16	1.370453710	5.042333950	1.108934360
16	-3.283585720	3.101763480	2.428366520
79	-0.596001610	-0.825565620	-2.690206420
79	0.324478990	-2.779950380	-0.522106470
79	2.343490030	-0.936815330	-1.737094930
79	-2.355808540	-1.223254300	-0.191903430
79	-1.965978470	1.541462140	-1.309773700
79	-3.408703060	-0.754622720	-2.755831050
79	1.874741790	-0.053165820	-4.356657190
79	-2.244023120	-3.072273010	-2.267081680
79	3.685726520	1.199285050	-2.892082280
79	0.979555940	1.730062010	-2.355708460

79	1.433693690	-3.921559940	1.800466300
79	2.994660450	-3.594165000	-0.303481250
16	0.560747850	3.811738060	-3.655549430
16	-3.826357530	1.588374880	-3.030767840
16	-4.307376890	-2.347645700	0.976938180
16	-0.190621600	-0.954162420	-5.175755980
16	-0.729397600	-4.792362000	-1.582638450
16	4.196033800	-2.635959120	-2.141557400
6	6.194539880	1.197868620	-0.604008780
1	7.088233240	1.470389290	-1.185538290
1	6.383907540	1.350199950	0.469382250
1	5.934574300	0.148775940	-0.800980400
6	0.248982180	5.789081560	2.371713440
1	0.810145400	6.572906530	2.902156420
1	-0.609014430	6.231867780	1.843945110
1	-0.106873850	5.036310880	3.086476890
6	5.682277460	-1.891127590	2.093661290
1	5.804203650	-1.323262690	1.162593080
1	6.551378380	-1.727892410	2.748411110
1	5.579434060	-2.962020380	1.862510060
6	-5.025830760	2.500568890	2.326087780
1	-5.695120150	3.348720020	2.534820820
1	-5.244140690	2.093614950	1.329902870
1	-5.161002920	1.716143850	3.086706930
6	-5.325036090	2.069484200	-2.066315940
1	-5.214519430	3.122390810	-1.765231260
1	-6.203491160	1.954719400	-2.719017080
1	-5.440904080	1.436969330	-1.176466750
6	-5.790587920	-1.447196500	0.347654830
1	-5.676556550	-0.362607040	0.475746230
1	-5.910856750	-1.686810680	-0.719965720
1	-6.667365880	-1.795784200	0.913956770
6	0.090590220	2.948547530	5.341831100
1	0.997671080	3.548254120	5.173140370

1	-0.719847880	3.282940980	4.679522970
1	-0.230155030	3.039734440	6.390598350
6	3.680629340	-3.533330850	-3.670903770
1	3.722420510	-2.826589640	-4.513863780
1	4.387542040	-4.360411100	-3.835814830
1	2.663729660	-3.934273410	-3.565005480
6	0.016581080	-2.758313500	-5.507904940
1	0.405134000	-2.875869490	-6.530550540
1	0.708435170	-3.217689590	-4.790224720
1	-0.972070950	-3.234063210	-5.422376130
6	-1.543939400	-5.656396830	-0.166269870
1	-2.190968820	-4.968556930	0.395026800
1	-2.144446710	-6.482111830	-0.576157600
1	-0.754598110	-6.050760930	0.491136380
6	0.734338660	-3.077138250	5.009081430
1	0.059496160	-2.456435670	5.617343450
1	1.043538950	-3.968035450	5.575844330
1	1.620109220	-2.496015920	4.717844840
6	-0.395833780	3.219525330	-5.122063690
1	-0.745211580	4.105735960	-5.672540970
1	0.279695490	2.623993350	-5.754004290
1	-1.257094590	2.610801860	-4.814657320

[Au$_{25}$(SMe)$_{12}$]$^-$ (asymmetrical): atomic coordinates, minimum harmonic frequency (v_1, cm^{-1}) and total energy (E, Hartree)

$v1 = 4.8$

$E = -480867.25496682$

79	1.392713020	2.129444140	-1.961430730
79	3.937647570	1.258050240	-0.372906650
79	-3.275444660	-0.663270100	-2.342348880
79	-1.023046820	1.227987200	-2.965887890
79	-0.962565870	2.344689290	-0.219759250
79	-0.280498210	3.903056780	-3.318078020
79	1.018416250	2.057823800	-4.726083740
79	1.138352520	-0.761414320	-2.566836090
79	2.747087780	2.348291540	1.929796600
79	4.344039270	-1.400145680	-0.503138180
79	1.257383980	0.518924560	0.322173230
16	3.558406840	3.271297600	-1.563353100
16	-3.174422940	0.855783010	-4.138537350
16	2.129560130	-0.120992810	-4.758537490
16	-1.561148490	4.479416790	-1.330462800
6	4.422212680	3.050336050	-3.185197970
1	4.332363960	2.019262700	-3.551345610
1	3.944086090	3.732400510	-3.904913830
6	-2.712431480	-0.145375700	-5.624846580
1	-2.090133450	-1.003782780	-5.341347120
1	-2.163732020	0.510502000	-6.317761800
6	1.305308020	-1.250664670	-5.964439920
1	1.544039540	-2.288500050	-5.687569010
1	0.217382110	-1.105012890	-5.954591770
6	-0.582894430	5.724030710	-0.378894960
1	-0.946308110	5.735407820	0.659568970
1	0.487776840	5.479913130	-0.398093620
79	-2.535709080	-2.041619570	2.447834760
79	-3.151600240	-2.590101880	-0.495763690

79	3.750806980	-0.289543080	1.871223300
79	1.141985820	0.429843760	3.505148600
79	1.319583040	-2.269344720	-0.108368440
79	-1.128993290	0.311439350	1.926470950
79	-1.047513850	-0.698671010	-0.738747790
79	-0.225391860	-3.296082790	-2.215930720
79	2.500873860	-3.147726480	-2.433739900
79	-3.727528570	-0.111639120	0.444623100
16	-3.866360190	-3.837513620	1.641563330
16	3.279634010	-0.439571340	4.229851870
6	-5.610344440	-3.259534160	1.859145770
1	-5.712063900	-2.215219310	1.530678830
1	-5.888933750	-3.352452490	2.918911680
6	4.317558200	0.896743410	4.977647510
1	4.294801130	1.801597680	4.354053380
1	3.924209270	1.111061260	5.982259140
16	4.878226300	-3.137209140	-2.075992380
6	5.560879220	-2.215370810	-3.529496070
1	4.871101930	-1.423300710	-3.853261610
1	6.533234700	-1.788954870	-3.243192460
16	-2.399185100	-4.294306620	-2.169834250
6	-2.204640980	-5.857717590	-1.203430610
1	-1.773851260	-6.625621670	-1.862968490
1	-1.555106430	-5.708969400	-0.330821710
79	-2.786243440	2.485020450	1.914262500
79	-0.202251460	2.985864400	2.455656250
16	1.826156190	4.242080640	3.014944380
6	2.049828020	3.951063510	4.828842640
1	1.371743170	4.640941780	5.353018700
1	1.794060440	2.913308960	5.088760370
16	-4.999858820	1.740692950	1.397414250
6	-5.462550860	2.740311170	-0.092432100
1	-4.590812740	2.913418350	-0.737860150
1	-6.234626330	2.186792110	-0.646420270

79	0.207736210	-2.092665520	2.567383990
79	-1.251521210	-0.716101360	4.541860660
16	-1.734804240	-0.271213300	6.756975170
6	-2.776382910	1.254531340	6.675204720
1	-2.231483290	2.079348220	6.193135800
1	-3.709165280	1.065346950	6.124861680
16	1.908917490	-3.598802460	1.867434760
6	1.039742580	-5.209664410	1.595697740
1	1.024094340	-5.750059240	2.553930730
1	0.011929570	-5.044401130	1.248245270
1	-3.640015730	-0.502800640	-6.096752810
1	-6.255160050	-3.903824700	1.242193190
1	-5.864585780	3.702894070	0.256357150
1	-3.203826530	-6.169288240	-0.864198030
1	-3.018542290	1.536134360	7.712255570
1	3.092528370	4.172599020	5.099054990
1	-0.749092650	6.704683820	-0.849882370
1	1.702635530	-1.024383370	-6.965189540
1	5.697182460	-2.943702920	-4.343199450
1	5.348649420	0.519301480	5.049212370
1	5.481151310	3.314899640	-3.047567420
1	1.604746890	-5.779999860	0.843758710

[Au₂₅(SCH₂CH₂Ph)₁₂]⁻ (symmetrical): atomic coordinates and total energy (*E*, Hartree)

E = -484109.54890762

79	-0.220022650	2.960976720	0.440487320
79	2.121287950	3.455871580	2.605852770
79	-3.380223180	-0.923055210	-2.966879590
79	-2.047832370	1.631041350	-1.464907710
79	-2.039014570	0.930113050	1.595619510
79	-2.849360810	3.793982340	0.108311440
79	-1.137126290	4.378484420	-1.820525550
79	0.706890120	2.030890610	-2.228728160
79	0.757514940	0.993936790	2.514806410
79	-1.751844540	-0.076193110	4.251548960
79	-3.470635880	-1.236943450	2.636452160
79	2.498859420	1.851049010	0.338913850
79	0.229537380	0.110692210	-0.212241240
16	0.207625730	4.846948350	2.071308230
16	-4.113107820	1.344762050	-2.805018610
16	0.829070660	4.329545820	-3.259343060
16	-3.964434330	2.503674130	1.774611760
16	0.397221860	0.682216620	5.004618200
16	-4.417540720	-2.138587560	0.630934670
6	0.881506950	6.287561470	1.126580090
1	1.503244450	5.922923000	0.294863830
1	0.008076200	6.810157430	0.702355050
6	1.691412520	7.246131610	2.028413350
1	1.100594790	7.472215290	2.933052320
1	1.813233570	8.193423470	1.471761970
6	3.056228250	6.722917230	2.405829530
6	4.162799600	6.968796830	1.581855710
1	4.038470590	7.570838290	0.675715310
6	5.424901570	6.459592580	1.899624010
1	6.271155950	6.672773100	1.240915620
6	5.602544670	5.680335310	3.045482180

1	6.586508890	5.270969670	3.287766630
6	4.513599910	5.425897400	3.879566020
1	4.636857990	4.819335890	4.780765690
6	3.248454370	5.944380830	3.565274070
1	2.417477680	5.801412040	4.262827180
6	-3.637534610	2.090001700	-4.436443790
1	-2.576603180	1.871105220	-4.625052770
1	-3.762481910	3.179380130	-4.328089030
6	-4.507021830	1.538130870	-5.576236520
1	-5.574108240	1.676470720	-5.328335360
1	-4.330592130	0.448744520	-5.645253670
6	-4.187371820	2.208452900	-6.894181050
6	-5.086255840	3.104136300	-7.489997260
1	-6.048926980	3.293786710	-7.004498100
6	-4.772487960	3.750032250	-8.688711690
1	-5.489492760	4.443343350	-9.137249650
6	-3.546146690	3.510147130	-9.312369410
1	-3.296854020	4.014437530	-10.249828040
6	-2.642035800	2.616145010	-8.730522040
1	-1.680404760	2.417564970	-9.212314420
6	-2.959818870	1.970458330	-7.534690510
1	-2.244157730	1.271959980	-7.085414620
6	0.203665630	4.251054360	-5.000835030
1	1.053748860	3.913671930	-5.615996230
1	-0.593864850	3.496241750	-5.069682770
6	-0.301333090	5.622696530	-5.499965600
1	0.463808990	6.387429660	-5.279655000
1	-0.387089440	5.555470770	-6.599882100
6	-1.638853730	6.033543860	-4.931211110
6	-1.736135020	6.728068010	-3.710964700
1	-0.823386870	7.041250970	-3.196022840
6	-2.984839990	7.063676390	-3.172985180
1	-3.036037640	7.590698980	-2.216347750
6	-4.155354080	6.716191030	-3.848418250

1	-5.130087410	6.973897760	-3.426285060
6	-4.070824630	6.035440870	-5.065188360
1	-4.979340250	5.761735420	-5.608199270
6	-2.824875820	5.694343670	-5.597130210
1	-2.775836340	5.153326780	-6.547677970
6	-3.694878320	3.345261290	3.407243570
1	-3.661832490	2.542957990	4.164194630
1	-2.724884300	3.865159890	3.396086690
6	-4.848839240	4.322179570	3.683734820
1	-4.858356030	5.091613490	2.892755180
1	-5.803481200	3.772680010	3.614522030
6	-4.733371970	4.977372420	5.041486530
6	-5.211442760	4.332002610	6.192456130
1	-5.680733160	3.347401760	6.097121850
6	-5.103975240	4.930743770	7.448675330
1	-5.486845800	4.412944380	8.332393480
6	-4.515403600	6.191893290	7.576517540
1	-4.438710430	6.665172100	8.558981450
6	-4.028078380	6.842003940	6.440244740
1	-3.565026650	7.828719240	6.528465690
6	-4.133703080	6.236599610	5.186196870
6	0.369564800	2.391339370	5.724688310
1	1.384281510	2.797157990	5.571908310
1	-0.337265170	3.018166380	5.161320290
6	0.010789830	2.355746050	7.218505360
1	-1.030307010	2.006325780	7.328092150
1	0.657884090	1.619775120	7.726436390
6	0.184863490	3.714942130	7.858505650
6	1.402616890	4.067407920	8.459858850
1	2.213950460	3.332910530	8.491975720
6	1.589116100	5.332623910	9.019337450
1	2.544759570	5.584836330	9.487119980
6	0.555749300	6.272073360	8.984302000
1	0.698271550	7.263355970	9.422668200

6	-0.660982470	5.933969120	8.387630520
1	-1.479683060	6.657065340	8.353160260
6	-0.844408560	4.667270570	7.829620390
1	-1.804734930	4.416201590	7.368172880
6	-4.194752820	-3.971830810	0.815868810
1	-4.457213670	-4.421419640	-0.155737650
1	-3.133892530	-4.171153250	1.025901880
6	-5.072451030	-4.526436190	1.948038430
1	-4.756984920	-4.041014270	2.890075260
1	-6.125297980	-4.244137550	1.775981460
6	-4.950696670	-6.029531820	2.065323940
6	-6.011015900	-6.874104750	1.708285030
1	-6.950999290	-6.431837060	1.362999850
6	-5.884322750	-8.263372120	1.788913660
1	-6.724787890	-8.903826820	1.507192220
6	-4.686776910	-8.832481940	2.227439910
1	-4.583518220	-9.919050270	2.289918450
6	-3.622579850	-8.001108590	2.590048480
1	-2.681974680	-8.436454250	2.939597350
6	-3.753725660	-6.613875270	2.511843170
1	-2.914819750	-5.968840790	2.798553730
1	-3.750241410	6.749805470	4.298717330
79	0.318278200	-2.790412720	-0.545944090
79	-2.013771090	-3.165386910	-2.651056000
79	3.514270300	1.213856260	2.872626920
79	2.118125140	-1.423935160	1.356275200
79	2.197599730	-1.136040050	-2.014644880
79	2.989376700	-3.586794530	-0.223598250
79	1.305532920	-4.076356520	1.754382390
79	-0.736190420	-1.598182370	2.069405210
79	-0.627312580	-0.721739040	-2.805858910
79	1.629462450	0.338058300	-4.300358290
79	3.360245630	1.340263950	-2.558872030
79	-2.284290140	-1.433568670	-0.444987020

16	-0.265288110	-4.714726490	-2.076915670
16	4.149576820	-1.085105240	2.719465330
16	-0.686876650	-3.931828470	3.080051180
16	4.082455970	-2.720625410	-2.183622520
16	-0.382854790	-0.347783530	-5.394455190
16	4.611330260	2.394414070	-0.839698140
6	-0.946491480	-6.061824590	-1.001266720
1	-1.676333200	-5.634432600	-0.298016320
1	-0.086314510	-6.437356180	-0.421869280
6	-1.582358680	-7.204260980	-1.818218290
1	-0.879116070	-7.516030120	-2.609928580
1	-1.702013320	-8.063055260	-1.132420190
6	-2.928942220	-6.864769140	-2.414313130
6	-4.102338590	-7.085237150	-1.678126000
1	-4.039239960	-7.527566390	-0.678610370
6	-5.351672000	-6.746335900	-2.201731080
1	-6.251144300	-6.927171390	-1.607138800
6	-5.450078410	-6.176181070	-3.473250580
1	-6.426936930	-5.903850940	-3.881369210
6	-4.290741020	-5.952146660	-4.217618940
1	-4.352937710	-5.499207140	-5.210838400
6	-3.041538990	-6.296211970	-3.693229410
1	-2.139041880	-6.123717440	-4.286640830
6	3.633960760	-1.778365660	4.363566210
1	2.576679840	-1.524444140	4.528517950
1	3.730247660	-2.873773030	4.286964010
6	4.499047840	-1.213099940	5.499458380
1	5.564651300	-1.410889340	5.291662140
1	4.369631400	-0.114687030	5.506826740
6	4.115127840	-1.793832140	6.842408410
6	4.971217280	-2.666831980	7.527849150
1	5.942865130	-2.914318810	7.088443880
6	4.603448570	-3.218482140	8.757983810
1	5.287099480	-3.896586370	9.276392630

6	3.365329250	-2.905846230	9.323184480
1	3.073679790	-3.337482330	10.284336500
6	2.502345270	-2.035451280	8.650222380
1	1.530270350	-1.782967780	9.083455350
6	2.873850220	-1.484114500	7.423077480
1	2.188857840	-0.806594030	6.899809930
6	-0.252854050	-3.697018440	4.867364340
1	-1.120720200	-3.180026700	5.310688910
1	0.620283170	-3.032401370	4.944338510
6	0.005768180	-5.029537490	5.596947480
1	-0.830485910	-5.719901880	5.391151180
1	-0.013559370	-4.809534710	6.680278800
6	1.324267270	-5.683849570	5.254399790
6	1.424423790	-6.627888220	4.220773240
1	0.525877570	-6.909116530	3.663925020
6	2.653259210	-7.206544260	3.893067280
1	2.709553520	-7.931109100	3.076057640
6	3.805007310	-6.852718180	4.597824640
1	4.767389780	-7.303128710	4.340956630
6	3.718709290	-5.915996490	5.630589290
1	4.612335310	-5.626388260	6.189693170
6	2.489614430	-5.338164960	5.954656930
1	2.437210200	-4.603649460	6.764831900
6	3.567116090	-3.924506930	-3.503839990
1	3.878785750	-3.487715820	-4.467100640
1	2.471380940	-4.018953830	-3.490153220
6	4.229945130	-5.289857060	-3.267520470
1	3.902370900	-5.652435150	-2.275288100
1	5.325196190	-5.165104860	-3.215750900
6	3.875470070	-6.306022340	-4.330188350
6	4.829240950	-6.748062700	-5.257437200
1	5.845664780	-6.344186370	-5.211248600
6	4.503857300	-7.702037270	-6.225318660
1	5.265554720	-8.039476700	-6.933789840

6	3.211155380	-8.226892270	-6.282902790
1	2.954122280	-8.978117920	-7.034525620
6	2.246776670	-7.784463900	-5.372186240
1	1.229625670	-8.183129660	-5.415782710
6	2.575822010	-6.833699320	-4.406060930
1	1.814625790	-6.489962310	-3.696650280
6	-0.169296420	-2.030975240	-6.141243000
1	-1.179193990	-2.471513620	-6.191873090
1	0.439316120	-2.653492360	-5.469343120
6	0.464869670	-1.941042950	-7.537922790
1	1.481565020	-1.523070950	-7.434430180
1	-0.114907750	-1.231552990	-8.153026160
6	0.515279950	-3.288956500	-8.221467830
6	-0.453909240	-3.652657790	-9.167525740
1	-1.238757440	-2.936059790	-9.430127240
6	-0.425958180	-4.907978860	-9.778638910
1	-1.188708280	-5.169826910	-10.517214040
6	0.573878480	-5.825336460	-9.447894530
1	0.597343760	-6.808963410	-9.924460110
6	1.543756250	-5.478511740	-8.503671200
1	2.325473200	-6.190127590	-8.226576710
6	1.512787960	-4.221171870	-7.898885990
1	2.277402490	-3.958446320	-7.161120760
6	4.416699860	4.213667830	-1.154729600
1	4.707741660	4.710211040	-0.215233190
1	3.355945730	4.427076730	-1.350602430
6	5.285145400	4.689801480	-2.327817650
1	4.921782200	4.202895100	-3.250377770
1	6.327850440	4.361861830	-2.175488280
6	5.230812780	6.195462950	-2.464794210
6	6.316403780	6.996876940	-2.083946370
1	7.230924110	6.517458100	-1.720017710
6	6.247894700	8.389896120	-2.167959490
1	7.107635890	8.995984060	-1.868949300

6	5.084865080	9.006237530	-2.634496600
1	5.027728500	10.095963340	-2.701252800
6	3.995607000	8.218448590	-3.018296980
1	3.080396690	8.691345920	-3.385932690
6	4.067841180	6.827183110	-2.934957290
1	3.206398570	6.216621240	-3.229470070

[Au₂₅(SCH₂CH₂Ph)₁₂]⁻ (asymmetrical): atomic coordinates and total energy (*E*, Hartree)

E = -484109.61187806

79	1.506604660	3.193566380	-2.603920600
79	3.941116190	2.325509450	-0.804755020
79	-3.339490970	0.921617430	-3.187423420
79	-0.945812430	2.576974980	-3.700186790
79	-0.850290550	3.742396460	-0.973792520
79	0.134749540	5.113502040	-4.093046120
79	1.246653490	3.083160260	-5.401539570
79	0.820624740	0.313231910	-3.272874380
79	2.212960140	3.346759380	1.233758940
79	3.818446480	-0.402093700	-0.930874490
79	1.380604290	1.255555780	-0.529365400
16	3.739328970	4.235486480	-2.171451350
16	-3.083665890	2.448514610	-4.962748440
16	2.101953770	0.788011950	-5.349180550
16	-1.119136170	5.915690180	-2.180605020
6	4.648592240	3.802239770	-3.734848640
1	4.411106430	2.764252040	-4.008701320
1	4.212468230	4.455785070	-4.509602390
6	6.160409430	4.033831640	-3.621905400
1	6.350578500	5.085230580	-3.345902800
1	6.580494180	3.891226130	-4.637225430
6	6.886470350	3.122638030	-2.655366830
6	6.791268790	1.726001980	-2.766192240
1	6.172587840	1.280514800	-3.552165500
6	7.472102620	0.888496590	-1.880677800
1	7.364907530	-0.195184740	-1.978748110
6	8.267763320	1.432576030	-0.869727510
1	8.797230670	0.776932470	-0.173435420
6	8.370760070	2.819425700	-0.747988480
1	8.984528080	3.256642010	0.044473280
6	7.682687920	3.653696350	-1.632119010

1	7.755489060	4.740467110	-1.523338780
6	-2.646163760	1.363024320	-6.406303760
1	-1.839854860	0.682393680	-6.098438580
1	-2.250059070	2.034498170	-7.185900780
6	-3.855782410	0.563096500	-6.911882690
1	-4.669606880	1.255102180	-7.188945960
1	-4.225709030	-0.064704890	-6.081930790
6	-3.475044450	-0.301840770	-8.091970390
6	-3.710461480	0.118627930	-9.408795080
1	-4.221533370	1.071409310	-9.580881400
6	-3.306015360	-0.660044710	-10.495765170
1	-3.502072340	-0.315727180	-11.515103120
6	-2.654305620	-1.877001920	-10.281297520
1	-2.336812040	-2.488602060	-11.130077350
6	-2.418401610	-2.310199290	-8.973268060
1	-1.917033040	-3.265496140	-8.793517050
6	-2.826064400	-1.530438600	-7.889576570
1	-2.646578220	-1.879851820	-6.866475230
6	1.318912740	-0.196725320	-6.707708420
1	1.581453720	-1.248113820	-6.506403490
1	0.225100740	-0.094896010	-6.652416020
6	1.830675360	0.227690200	-8.100654930
1	2.932428480	0.290704640	-8.075947880
1	1.566533790	-0.583970280	-8.803181420
6	1.236451950	1.521950050	-8.603609330
6	1.876193800	2.755666210	-8.389843980
1	2.858739570	2.775802530	-7.908798260
6	1.290230930	3.952606750	-8.819632480
1	1.799632260	4.901177720	-8.629452960
6	0.057950180	3.933699450	-9.473707280
1	-0.402797550	4.868310240	-9.803949100
6	-0.583653600	2.712874020	-9.698399200
1	-1.547339710	2.684048850	-10.214247450
6	-0.000368710	1.520592410	-9.264107220

1	-0.517924180	0.572047240	-9.441033850
6	0.046760030	7.036725400	-1.270643730
1	-0.433014460	7.282336410	-0.308642150
1	0.978856700	6.490953930	-1.063250770
6	0.335488770	8.304409110	-2.088041880
1	0.812923620	7.998143370	-3.037011740
1	-0.615314290	8.798970540	-2.351276150
6	1.228205520	9.264791220	-1.335057430
6	0.708760860	10.424823530	-0.743980130
1	-0.358182180	10.645183270	-0.850476350
6	1.531332770	11.299051320	-0.029714220
1	1.105755370	12.200498460	0.419994790
6	2.892986880	11.023031540	0.108706360
1	3.539565660	11.705514210	0.666698410
6	3.423518890	9.867966800	-0.472410100
1	4.488255340	9.641640360	-0.368900080
6	2.598640640	8.998760850	-1.186985470
1	3.021665540	8.095374630	-1.638437830
79	-2.381310410	-0.444790140	1.288281510
79	-3.381559120	-1.127521180	-1.483823430
79	3.532283460	0.831341750	1.462576640
79	1.201471380	1.535328840	3.321857540
79	0.591343640	-1.498066740	-0.851479970
79	0.324303600	-0.590375150	1.798920860
79	-1.371477470	0.672887080	3.718086500
79	-0.792038330	1.925911390	1.275437250
79	-1.238541130	0.768774750	-1.343098470
79	-3.930844940	1.343045240	-0.443563470
16	-3.835296440	-2.297954230	0.777819100
16	3.463376220	0.962929960	3.892088580
16	-2.533187410	0.907016660	5.699098950
16	1.471874230	-2.588824430	1.178943750
6	-5.500168840	-1.624485170	1.268955640
1	-5.621776510	-0.643952060	0.780929690

1	-5.474147350	-1.460659400	2.358219820
6	-6.642823040	-2.583894490	0.921073030
1	-6.496509640	-3.536927250	1.458988800
1	-7.568933510	-2.135674340	1.333940490
6	-6.856775940	-2.876138600	-0.550417730
6	-6.808169250	-1.862738610	-1.520080850
1	-6.572492990	-0.833758990	-1.229890810
6	-7.036136530	-2.148937520	-2.867090100
1	-6.967880370	-1.344423800	-3.604421870
6	-7.326397080	-3.454064990	-3.272152800
1	-7.498439400	-3.677463060	-4.328378880
6	-7.382122020	-4.472084280	-2.317779910
1	-7.600549650	-5.499672030	-2.621514120
6	-7.145824850	-4.181463240	-0.971872280
1	-7.186001590	-4.984675810	-0.228791870
6	4.465175320	2.506042720	4.189081550
1	4.141313470	3.258174880	3.452760010
1	4.208227900	2.850481560	5.204461180
6	5.974653560	2.252862270	4.052011710
1	6.172716480	1.857750810	3.040230870
1	6.472763090	3.238305350	4.116053340
6	6.552175590	1.331548630	5.101762060
6	6.748423920	-0.032000570	4.841667190
1	6.489821000	-0.430349980	3.855935590
6	7.259734140	-0.882060450	5.824828720
1	7.402094360	-1.942987440	5.602340730
6	7.586000480	-0.380911650	7.086555740
1	7.988286320	-1.045323450	7.855755190
6	7.397553710	0.976635290	7.358263400
1	7.654927200	1.379998470	8.341403690
6	6.885278670	1.822253200	6.373271190
1	6.745445730	2.886150790	6.591188340
6	-1.764318950	-0.185748380	6.989414230
1	-1.647224680	0.467726430	7.870220080

1	-0.760849010	-0.493922410	6.660662360
6	-2.617171660	-1.412771610	7.376669560
1	-3.675575500	-1.103187280	7.430190910
1	-2.318965770	-1.716084010	8.397567520
6	-2.459934260	-2.603767160	6.460589980
6	-3.108968870	-2.666456220	5.218200530
1	-3.746466260	-1.834213370	4.907671780
6	-2.928230470	-3.761977100	4.371433630
1	-3.420247170	-3.772995490	3.393952470
6	-2.104540510	-4.822869460	4.756277100
1	-1.961727760	-5.681814050	4.095278600
6	-1.454144000	-4.773925900	5.991533750
1	-0.806546400	-5.599807150	6.298903130
6	-1.629688880	-3.672292780	6.831209610
1	-1.117951000	-3.639040260	7.799152890
6	0.378068710	-3.953818190	1.816896360
1	-0.666977180	-3.756207920	1.537515860
1	0.451883580	-3.912941050	2.914946000
6	0.880549180	-5.306056840	1.283523100
1	1.981133820	-5.330693330	1.367324710
1	0.631408700	-5.386963330	0.212013210
6	0.301708390	-6.474276920	2.052086900
6	-0.855614950	-7.134664520	1.617522770
1	-1.343167280	-6.824447450	0.688842830
6	-1.394850370	-8.192841270	2.353686290
1	-2.296320490	-8.692131970	1.989203460
6	-0.784254660	-8.608545530	3.538815580
1	-1.205643430	-9.436167010	4.115489690
6	0.373147440	-7.961059240	3.980621140
1	0.863417450	-8.282786350	4.903585230
6	0.908771540	-6.904786590	3.242502740
1	1.816492840	-6.402059170	3.591562500
79	-0.620477740	-2.149865740	-3.220859710
79	2.112619630	-2.113439620	-3.038212050

16	-2.951997050	-2.578772610	-3.489876910
16	4.445426300	-2.149180930	-2.458716400
6	-3.280802110	-4.353126970	-3.069036080
1	-4.364529390	-4.411261350	-2.873709860
1	-3.061596000	-4.931441960	-3.982435450
6	-2.485566930	-4.900471400	-1.879536850
1	-1.407460620	-4.790351160	-2.095428520
1	-2.710925330	-4.280601150	-0.994624080
6	-2.834604380	-6.346576690	-1.615373680
6	-3.907742540	-6.681856300	-0.774734600
1	-4.468203630	-5.878911160	-0.285987350
6	-4.255961150	-8.015747310	-0.553961570
1	-5.092718070	-8.256039550	0.107992070
6	-3.535793460	-9.041892800	-1.171969290
1	-3.805353980	-10.086859600	-0.997365760
6	-2.465550020	-8.722552480	-2.011167830
1	-1.891633030	-9.518250500	-2.493981530
6	-2.121918880	-7.387043360	-2.230835820
1	-1.278965130	-7.141489380	-2.885202340
6	4.634483430	-3.645644530	-1.368070640
1	5.576086410	-3.506991830	-0.811796650
1	3.802352750	-3.671261910	-0.648224570
6	4.681157020	-4.927401810	-2.212948130
1	3.728969620	-5.018188710	-2.764710770
1	5.485581970	-4.840556390	-2.963798940
6	4.905517250	-6.147485970	-1.348119290
6	6.201296200	-6.601360960	-1.062178420
1	7.059146460	-6.085597520	-1.505745980
6	6.407983990	-7.701412550	-0.227383120
1	7.425971900	-8.042637120	-0.020230870
6	5.317985040	-8.365567340	0.340371450
1	5.477969650	-9.225971510	0.995213000
6	4.021311490	-7.925336340	0.063093240
1	3.160126350	-8.436300440	0.501929650

6	3.820618080	-6.827522610	-0.775684770
1	2.803157140	-6.489034530	-0.993226880
79	-2.849899650	3.792555340	1.042810560
79	-0.411480590	4.667701180	1.640576550
16	-5.123183710	3.158128100	0.611126210
16	1.804051380	5.548760390	2.101441860
6	-5.776812580	2.469087870	2.213532780
1	-6.718071670	1.957236940	1.951783230
1	-5.070052480	1.724497090	2.608208600
6	-6.036186380	3.587280340	3.233909600
1	-5.065211890	4.010977590	3.545305140
1	-6.602479150	4.398562380	2.744502130
6	-6.805737050	3.077786480	4.432823310
6	-8.191661220	3.272478500	4.527745970
1	-8.708115400	3.827527870	3.737715770
6	-8.915350120	2.776078510	5.614089850
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6	-6.880926670	1.867726730	6.541467720
1	-6.355435260	1.317841080	7.327200000
6	-6.159511960	2.367018430	5.455790720
1	-5.078535530	2.195266920	5.408152870
6	2.039416000	5.575091720	3.947665040
1	3.037580910	5.161170560	4.157824260
1	2.064906350	6.651961830	4.187770230
6	0.963723850	4.866925510	4.776546720
1	-0.021580210	5.308600460	4.541551130
1	0.911536290	3.801979290	4.473378260
6	1.255249350	4.960797170	6.257368670
6	1.739111420	3.850685720	6.964615890
1	1.857427630	2.895891140	6.440608080
6	2.041295410	3.943325770	8.325107830
1	2.411033260	3.063137080	8.858403440

6	1.863357960	5.151432910	9.002600570
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6	1.373269560	6.263046260	8.311773570
1	1.218145530	7.209659670	8.836801880
6	1.071993820	6.166357310	6.952598150
1	0.677182910	7.038248160	6.420828870

[Au₂₅(SCH₂CH₂Ph)₁₈]: atomic coordinates and total energy (*E*, Hartree)

E = -488365.26951219

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79	2.416805770	3.619541280	2.396442380
79	-4.233158830	-0.619251700	-2.719349580
79	-2.055825310	1.556505160	-1.260843710
79	-2.085072720	0.860901620	1.714706430
79	-3.173636930	3.870282760	0.449327390
79	-0.902326030	4.459474540	-2.250054600
79	0.806471730	1.603585340	-2.207210680
79	0.967235660	0.859059830	2.529034710
79	-1.532334900	0.171981120	4.773257350
79	-3.999969840	-1.388540950	2.752485560
79	2.512833520	1.325721170	0.249564460
79	0.000461350	0.000569990	-0.000501680
16	0.348703760	4.588562410	1.887743620
16	4.579454860	2.923382230	2.969862570
16	-4.082756290	1.715998510	-2.607727990
16	-2.654854990	5.528577450	-1.118271500
16	0.908512910	3.662531960	-3.513713470
16	-3.822952930	2.454227080	2.197323560
16	0.699226820	0.851739280	4.917979450
16	-3.787828840	-0.438983070	4.885931950
16	-4.527894680	-2.347504280	0.686827560
6	0.750484870	6.131457370	0.923006790
1	1.622494850	5.940737400	0.281401330
1	-0.126082220	6.304276940	0.276613560
6	0.974079740	7.343357560	1.840692260
1	0.099278080	7.461145590	2.502557030
1	1.000055730	8.231176900	1.181330660
6	2.241780640	7.301660950	2.663422000
6	3.486576460	7.540265890	2.060316740
1	3.538040540	7.763833280	0.989504140

6	4.661139210	7.507559420	2.812612690
1	5.620525190	7.701654420	2.325678290
6	4.610381320	7.243565130	4.184621700
1	5.529850480	7.234317160	4.776192880
6	3.378002170	7.006249920	4.796992600
1	3.319404720	6.801044590	5.869452620
6	2.204462140	7.032841130	4.038416900
1	1.243311770	6.842328890	4.526511890
6	4.663762140	3.180148950	4.813346300
1	4.492253340	4.256827760	4.972278480
1	3.847861390	2.616994210	5.288052870
6	6.022150160	2.740267080	5.375823270
1	6.191827820	1.680649300	5.115454950
1	6.825580910	3.326336370	4.898341300
6	6.057007140	2.923705790	6.877069290
6	6.477775890	4.135185190	7.444364810
1	6.829043120	4.939570230	6.790252120
6	6.462277850	4.322752840	8.827997850
1	6.803448970	5.271044840	9.251797620
6	6.020904870	3.298657130	9.669660380
1	6.011333680	3.442543370	10.752916170
6	5.601610320	2.085511500	9.117772750
1	5.263545610	1.273148230	9.766419810
6	5.620044210	1.902007460	7.733651510
1	5.295508720	0.944695220	7.312834840
6	-3.505105810	2.128403480	-4.325388870
1	-2.614373210	1.520723490	-4.543406920
1	-3.212877140	3.192272330	-4.305832710
6	-4.617755320	1.876501860	-5.351054170
1	-5.528999250	2.419653490	-5.047874730
1	-4.864494520	0.798581540	-5.322699440
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6	-4.890509480	3.328562530	-7.410951290
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6	-2.785522760	2.038411300	-8.703462290
1	-1.957768430	1.528385410	-9.204173670
6	-3.160857580	1.648078920	-7.416611970
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6	-4.044157380	5.473195090	-2.354443740
1	-3.693111690	6.047446710	-3.226527680
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6	-5.342363290	6.057216520	-1.783658400
1	-5.177083300	7.098846550	-1.460324340
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6	-6.433964090	5.997452160	-2.829901150
6	-6.728629600	7.108834970	-3.631897790
1	-6.192563210	8.048269830	-3.463380900
6	-7.699658940	7.033389560	-4.633098290
1	-7.921510780	7.913239720	-5.242882040
6	-8.390549740	5.839089440	-4.850134330
1	-9.154578070	5.779306520	-5.629435720
6	-8.106089030	4.723895130	-4.057018890
1	-8.647926930	3.786985460	-4.213038140
6	-7.135874560	4.803382750	-3.056511020
1	-6.916917250	3.925721300	-2.439365450
6	0.210691890	3.300174360	-5.204108920
1	0.785887990	2.431955680	-5.572819480
1	-0.836541360	2.985899900	-5.098919860
6	0.347461410	4.487997030	-6.169611420
1	1.393183550	4.840203140	-6.175010270
1	0.137288240	4.092852510	-7.181033790
6	-0.588751530	5.641453130	-5.889307550
6	-0.147022350	6.792047770	-5.221456220
1	0.898749380	6.858967470	-4.905279390

6	-1.021576730	7.849392950	-4.960398310
1	-0.658148840	8.740370670	-4.441265710
6	-2.355561740	7.772399560	-5.366150520
1	-3.039247030	8.602654300	-5.170925230
6	-2.807078930	6.632338430	-6.037167440
1	-3.846580880	6.565729890	-6.369299140
6	-1.929714010	5.578277670	-6.297796320
1	-2.290826800	4.699082760	-6.840501490
6	-3.346004690	3.439513820	3.702965210
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1	-2.347850370	3.876723630	3.548471790
6	-4.403703770	4.520168880	3.969620350
1	-4.432931310	5.206173440	3.105205020
1	-5.395183120	4.039328980	4.034236930
6	-4.128910420	5.297961520	5.237358360
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6	-4.243379250	5.493282520	7.661869150
1	-4.534775210	5.072580870	8.627954250
6	-3.642836190	6.753766940	7.600460570
1	-3.465718400	7.322373280	8.516881790
6	-3.277546100	7.283183690	6.360693700
1	-2.812610550	8.271008370	6.301397880
6	-3.515408500	6.557647060	5.191092310
6	0.674095900	2.609371600	5.529819300
1	1.628320120	3.047746310	5.193044800
1	-0.136917980	3.158883640	5.030985100
6	0.547587140	2.662343230	7.059194660
1	-0.473819970	2.357837530	7.346975110
1	1.243687790	1.931612220	7.505666670
6	0.865719600	4.045285540	7.586244010
6	2.141798590	4.334628100	8.092079430
1	2.899528950	3.545884840	8.138849160
6	2.458036030	5.616098480	8.548213870

1	3.456974670	5.812988390	8.946424670
6	1.501284540	6.632799250	8.499152050
1	1.744854550	7.636281020	8.857543530
6	0.227196990	6.355766810	7.996599690
1	-0.533481190	7.139334540	7.959508030
6	-0.088567830	5.072831640	7.545278300
1	-1.095051290	4.869724660	7.165244680
6	-3.833687380	-1.905193760	6.034709640
1	-3.128492920	-2.664201200	5.666109770
1	-3.484808900	-1.540500310	7.014414890
6	-5.251499470	-2.484348590	6.132250010
1	-5.943155670	-1.707521270	6.499824120
1	-5.587550780	-2.766714400	5.118752040
6	-5.275044350	-3.686770150	7.049632280
6	-4.971606740	-4.965744820	6.558928120
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6	-5.231823560	-5.917124960	8.768885510
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6	-5.537420450	-4.649707440	9.269579230
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6	-5.557165160	-3.545129940	8.415661920
1	-5.803616740	-2.555186940	8.812732230
6	-4.019504030	-4.125677430	0.870248540
1	-4.172664890	-4.571032730	-0.128295780
1	-2.944684800	-4.156833780	1.104249360
6	-4.840044810	-4.860930990	1.936777690
1	-4.613519880	-4.404993990	2.917733520
1	-5.916426400	-4.707500240	1.748840830
6	-4.521560560	-6.340128680	1.951220200
6	-5.444969680	-7.282671950	1.477600810
1	-6.421799970	-6.941275550	1.120896690
6	-5.136220880	-8.645231270	1.460401000

1	-5.872493000	-9.365036460	1.092925460
6	-3.890169290	-9.087190700	1.910736290
1	-3.646164350	-10.152453170	1.895648150
6	-2.959755790	-8.157178840	2.383714260
1	-1.980431490	-8.491901940	2.737848580
6	-3.273941870	-6.797205880	2.406849680
1	-2.540079770	-6.074775980	2.782221180
1	-3.235252820	6.980014890	4.220813520
79	0.133003950	-2.823387810	-0.317225090
79	-2.416337430	-3.617116740	-2.398553050
79	4.235135850	0.621007220	2.717272550
79	2.056283100	-1.554398860	1.260960980
79	2.084697060	-0.860168800	-1.717204670
79	3.174420780	-3.867660900	-0.447914280
79	0.901999500	-4.457268920	2.251010530
79	-0.805046420	-1.602796170	2.205115660
79	-0.966035640	-0.855109660	-2.531218780
79	1.533841730	-0.170952480	-4.775222850
79	4.001525640	1.389569060	-2.754597500
79	-2.511819530	-1.324427640	-0.251685060
16	-0.347360110	-4.584812640	-1.890838200
16	-4.580079710	-2.921554400	-2.968824820
16	4.083806380	-1.714186400	2.605986370
16	2.654439870	-5.526168120	1.119009880
16	-0.908331330	-3.659504740	3.515002390
16	3.823774590	-2.452939930	-2.197328800
16	-0.697973200	-0.850013050	-4.920120890
16	3.789262430	0.440000920	-4.887731840
16	4.529058670	2.348223510	-0.688757570
6	-0.747652250	-6.129168140	-0.927763990
1	-1.620227610	-5.940171680	-0.286403530
1	0.128857110	-6.301536300	-0.281194460
6	-0.969370120	-7.340315330	-1.846852430
1	-0.094370960	-7.456118270	-2.508807090

1	-0.994227610	-8.229007030	-1.188621700
6	-2.237133520	-7.299178710	-2.669520370
6	-3.481706210	-7.539258540	-2.066474200
1	-3.532903160	-7.763397360	-0.995754360
6	-4.656303870	-7.507291820	-2.818734750
1	-5.615497800	-7.702601910	-2.331917060
6	-4.605789780	-7.242555140	-4.190622160
1	-5.525251120	-7.233942050	-4.782218550
6	-3.373675780	-7.003644930	-4.802888510
1	-3.315377140	-6.797649290	-5.875205660
6	-2.200094910	-7.029587860	-4.044349920
1	-1.239136380	-6.837949280	-4.532384180
6	-4.668431150	-3.180439290	-4.811872950
1	-4.495020570	-4.256851830	-4.970411640
1	-3.854903270	-2.615903820	-5.289084210
6	-6.029127380	-2.743821220	-5.371303800
1	-6.200054820	-1.684087570	-5.112290890
1	-6.830329320	-3.330539140	-4.890886770
6	-6.067497630	-2.929583480	-6.872208160
6	-6.488805360	-4.142188420	-7.436663290
1	-6.837817390	-4.945844950	-6.780457500
6	-6.476632220	-4.331781580	-8.820046420
1	-6.818258570	-5.280906280	-9.241608820
6	-6.037995080	-3.308654850	-9.664308500
1	-6.031186710	-3.454075980	-10.747382970
6	-5.617871590	-2.094501090	-9.115249070
1	-5.281709950	-1.283024960	-9.765987500
6	-5.633047830	-1.908964920	-7.731360060
1	-5.307828230	-0.950949090	-7.312651310
6	3.508603730	-2.127352670	4.324277210
1	2.620919730	-1.516462520	4.545852300
1	3.211745200	-3.189922630	4.303273910
6	4.624725190	-1.882405670	5.347847400
1	5.531864450	-2.431974500	5.043944280

1	4.878798060	-0.806283820	5.317965220
6	4.225293340	-2.290969050	6.748804550
6	4.893168650	-3.331519820	7.410432270
1	5.716387500	-3.844944750	6.903349530
6	4.522254860	-3.716356200	8.701366750
1	5.057043590	-4.528432620	9.200909030
6	3.470059450	-3.067903400	9.351352980
1	3.176662990	-3.369583500	10.359977040
6	2.795017390	-2.029852120	8.702428160
1	1.969918410	-1.515288270	9.202873780
6	3.170508180	-1.643963780	7.414278140
1	2.631569490	-0.831296020	6.914475550
6	4.043240480	-5.473069320	2.355823300
1	3.691532030	-6.048418000	3.226940350
1	4.197479940	-4.424172820	2.649018900
6	5.341555670	-6.056843730	1.784990540
1	5.176745520	-7.098932550	1.462904620
1	5.630944460	-5.475151090	0.891829990
6	6.433518740	-5.995294060	2.830751630
6	6.727873110	-7.105021040	3.635155810
1	6.191241380	-8.044546440	3.468945330
6	7.699227170	-7.027797020	4.635890010
1	7.920779090	-7.906343180	5.247656310
6	8.390972380	-5.833431520	4.849847930
1	9.155440940	-5.772326080	5.628624940
6	8.106814110	-4.719875400	4.054348810
1	8.649217160	-3.782906820	4.208007020
6	7.136097270	-4.801079370	3.054456190
1	6.917347270	-3.924662290	2.435472280
6	-0.209504700	-3.295502330	5.204535380
1	-0.784568880	-2.426977190	5.572781170
1	0.837659590	-2.981241100	5.098464660
6	-0.345433380	-4.482475090	6.171169920
1	-1.390821190	-4.835652150	6.176870290

1	-0.135730250	-4.086314760	7.182289570
6	0.592056380	-5.635070820	5.891660060
6	0.151919880	-6.786380250	5.223982990
1	-0.893590690	-6.854525370	4.907207300
6	1.027737630	-7.842907290	4.963848540
1	0.665532540	-8.734443850	4.444822710
6	2.361414050	-7.764388140	5.370390520
1	3.046077590	-8.594012470	5.175903310
6	2.811338680	-6.623575550	6.041187070
1	3.850586580	-6.555600420	6.373842540
6	1.932724640	-5.570326610	6.300851250
1	2.292672050	-4.690526540	6.843353000
6	3.344923360	-3.441112790	-3.700618520
1	3.293864280	-2.717460070	-4.531702220
1	2.346157910	-3.876155820	-3.543922960
6	4.400459280	-4.524305740	-3.965309930
1	4.431480670	-5.206004640	-3.097525140
1	5.392335750	-4.045141820	-4.035585480
6	4.120208950	-5.308044060	-5.228145190
6	4.480451210	-4.795709810	-6.484101600
1	4.972852130	-3.819527150	-6.543902050
6	4.234228580	-5.520323540	-7.651240830
1	4.529683280	-5.108476510	-8.619905890
6	3.623313460	-6.775361220	-7.581844100
1	3.442373200	-7.348706320	-8.494559130
6	3.252790070	-7.293461420	-6.338814400
1	2.779598300	-8.276963050	-6.273301110
6	3.496051800	-6.562221490	-5.173919760
1	3.211839530	-6.975809430	-4.201030330
6	-0.673752100	-2.607932930	-5.531021800
1	-1.630130140	-3.044253260	-5.197756130
1	0.134349590	-3.158564180	-5.028670700
6	-0.541650660	-2.662077070	-7.059941940
1	0.482124420	-2.362191620	-7.344098260

1	-1.232810660	-1.928236200	-7.509037130
6	-0.864049540	-4.043680440	-7.587853630
6	-2.139510630	-4.327561540	-8.098233860
1	-2.893688270	-3.535616870	-8.147890340
6	-2.459598130	-5.607626140	-8.555727760
1	-3.457955040	-5.800193720	-8.957433630
6	-1.507296770	-6.628338650	-8.503493600
1	-1.753778650	-7.630682080	-8.863078900
6	-0.233875860	-6.356815510	-7.996247560
1	0.523289360	-7.143654630	-7.956398960
6	0.085694040	-5.075302420	-7.543567780
1	1.091576360	-4.876613310	-7.159636050
6	3.835169850	1.906031340	-6.036764270
1	3.130537140	2.665471400	-5.667973080
1	3.485660600	1.541353880	-7.016240910
6	5.253254570	2.484365760	-6.135110840
1	5.944211960	1.707099430	-6.503082780
1	5.590059780	2.766498370	-5.121817500
6	5.276978560	3.686651850	-7.052661230
6	4.974751190	4.965921020	-6.561978160
1	4.762894360	5.098137440	-5.495870900
6	4.953666550	6.072558440	-7.412569190
1	4.723417970	7.062062470	-7.009272090
6	5.234078410	5.916717580	-8.772301340
1	5.221397480	6.782652550	-9.438797800
6	5.538436230	4.648998440	-9.272992670
1	5.766519550	4.519384980	-10.334206190
6	5.558067510	3.544558550	-8.418864950
1	5.803549940	2.554382310	-8.815947740
6	4.022030930	4.126737070	-0.872263980
1	4.175132610	4.572043470	0.126307130
1	2.947361490	4.158736200	-1.106806760
6	4.843989680	4.860957170	-1.938442600
1	4.618387630	4.404526540	-2.919403140

1	5.920079900	4.707055500	-1.749178010
6	4.526697180	6.340417820	-1.954505700
6	5.451608880	7.282783900	-1.483465150
1	6.428414780	6.940927210	-1.127150680
6	5.144414010	8.645723240	-1.468342060
1	5.881822870	9.365321030	-1.102747750
6	3.898462740	9.088313450	-1.918318260
1	3.655652610	10.153868970	-1.904820070
6	2.966592040	8.158518830	-2.388833630
1	1.987319260	8.493702070	-2.742678370
6	3.279173830	6.798132420	-2.409783830
1	2.544169480	6.075944960	-2.783381840

Au₂₅(SMe)₁₂ (symmetrical): atomic coordinates and total energy (*E*, Hartree)

E = -480867.05115868

79	0.208063280	0.091421020	-0.059503040
79	0.962464290	1.078758650	2.601173780
79	0.204453180	2.966515200	0.377033540
79	-1.904107670	1.172246320	1.630616960
79	2.825881430	1.386150950	0.038569150
79	2.364387290	-1.296069010	1.291256350
79	3.757743320	0.947269290	2.649111500
79	-1.445565390	0.198275270	4.189323210
79	2.621145420	3.284013150	2.075435490
79	-3.250845040	-1.052087020	2.699369610
79	-0.534581320	-1.587623070	2.213856900
79	-1.005516130	4.014995250	-1.919802180
79	-2.493777130	3.755148950	0.270710400
16	-0.241258990	-3.693217690	3.555352650
16	4.211471480	-1.372981920	3.024487150
16	4.829365940	2.375399380	-1.136385880
16	0.537655980	1.187002760	5.080898030
16	1.374410860	5.080092240	1.108490030
16	-3.313537990	3.142146120	2.437401620
79	-0.564932210	-0.827188330	-2.708353530
79	0.267907690	-2.789511830	-0.545872610
79	2.340759660	-0.989771770	-1.718638060
79	-2.388795480	-1.219417940	-0.135292560
79	-2.005474350	1.498804620	-1.326999750
79	-3.370930240	-0.732981680	-2.717394300
79	1.819300380	-0.078204690	-4.306873480
79	-2.199582800	-3.060436230	-2.207880810
79	3.640907470	1.192629710	-2.841085760
79	0.938180670	1.757801210	-2.351652240
79	1.376186160	-3.846600830	1.806227010
79	2.952864230	-3.535550770	-0.308781980

16	0.591175940	3.843897860	-3.684838770
16	-3.855887930	1.585756030	-3.063489160
16	-4.347414100	-2.357963460	1.016174390
16	-0.211589250	-0.966438830	-5.210581500
16	-0.729825940	-4.844466690	-1.601957240
16	4.213300180	-2.665835570	-2.147534080
6	6.241635350	1.286377170	-0.655486150
1	7.098596890	1.553236160	-1.291742940
1	6.482752380	1.484678250	0.399388940
1	5.993042300	0.226651460	-0.799428450
6	0.284034600	5.810389780	2.407078790
1	0.877359510	6.547154690	2.968279990
1	-0.553772820	6.311658630	1.900111700
1	-0.100929870	5.041961490	3.088767760
6	5.729634200	-1.858101650	2.092911570
1	5.804035950	-1.319349350	1.140179860
1	6.599670980	-1.626030840	2.724558460
1	5.679530750	-2.940870310	1.904978670
6	-5.065173320	2.577324130	2.299518560
1	-5.715264240	3.455283530	2.428404510
1	-5.256857840	2.114351380	1.323134380
1	-5.252547860	1.849408820	3.103247440
6	-5.378972690	2.034579580	-2.122573970
1	-5.318437840	3.102508140	-1.865103530
1	-6.244336340	1.855531890	-2.777693190
1	-5.474664630	1.432251540	-1.210251800
6	-5.842053650	-1.449272100	0.427747260
1	-5.698575460	-0.363297330	0.495500320
1	-6.030137560	-1.739582150	-0.616739690
1	-6.690253400	-1.751133970	1.059863120
6	0.111799840	2.950705540	5.427242390
1	1.025621890	3.552102380	5.312046670
1	-0.672908740	3.308156770	4.747336070
1	-0.245795980	3.008875110	6.466051870

6	3.706298600	-3.604848100	-3.654435410
1	3.811435020	-2.938964690	-4.524002990
1	4.383140330	-4.466092730	-3.756179890
1	2.670547000	-3.958245510	-3.569782240
6	0.023562420	-2.763868480	-5.559568210
1	0.475542860	-2.859106990	-6.557724790
1	0.669089750	-3.236309380	-4.808553250
1	-0.967792810	-3.240858470	-5.548951740
6	-1.549936800	-5.737953980	-0.207866970
1	-2.152453980	-5.053563280	0.403915960
1	-2.194713870	-6.514881150	-0.644149690
1	-0.764104550	-6.201069770	0.406868700
6	0.693374020	-3.159543320	5.057537180
1	0.001144840	-2.603092660	5.706493510
1	1.043821030	-4.067036700	5.570743660
1	1.550923000	-2.527559330	4.790988580
6	-0.358595460	3.282509610	-5.167226760
1	-0.740595020	4.180282640	-5.674932670
1	0.333943070	2.741966080	-5.829034370
1	-1.195664720	2.630710820	-4.884038090

Au₂₅(SCH₂CH₂Ph)₁₂ (symmetrical): atomic coordinates and total energy (*E*, Hartree)

E = -484109.42474252

79	-0.176012570	3.000423560	0.387295330
79	2.094918420	3.523006390	2.590354300
79	-3.415998660	-1.111765890	-2.907983200
79	-2.057708740	1.562032920	-1.492433840
79	-2.016863780	1.033843690	1.605226620
79	-2.839764940	3.763028220	0.065441260
79	-1.093462130	4.351570780	-1.867417150
79	0.654122530	1.966344610	-2.200024230
79	0.742008110	1.081578970	2.532632640
79	-1.603489690	0.002934630	4.233432810
79	-3.357215880	-1.185040300	2.654072870
79	2.483714150	1.876809720	0.335184390
79	0.192547060	0.088111810	-0.156385120
16	0.140980890	4.898421970	2.001540840
16	-4.095380150	1.165710580	-2.801482370
16	0.919270570	4.213128170	-3.309705300
16	-4.011374060	2.511411110	1.708895980
16	0.474364500	0.830750000	5.075929710
16	-4.468547360	-2.129527870	0.774599200
6	0.926819250	6.348251000	1.165827500
1	1.512394560	6.002126440	0.300529110
1	0.104849350	6.985505820	0.800506600
6	1.822453170	7.148662280	2.141071370
1	1.244540690	7.375149060	3.053987280
1	2.057965350	8.112398440	1.654732120
6	3.111155810	6.448351870	2.490739780
6	4.257877010	6.632688560	1.712663740
1	4.226369570	7.318766050	0.860250150
6	5.451932750	5.966411830	2.014322560
1	6.336614960	6.146485450	1.397831680
6	5.519313750	5.083737060	3.093030570

1	6.449403340	4.557977550	3.321073040
6	4.391306790	4.884691840	3.890887590
1	4.439785230	4.232128670	4.766400620
6	3.183609790	5.556244390	3.593874630
1	2.368758310	5.544611860	4.327193200
6	-3.607998530	1.863073020	-4.450404560
1	-2.553310300	1.615101520	-4.637928610
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6	-4.491229890	1.330015430	-5.586163910
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