

New Structural Insights into the Stability of $\text{Au}_{22}(\text{SR})_{16}$ Nanoclusters under Ring Model Guidance

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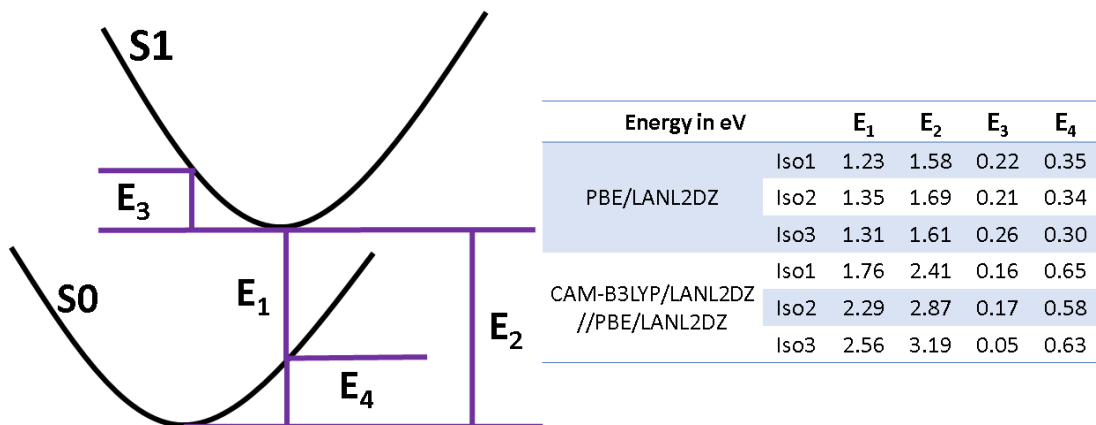


Figure S1 E_3 or E_4 corresponds to the reorganization energy, where $E_3 = E_{S1_using\ the\ geometry\ of\ S0\ minimum} - E_{S1_minimum}$, $E_4 = E_{S0_using\ the\ geometry\ of\ S1\ minimum} - E_{S0_minimum}$.

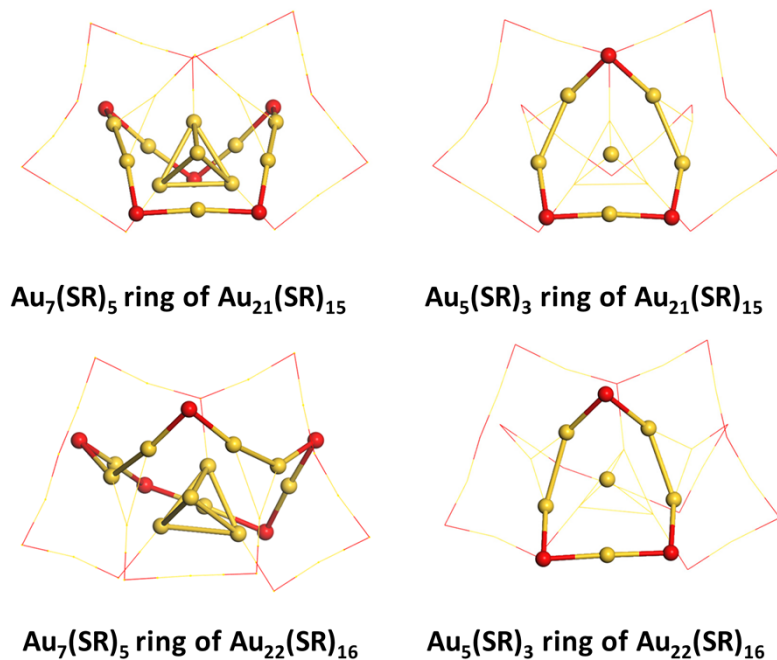


Figure S2. $[Au_7(SR)_5]$, and $[Au_5(SR)_3]$ ring in the $Au_{21}(SR)_{15}$ cluster; $Au_7(SR)_5$, $Au_5(SR)_3$ rings in the $Au_{22}(SR)_{16}$ cluster.

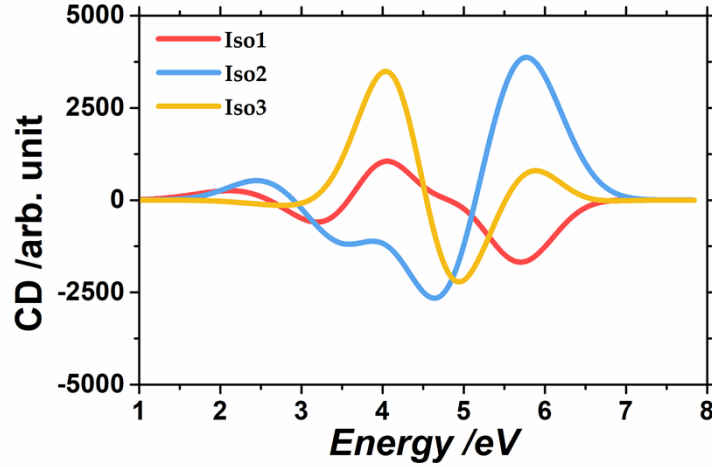


Figure S3 Circular dichroism spectra of the three clusters”

Table S1. The number of gold core atoms ($N_{\text{Au-core}}$), the elementary blocks (N_{eb}) that the gold-core atoms belong to, the number of gold atoms in the protection motifs (N_{Au}), and the number of S atoms in the protection motifs (N_{S}) in $[\text{Au}_m(\text{SR})_n]$ ($m = 5 - 8$, $0 \leq n \leq m$) rings. For every ring class, two equations to describe the relationship among $N_{\text{Au-core}}$, N_{eb} , N_{Au} , and N_{S} are also presented. The superscripts, 1a and 1b, in the table denote the corresponding ring structures shown in Figure 1a and Figure 1b, respectively¹.

Ring Class	Specific Rings	$N_{\text{Au-core}}$	N_{eb}	N_{Au}	N_{S}	Protection Motifs	Equations
$[\text{Au}_5(\text{SR})_n]$ ($1 \leq n < 5$)	$[\text{Au}_5(\text{SR})_4]^{2a}$	2	1	3	4	$\text{SR}[\text{Au}(\text{SR})]_3$	$N_{\text{Au}} = 5 - N_{\text{Au-core}}$ $N_{\text{S}} = 5 - N_{\text{eb}}$
	$[\text{Au}_5(\text{SR})_3]^{2b,2c}$	4	2	1	3	$\text{SR} + \text{SR}[\text{Au}(\text{SR})]$	
	$[\text{Au}_5(\text{SR})_2]^{2d}$	4	3	1	2	$\text{SR}[\text{Au}(\text{SR})]$	
	$[\text{Au}_5(\text{SR})]^{2e}$	5	4	0	1	SR	
$[\text{Au}_6(\text{SR})_n]$ ($0 \leq n \leq 6$)	$[\text{Au}_6(\text{SR})_6]^{3a}$	0	0	6	6	$[\text{Au}_6(\text{SR})_6]$ ring	$N_{\text{Au}} = 6 - N_{\text{Au-core}}$ $N_{\text{S}} = 6 - N_{\text{eb}}$
	$[\text{Au}_6(\text{SR})_5]^{3b}$	2	1	4	5	$\text{SR}[\text{Au}(\text{SR})]_4$	
	$[\text{Au}_6(\text{SR})_4]^{3c}$	3	2	3	4	$\text{SR}[\text{Au}(\text{SR})]_3$	
	$[\text{Au}_6(\text{SR})_4]^{3d}$	4	2	2	4	$2\text{SR}[\text{Au}(\text{SR})]$	
	$[\text{Au}_6(\text{SR})_3]^{3e}$	5	3	1	3	$\text{SR} + \text{SR}[\text{Au}(\text{SR})]$	
	$[\text{Au}_6(\text{SR})_3]^{3f}$	4	3	2	3	$\text{SR}[\text{Au}(\text{SR})]_2$	
	$[\text{Au}_6(\text{SR})_3]^{3g}$	6	3	0	3	3SR	
	$[\text{Au}_6(\text{SR})_2]^{3h}$	5	4	1	2	$\text{SR}[\text{Au}(\text{SR})]$	
	$[\text{Au}_6(\text{SR})_2]^{3i}$	6	4	0	2	2SR	
	$[\text{Au}_6(\text{SR})]^{3j}$	6	5	0	1	SR	
	$[\text{Au}_6]^{3k}$	6	6	0	0	-	
$[\text{Au}_7(\text{SR})_n]$ ($n = 4$ or 5)	$[\text{Au}_7(\text{SR})_5]^{4a}$	4	2	3	5	$\text{SR}[\text{Au}(\text{SR})] + \text{SR}[\text{Au}(\text{SR})]_2$	$N_{\text{Au}} = 7 - N_{\text{Au-core}}$ $N_{\text{S}} = 7 - N_{\text{eb}}$
	$[\text{Au}_7(\text{SR})_4]^{4b}$	5	3	2	4	$\text{SR} + \text{SR}[\text{Au}(\text{SR})]_2$	
	$[\text{Au}_7(\text{SR})_4]^{4c}$	5	3	2	4	$2\text{SR}[\text{Au}(\text{SR})]$	
$[\text{Au}_8(\text{SR})_n]$ ($n = 4, 6$, or 8)	$[\text{Au}_8(\text{SR})_8]^{5a}$	0	0	8	8	$[\text{Au}_8(\text{SR})_8]$ ring	$N_{\text{Au}} = 8 - N_{\text{Au-core}}$ $N_{\text{S}} = 8 - N_{\text{eb}}$
	$[\text{Au}_8(\mu_3\text{-S})_2(\text{SR})_4]^{5b}$	4	2	4	6	$\text{SR} + \text{SR}[\text{Au}(\mu_3\text{-S})\text{Au}(\text{SR})]_2$	
	$[\text{Au}_8(\text{SR})_4]^{5c}$	6	4	2	4	$2\text{SR}[\text{Au}(\text{SR})]$	

Coordinates of Iso1 via PBE functional:

Au	-1.33773757347076	2.50122901545726	-0.97567607445002
Au	2.94088695178049	0.16959489782186	0.68000775438402
Au	-0.16421433297062	-0.15042567086341	-0.58204071213368
Au	1.43528725003628	-2.08700446717718	0.88960285050758
Au	-1.60691274506764	-2.19792099774937	0.68896711345656
Au	2.37278495059905	-1.16882806914892	-1.60118690558259
Au	-2.37482167868727	-1.33681489138928	-1.92352910304420
Au	-3.03037416530189	0.12045959555909	0.24843660808008
Au	3.96105530359357	-3.03943637517399	2.12387015989110
Au	0.32993771315190	2.05283615660199	1.13391437482906
Au	1.46106179507797	2.04858773088184	-1.35653424127077
Au	5.22778754544232	-2.13364504462980	-0.98404562065292
Au	-3.06393225759114	3.40320750083553	1.52023290947643
Au	-1.77527384165809	-0.53319142454343	3.53968148143947
Au	1.85639408891995	-0.59558857996579	3.68003190175976
Au	4.40582660223274	1.02263069441286	-2.65939196402184
Au	-4.39208644780233	1.32753849726840	-2.42503023712098
Au	-0.01486825171427	-2.21357447233341	-4.00166517789523
Au	3.17318147528696	3.50931031651780	0.79253510840107
Au	-4.12248321780815	-2.92869923068987	2.01291879913933
Au	0.07222300081880	5.12800927395862	0.43501072352619
Au	-5.27687557538933	-2.06470465905967	-1.16863725583541
S	0.07816921096688	0.94875434991087	3.36106204990708
S	-0.09463083379510	-3.81788719410117	1.75015481772699
S	4.44524947023165	-4.12062634423922	0.06551281300292
S	-2.86469182826899	3.10494371336596	-2.74381546268481
S	2.75195541032840	2.57107483326132	-3.33697635390786
S	4.19558384255689	1.78260739587943	2.04785758269430
S	2.34267506722777	-2.09249369963782	-3.87636235493565
S	3.56722937000743	-2.11933083779218	4.27875319393309
S	6.28259674795409	-0.30610099626268	-2.05869402027033
S	-4.27436755689686	1.41406083906775	1.90411620841807
S	-2.09490546765370	5.55252079331177	1.30592514414577
S	-2.38350930069457	-2.27260674368631	-4.18143081074202
S	-3.57892277915194	-1.95711883020967	4.11087764313139
S	2.26968686199864	5.31093692512169	-0.46304747802429
S	-6.17130575550298	-0.24729592822208	-2.39498850030327
C	0.02814092073992	2.04604919354423	4.84159933582219
C	-2.81013252131697	-4.04493357622815	-3.87040430708125
C	5.91179735891114	1.68424640082265	1.36904100763041
C	-3.79531617868318	4.58385439897393	-2.14383452990248
C	6.00381251080631	-5.05849825351271	0.40990534284443
C	-1.76035276827646	6.04130930439812	3.05740341562910
C	1.79357530745514	1.72585771789501	-4.67177332054208
C	2.84513322561216	-3.84934156369205	-3.60028616918607

C	6.78053373213833	-1.01271223818045	-3.69325120641727
C	2.91968450010565	6.81875307194590	0.39347119313515
C	-6.38715654339507	-4.78301694608389	0.39098856208260
S	-4.72727186338972	-4.05506994000753	0.01208651723394
C	-5.92258376863377	1.73665900074495	1.13109709149304
C	2.60882187384035	-3.47404748607088	5.09679972447357
C	-6.14279689994864	-0.87015358872093	-4.13537286448765
C	0.07008733006083	-5.13832695155299	0.46822742862077
C	-2.70682794329443	-3.35735475965014	4.94892140922849
H	-0.86380525273844	2.68597551370263	4.75754953478227
H	0.94359228115223	2.65678354901727	4.84166544513061
H	-0.02493320656349	1.43239604284401	5.75241532546490
H	-2.57559140716246	-4.62632042606019	-4.77596002079214
H	-3.89040885367946	-4.09740907288002	-3.66091684046769
H	-2.25721077469481	-4.44551210038146	-3.01002962554200
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H	5.91137677417867	1.72913757588902	0.27017888040634
H	6.34688683604212	0.72778835411929	1.69923209395742
H	-3.10259784271220	5.44050022905638	-2.15634645725029
H	-4.17081244896418	4.43380357525202	-1.12110815408984
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H	3.92127029693614	-3.85376059805588	-3.36457505218639
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H	5.92133096259283	-1.46799824189652	-4.20558638464929
H	2.38805689090550	7.69468166981093	-0.00968399079571
H	3.99352679786610	6.90050048161882	0.16212037226758
H	2.77543687020135	6.75826968952720	1.48115282292354
H	-7.05961576070340	-4.03455354068225	0.83195582644144
H	-6.24069334709630	-5.61821047166191	1.09383250084082
H	-6.81489200349000	-5.16241279642849	-0.55012969118410
H	-5.81403456519361	2.10230133028802	0.09927841177052
H	-6.46171694200957	2.47436358372946	1.74548340034788
H	-6.47414900379422	0.78285687368991	1.12332864622488
H	2.21609284801100	-3.08756108961125	6.04970040558700

H	3.30212500119484	-4.30684106678173	5.29154189013992
H	1.78305078540963	-3.81328684517077	4.45426225753176
H	-5.13660754086903	-1.21739228981103	-4.41273346469015
H	-6.44938669166927	-0.04326363986585	-4.79478241998965
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H	0.07144200114556	-4.70308516833921	-0.54169852638831
H	-0.77802700047140	-5.83424867210098	0.57170964109179
H	1.01737198307473	-5.67490686098747	0.63962480773859
H	-2.27132656351150	-2.97622262560264	5.88535867807793
H	-1.91891166553289	-3.77114934625036	4.30259471435853
H	-3.45561685429336	-4.13180347952985	5.17654814297731

Coordinates of Iso2 via PBE functional:

Au	-1.76265072256505	-0.64254187513040	1.20887731755385
Au	-3.62846819757572	3.13488645288346	-2.05286454728043
Au	4.83700498952929	0.99058014789621	-1.96698632178565
Au	-1.29075170355799	-2.36138346408867	-1.25591392650116
S	3.79039919568390	-0.38454513323013	-3.57659693855262
S	6.18989357413406	2.35821613829335	-0.59245331117525
Au	-4.25360732230022	-0.47944187297948	-2.17879977960228
Au	-1.46130007544196	0.72704046404189	-1.27351100647987
Au	-0.27902920857293	4.19743560012753	-1.08001419452593
Au	0.59488117008989	-3.51886132170122	0.48974109716515
Au	1.25140384095207	-2.97235899237094	-2.17659026932447
Au	0.91049122858766	-0.84721866236354	-0.41125982101457
Au	4.99634261331535	2.20656263421922	1.44801506182596
S	0.91327882500827	-0.64402579041836	4.47229624122420
Au	2.02713709470053	1.72459354889078	0.02036784536297
Au	1.44542663296789	0.11572872165483	2.19527655038214
Au	3.59624924521301	-0.52910713532031	0.44348293817679
Au	-3.55233804781806	1.40623268453972	0.45476327885393
Au	-0.85012116270787	2.01725500515527	1.10888497929754
Au	1.49110884663761	0.15950202816292	-3.32882090699653
S	-0.28334007764912	3.74010552238657	2.74693583769861
Au	1.92532954924919	2.97269371417058	3.10970466621980
S	4.14104939178692	2.31346202874010	3.65544813780179
S	5.40182774622580	-2.13445206801599	0.21283830630641
Au	4.22650249669787	-3.29957826804805	-1.49328464312840
Au	1.05806443468388	-2.80858588765684	3.52045165123126
S	1.18702358960196	-4.88794309626890	2.37895446328561
S	2.91990602545165	-4.48561541389624	-3.11276147074249
S	2.03496297789849	3.76493556089925	-1.32031407446888
S	-2.53805221701230	4.91775623567415	-0.92887097666967
S	-4.86115561205553	1.53187722253570	-3.29471984476651
S	-3.69019758593398	-2.68602825312026	-1.49462271397172
S	-0.72996784290032	0.92607261824961	-3.60716598687536

S	-2.39216917331167	-2.40003154730440	2.78682378174390
S	-5.81979276325728	2.10921077818889	0.97501471046882
Au	-4.54952707262094	-2.58136830999527	1.83839785357783
Au	-6.34977330845034	-0.19913807418397	0.86407312809543
S	-6.70675081545482	-2.55502445026369	0.81433169212835
C	-2.59755760783983	6.28397841231937	-2.17678282645452
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H	-2.19311247162303	5.95861802758474	-3.14461271048700
C	-3.87185067448698	-3.65985637161500	-3.05649417869179
H	-3.44550476232496	-4.65933241285253	-2.87923955510362
H	-4.94571536432142	-3.75028585178094	-3.28210549757988
H	-3.35312122654658	-3.17789477480908	-3.89693186702812
C	4.18913371664317	0.49908185792180	-5.15651880646410
H	5.27622256454883	0.42861070034154	-5.31943726635540
H	3.65712258015786	-0.00959629255394	-5.97578068081642
H	3.88338103443512	1.55340758087402	-5.11099641211195
C	3.47098505543659	-3.88292455662033	-4.76593764900254
H	4.41656323323138	-4.38781186402376	-5.01832508448174
H	2.69885048033503	-4.15909179685858	-5.50138950304799
H	3.61808732553891	-2.79382096327844	-4.75589482536181
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H	5.55885600142499	-2.67204383771907	2.57236432635709
H	4.13616949248180	-3.49579154504586	1.83840663687990
H	5.79644017162024	-4.13039449382097	1.54417941528090
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H	-0.53809988131291	-6.56713568093528	2.09108663290788
H	-0.22378068329798	-6.22314754318664	3.83009522146951
H	-1.22453487340385	-5.08283490619164	2.85470358059476
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H	-8.90744492761171	-2.56005504046699	1.84416801272101
H	-7.89326173085592	-3.92726428338148	2.42534816298164
H	-7.63799833043696	-2.27407675196725	3.08805904016680
C	4.91358300943119	3.86454035656215	4.30695539777270
H	4.44588497132622	4.09481901138195	5.27662107499623
H	5.98897935767215	3.67602832590787	4.44976338220998
H	4.76907108462851	4.70459691302648	3.61389779642526
C	-6.62164003829769	1.84072897418728	-2.83108978919925
H	-6.92193205558086	2.80227046510553	-3.27586589731177
H	-7.23112295535116	1.02842837667490	-3.25639027123371
H	-6.75132650274533	1.87546108882431	-1.74059165124561
C	-1.15542786362164	3.12924354168363	4.25855878796141
H	-0.82946320771688	3.73569804957456	5.11818666467893
H	-2.23678901594219	3.26489962561962	4.09769142513438
H	-0.93503697025271	2.06742878478425	4.43983985323244
C	2.81114135240618	5.04480508198871	-0.23501774584430

H	3.87712114799805	4.78718640453306	-0.12479435043421
H	2.71315614704309	6.02377229249370	-0.73044513534243
H	2.33324855394200	5.07207532809277	0.75512501116215
C	7.65220241654716	1.26866495379310	-0.28186138204292
H	8.22240453139506	1.19538033188627	-1.22118508427289
H	8.27273208949106	1.74426383474562	0.49361213591896
H	7.33515668545651	0.26742884038487	0.04300168086612
C	2.45966386911175	-0.44298260340145	5.45836896637880
H	2.54899200949705	0.61909589172251	5.73277604832631
H	2.37174246529603	-1.06060305449293	6.36493357897068
H	3.34311686041900	-0.74410011763427	4.87937210694029
C	-2.75706682710983	-1.45105184099226	4.33305702026961
H	-3.30678653191066	-2.11304550653425	5.02041486842583
H	-1.79647135362196	-1.15912806829558	4.78431756254792
H	-3.35825150110106	-0.55792265069779	4.11078106052245
C	-5.76933464622466	2.45948556744494	2.78891736274065
H	-5.25392148098616	3.42284935988400	2.92735754771934
H	-6.80372491355354	2.53803505538188	3.15760453892340
H	-5.23653489776237	1.66777865127873	3.33287757671362
C	-1.49874074491344	-0.46081950189244	-4.55235255787558
H	-2.57767282664508	-0.25448871839858	-4.64152186686449
H	-1.03897407128164	-0.48863229543678	-5.55266825526242
H	-1.34326377230500	-1.42056204514368	-4.03547035709541

Coordinates of Iso3 via PBE functional:

Au	1.85491533647547	2.32049023817016	-0.28176701767565
Au	0.31819574675724	0.48274037268815	-2.82840641849953
Au	1.32125212278931	5.33251111099682	0.42335407177811
Au	3.83810593512207	0.42697496996134	-1.60422029743095
Au	-0.81427398606080	-0.21305823566985	0.40952823580471
Au	4.37952287671524	4.02084734277474	-1.15358756171712
Au	-1.17619939253710	2.51127082355304	0.65081996083407
Au	1.76321909187814	-0.90822541835219	-0.35632419005717
Au	3.43244741614022	-2.27194344548195	-2.14115608505001
Au	-2.08856111912123	-1.97468683400429	-2.29803856372181
Au	0.74675515328258	1.57522651655180	2.96391433908219
Au	-1.86259588220717	-0.61823731751723	3.69224703326693
Au	-3.22030538002419	-2.50014995785598	1.02582238147371
Au	4.43261272847133	-1.47798986968727	0.34977399008442
Au	1.48674265115777	-4.80595116391087	-2.09168870588540
Au	-0.22968861097906	-2.89431480477564	0.02011074827266
Au	0.78344868496185	-1.49384506624336	2.26172005479734
Au	3.77528861412429	-2.11309106221245	3.40748652889513
S	-2.62038306080924	-2.83812028314605	3.30240958501292
S	-0.17320497757070	-1.68408928298020	-3.67806205053233
S	-1.17864162999351	1.55852700132239	4.36264273601432

S	-0.43232930814755	-5.20488041978281	-0.75178485824881
S	1.66678424236312	-2.05657457975823	4.47828728045749
S	-4.12543910906516	-2.44314132208528	-1.17140146747524
S	3.42793118354742	-4.34123335968575	-3.39274583060572
S	5.82798941317540	-2.09782691383805	2.20951972440670
S	3.60176108600526	5.91383037180012	0.05271904782808
S	5.23773989464047	2.23688160236652	-2.45777912580162
S	0.69391333664289	2.77934038547027	-2.34751250497974
S	2.83352920880172	1.71779013490444	1.83628322633379
S	-0.94866267585593	4.91568240034337	0.97079047511747
Au	-2.44760922834108	1.04762002877125	-1.43871039906642
Au	-3.29522507977167	0.70362435461395	1.23281706446225
S	-3.44415819677910	1.46025273266263	-3.62582241641033
S	-5.35536260690301	0.69326007416429	2.53128392954340
Au	-5.58134733811938	1.19979107925208	-2.65692697139386
Au	-6.56000736889512	0.81021113760982	0.50394352851882
S	-7.67861672704052	0.90476007001037	-1.58814199679489
C	-4.34092106184161	-4.24741513971268	-1.53004656043245
H	-5.16936787782830	-4.62151715069514	-0.90807842091026
H	-4.59989099188510	-4.35259969049491	-2.59531261452171
H	-3.42000537622992	-4.80687081291135	-1.31055655027851
C	-4.27000689017880	-2.85046099308780	4.14030642759968
H	-4.79822613590824	-3.77034111530272	3.84294647162592
H	-4.09667145920298	-2.85832023255709	5.22808260018757
H	-4.86122945195652	-1.96635900193944	3.86072785691043
C	-0.42637785555999	1.23357427236616	6.02283911691514
H	0.10497968888701	2.14444398037047	6.34109101148180
H	-1.24339911138589	1.01686707725830	6.72867045295334
H	0.27016871507453	0.38372954636235	5.98023896381890
C	6.60158324720931	-0.49370755845035	2.71227257022599
H	7.01420830045234	-0.61336813799256	3.72602578572039
H	7.41723727834182	-0.27514676727245	2.00556579288997
H	5.86390567638158	0.32096586162939	2.69950388541814
C	1.19092780694228	-3.83019653246704	4.68988019925663
H	1.71981799527775	-4.23039606801083	5.56865850278141
H	0.10279055777452	-3.86461538303085	4.85648352779347
H	1.44604161804653	-4.41974210206288	3.79827739339184
C	2.76003179047759	-3.90518553166629	-5.05998249050109
H	3.56618126457824	-3.41594933737074	-5.62921373744546
H	2.46408398197506	-4.83763952034537	-5.56528813136171
H	1.89519101291037	-3.23262663509568	-4.97128603366591
C	-0.94532914981604	-1.25988311993130	-5.30767831225519
H	-0.14769958523959	-0.91369009117163	-5.98410481917519
H	-1.40375560338259	-2.17570861746202	-5.71325828602499
H	-1.70890269222653	-0.47655960842792	-5.19132486583968
C	-8.06621894132456	-0.87218817232690	-1.93078518106122

H	-8.89915539832529	-1.16959757260571	-1.27532913082785
H	-8.37713709855424	-0.95284651843611	-2.98381582545819
H	-7.19031214052014	-1.50924020724250	-1.74501450544286
C	-1.83957900281363	5.54201655092393	-0.52304132599918
H	-2.90634233454731	5.29459544187248	-0.40049932096832
H	-1.71631385970633	6.63559017683630	-0.57397092087417
H	-1.45183165304291	5.07148039328909	-1.43852926521430
C	3.54697695135371	3.26962458446299	2.53865289106858
H	3.86364516096910	3.05352275520794	3.57107708266289
H	4.42208391948014	3.55148426636538	1.93051923594847
H	2.81344370192860	4.08982710443358	2.53495200200559
C	1.93058989681139	3.27857799399370	-3.62275759346333
H	1.38371974396986	3.45056984721527	-4.56364444176532
H	2.41123115943339	4.21400258300753	-3.29380247470579
H	2.69319341834100	2.50206179857387	-3.77515382653129
C	6.86914059545592	1.83485528124290	-1.68839944849699
H	7.25121244301028	0.92503713348938	-2.17639180319246
H	7.55725446288439	2.67476485650927	-1.87375497839697
H	6.76794354747869	1.65909240943767	-0.60844082639334
C	0.20593546402809	-6.19262038295290	0.67437624472325
H	-0.56708722891146	-6.18669976388831	1.45918424794585
H	0.38184000711140	-7.22478873527614	0.33399116464346
H	1.13848166844960	-5.76468928547946	1.06750824601877
C	3.52245629640601	7.24741707703030	-1.22410480611422
H	3.06794743736154	8.13426712083782	-0.75595897061801
H	4.55181836149645	7.47983182570385	-1.53631288757553
H	2.92778217060655	6.93993153986295	-2.09505094048839
C	-5.41659610705279	2.40706063836633	3.22171984187828
H	-6.41530336097958	2.57144343049412	3.65530977582341
H	-4.64973324756249	2.47507201922763	4.00929753708453
H	-5.21436755087929	3.15611672364347	2.44441710439271
C	-3.24492701733333	3.28343400214549	-3.84790951142275
H	-2.16947245745236	3.48671109212323	-3.97260201827994
H	-3.79140107841441	3.58641419514903	-4.75468480453172
H	-3.62772666567307	3.83461279523487	-2.97788778356999

Coordinates of Iso1 via PW91 functional:

Au	-1.33810442282220	2.50772013844373	-0.97162642682504
Au	2.94324249078888	0.17100405216384	0.68437934530200
Au	-0.16314326071882	-0.14532170205283	-0.58081474077678
Au	1.43608303949073	-2.08305582072979	0.89159393996922
Au	-1.60603934925741	-2.19077699703069	0.69431457070459
Au	2.37492751062705	-1.16258128732080	-1.59834210367086
Au	-2.37482088033722	-1.33024981003621	-1.92066025276725
Au	-3.03045091462765	0.12432042754031	0.25155260631494
Au	3.95331196797306	-3.04640137610846	2.12093395919121
Au	0.33136146730956	2.06231078523225	1.13383181912969
Au	1.46151880277848	2.05338644910293	-1.35489178046701
Au	5.21461240532216	-2.13851921726487	-0.98145323819656
Au	-3.06013079219165	3.40757805067470	1.51491257319888
Au	-1.77778869816439	-0.52969761760265	3.52602584231629
Au	1.85506131213398	-0.59494290064227	3.67172944051273
Au	4.39995287632000	1.01939193254952	-2.65346754596600
Au	-4.38885314288905	1.32169960138079	-2.41479161498593
Au	-0.01341797052619	-2.20441956561745	-3.99922136268615
Au	3.17377283444081	3.50954392830532	0.79058341979138
Au	-4.11410410933403	-2.93676157660532	2.00767852446944
Au	0.07503452127141	5.12655244925486	0.42621763713128
Au	-5.26257617045229	-2.07416657718652	-1.16703855163814
S	0.07770173972663	0.95156545582903	3.35639607698774
S	-0.09431193562335	-3.81530014434010	1.75155540367756
S	4.43056465551962	-4.12860353718181	0.06165799453890
S	-2.86801043114812	3.10461871125637	-2.73926289984188
S	2.75040341451891	2.57007286243273	-3.33819173207430
S	4.19399471528773	1.78607132656114	2.05322767532612
S	2.34428908755147	-2.08414963553796	-3.87524815289748
S	3.56298864782756	-2.12062249517407	4.27391026448332
S	6.27532489336022	-0.31024670631107	-2.04948722086370
S	-4.27401304205019	1.42122421025463	1.90491298049234
S	-2.08962094587415	5.55649596772537	1.30053605803022
S	-2.38195467744240	-2.26379175037756	-4.17966872824532
S	-3.58080666502414	-1.95338417016914	4.10235599113038
S	2.27311286611268	5.30837836202657	-0.47172942996988
S	-6.16755289241554	-0.25487652032459	-2.38292503228470
C	0.02740248418640	2.04227140120526	4.84259407612308
C	-2.80719621476201	-4.03698939154727	-3.86707049092757
C	5.91141304783180	1.68567200735709	1.37555116594508
C	-3.80510622279897	4.57905616428821	-2.13605406830263
C	5.99084417301338	-5.06614554796732	0.40300646190137
C	-1.74809551858357	6.03936120148918	3.05314041816114
C	1.78721619582023	1.71867750037762	-4.66683070398891

C	2.84409735690064	-3.84247107559072	-3.59837222046129
C	6.77323983582400	-1.01690542453815	-3.68488602411271
C	2.92083171014173	6.81719033561804	0.38657346716443
C	-6.36302799300069	-4.80316286740656	0.37841715149875
S	-4.70432402671269	-4.06770895826518	0.00515987586306
C	-5.92035736451837	1.74403422582460	1.12590984448430
C	2.59966023902374	-3.47135623160294	5.09427697435602
C	-6.14109286782421	-0.87249442876315	-4.12598671623201
C	0.06629361526071	-5.13214453863983	0.46434937050901
C	-2.70309855585123	-3.34698118672411	4.94754707896465
H	-0.86422944001681	2.68023693792403	4.76238111626188
H	0.94103494874860	2.65286711998439	4.84398759406363
H	-0.02361372158673	1.42439722681682	5.74874457954841
H	-2.57280640600132	-4.61732522259264	-4.77132744884153
H	-3.88570453604844	-4.08951435800569	-3.65697531602202
H	-2.25355778040113	-4.43527726850177	-3.00807684146959
H	6.49657749602911	2.52177419265219	1.78473626930209
H	5.91051838777897	1.72744151612448	0.27816974885522
H	6.34498323476796	0.73137648919187	1.70865725969278
H	-3.11758971773663	5.43779970780411	-2.15044115351997
H	-4.17597392390321	4.42621568846332	-1.11365292998958
H	-4.64425565109911	4.76243923692750	-2.82222747107087
H	5.74434611272002	-5.91050842678378	1.06289502317293
H	6.74153562887738	-4.42456459529209	0.88040513004774
H	6.37559944466453	-5.44559756780367	-0.55448151116894
H	-2.71215395379947	6.13842886371589	3.57201329822528
H	-1.23015592573709	7.00912315589615	3.04086043733351
H	-1.12491367236590	5.29107128958800	3.55843717130436
H	2.41772951407033	1.64669197074891	-5.56438590660112
H	0.90457576282667	2.34005252518674	-4.87709572711124
H	1.46454304008956	0.71822429839641	-4.35390364844862
H	3.91864336827872	-3.84789224594408	-3.36269197595433
H	2.65794685998822	-4.40718106322228	-4.52360475001414
H	2.29186534507942	-4.28840503782859	-2.76218914432462
H	7.55251900826203	-1.77213857611337	-3.50814006534136
H	7.18009161566176	-0.19657353812684	-4.29410085971372
H	5.91433829579554	-1.46987837597211	-4.19637135560445
H	2.39019786575696	7.69120503090265	-0.01764237532194
H	3.99367554065514	6.89868376192582	0.15821347914425
H	2.77349662422354	6.75570987915910	1.47216304851384
H	-7.03882634387498	-4.05748110275249	0.81501209571487
H	-6.21533683383872	-5.63529186271472	1.08205502119271
H	-6.78420759096210	-5.18466189536270	-0.56291490405933
H	-5.80751131930840	2.10333649566926	0.09388049645103
H	-6.45764997998743	2.48553222009816	1.73438663873068
H	-6.47311040396505	0.79279948276838	1.12199747331221

H	2.20946742689053	-3.08212276459539	6.04529506739420
H	3.28947420939726	-4.30492517714756	5.28910653480254
H	1.77382750291983	-3.80754096498374	4.45294010315328
H	-5.13567886318371	-1.21549874137314	-4.40513867070915
H	-6.45047623773610	-0.04518926433669	-4.78084458900028
H	-6.86205621208874	-1.69898435520803	-4.20491238803953
H	0.06985075726698	-4.69308994257985	-0.54214392394588
H	-0.78359861672115	-5.82374580635955	0.56485872122883
H	1.01005932562264	-5.67185643359957	0.63454508724559
H	-2.26825765313579	-2.95916928880383	5.87968912831824
H	-1.91613565590137	-3.76067042361987	4.30277128003717
H	-3.44849971838533	-4.12107527855479	5.17967218373790

Coordinates of Iso2 via PW91functional:

Au	-1.76265072256505	-0.64254187513040	1.20887731755385
Au	-3.62846819757572	3.13488645288346	-2.05286454728043
Au	4.83700498952929	0.99058014789621	-1.96698632178565
Au	-1.29075170355799	-2.36138346408867	-1.25591392650116
S	3.79039919568390	-0.38454513323013	-3.57659693855262
S	6.18989357413406	2.35821613829335	-0.59245331117525
Au	-4.25360732230022	-0.47944187297948	-2.17879977960228
Au	-1.46130007544196	0.72704046404189	-1.27351100647987
Au	-0.27902920857293	4.19743560012753	-1.08001419452593
Au	0.59488117008989	-3.51886132170122	0.48974109716515
Au	1.25140384095207	-2.97235899237094	-2.17659026932447
Au	0.91049122858766	-0.84721866236354	-0.41125982101457
Au	4.99634261331535	2.20656263421922	1.44801506182596
S	0.91327882500827	-0.64402579041836	4.47229624122420
Au	2.02713709470053	1.72459354889078	0.02036784536297
Au	1.44542663296789	0.11572872165483	2.19527655038214
Au	3.59624924521301	-0.52910713532031	0.44348293817679
Au	-3.55233804781806	1.40623268453972	0.45476327885393
Au	-0.85012116270787	2.01725500515527	1.10888497929754
Au	1.49110884663761	0.15950202816292	-3.32882090699653
S	-0.28334007764912	3.74010552238657	2.74693583769861
Au	1.92532954924919	2.97269371417058	3.10970466621980
S	4.14104939178692	2.31346202874010	3.65544813780179
S	5.40182774622580	-2.13445206801599	0.21283830630641
Au	4.22650249669787	-3.29957826804805	-1.49328464312840
Au	1.05806443468388	-2.80858588765684	3.52045165123126
S	1.18702358960196	-4.88794309626890	2.37895446328561
S	2.91990602545165	-4.48561541389624	-3.11276147074249
S	2.03496297789849	3.76493556089925	-1.32031407446888
S	-2.53805221701230	4.91775623567415	-0.92887097666967

S	-4.86115561205553	1.53187722253570	-3.29471984476651
S	-3.69019758593398	-2.68602825312026	-1.49462271397172
S	-0.72996784290032	0.92607261824961	-3.60716598687536
S	-2.39216917331167	-2.40003154730440	2.78682378174390
S	-5.81979276325728	2.10921077818889	0.97501471046882
Au	-4.54952707262094	-2.58136830999527	1.83839785357783
Au	-6.34977330845034	-0.19913807418397	0.86407312809543
S	-6.70675081545482	-2.55502445026369	0.81433169212835
C	-2.59755760783983	6.28397841231937	-2.17678282645452
H	-3.64760270524749	6.59407010008782	-2.29299285402808
H	-2.00541533936970	7.12652489504784	-1.78614541127937
H	-2.19311247162303	5.95861802758474	-3.14461271048700
C	-3.87185067448698	-3.65985637161500	-3.05649417869179
H	-3.44550476232496	-4.65933241285253	-2.87923955510362
H	-4.94571536432142	-3.75028585178094	-3.28210549757988
H	-3.35312122654658	-3.17789477480908	-3.89693186702812
C	4.18913371664317	0.49908185792180	-5.15651880646410
H	5.27622256454883	0.42861070034154	-5.31943726635540
H	3.65712258015786	-0.00959629255394	-5.97578068081642
H	3.88338103443512	1.55340758087402	-5.11099641211195
C	3.47098505543659	-3.88292455662033	-4.76593764900254
H	4.41656323323138	-4.38781186402376	-5.01832508448174
H	2.69885048033503	-4.15909179685858	-5.50138950304799
H	3.61808732553891	-2.79382096327844	-4.75589482536181
C	5.19079918901740	-3.22358959843768	1.69289964240561
H	5.55885600142499	-2.67204383771907	2.57236432635709
H	4.13616949248180	-3.49579154504586	1.83840663687990
H	5.79644017162024	-4.13039449382097	1.54417941528090
C	-0.37012408659703	-5.77378442361276	2.83530026577618
H	-0.53809988131291	-6.56713568093528	2.09108663290788
H	-0.22378068329798	-6.22314754318664	3.83009522146951
H	-1.22453487340385	-5.08283490619164	2.85470358059476
C	-7.90425611356121	-2.85122777941498	2.19251228140202
H	-8.90744492761171	-2.56005504046699	1.84416801272101
H	-7.89326173085592	-3.92726428338148	2.42534816298164
H	-7.63799833043696	-2.27407675196725	3.08805904016680
C	4.91358300943119	3.86454035656215	4.30695539777270
H	4.44588497132622	4.09481901138195	5.27662107499623
H	5.98897935767215	3.67602832590787	4.44976338220998
H	4.76907108462851	4.70459691302648	3.61389779642526
C	-6.62164003829769	1.84072897418728	-2.83108978919925
H	-6.92193205558086	2.80227046510553	-3.27586589731177
H	-7.23112295535116	1.02842837667490	-3.25639027123371
H	-6.75132650274533	1.87546108882431	-1.74059165124561
C	-1.15542786362164	3.12924354168363	4.25855878796141
H	-0.82946320771688	3.73569804957456	5.11818666467893

H	-2.23678901594219	3.26489962561962	4.09769142513438
H	-0.93503697025271	2.06742878478425	4.43983985323244
C	2.81114135240618	5.04480508198871	-0.23501774584430
H	3.87712114799805	4.78718640453306	-0.12479435043421
H	2.71315614704309	6.02377229249370	-0.73044513534243
H	2.33324855394200	5.07207532809277	0.75512501116215
C	7.65220241654716	1.26866495379310	-0.28186138204292
H	8.22240453139506	1.19538033188627	-1.22118508427289
H	8.27273208949106	1.74426383474562	0.49361213591896
H	7.33515668545651	0.26742884038487	0.04300168086612
C	2.45966386911175	-0.44298260340145	5.45836896637880
H	2.54899200949705	0.61909589172251	5.73277604832631
H	2.37174246529603	-1.06060305449293	6.36493357897068
H	3.34311686041900	-0.74410011763427	4.87937210694029
C	-2.75706682710983	-1.45105184099226	4.33305702026961
H	-3.30678653191066	-2.11304550653425	5.02041486842583
H	-1.79647135362196	-1.15912806829558	4.78431756254792
H	-3.35825150110106	-0.55792265069779	4.11078106052245
C	-5.76933464622466	2.45948556744494	2.78891736274065
H	-5.25392148098616	3.42284935988400	2.92735754771934
H	-6.80372491355354	2.53803505538188	3.15760453892340
H	-5.23653489776237	1.66777865127873	3.33287757671362
C	-1.49874074491344	-0.46081950189244	-4.55235255787558
H	-2.57767282664508	-0.25448871839858	-4.64152186686449
H	-1.03897407128164	-0.48863229543678	-5.55266825526242
H	-1.34326377230500	-1.42056204514368	-4.03547035709541

Coordinates of Iso3 via PW91functional:

Au	1.85523429642922	2.32235263297547	-0.28038635684777
Au	0.32071903458883	0.48362681230375	-2.82376453082998
Au	1.32204899767311	5.32868685654936	0.42947619331133
Au	3.83229506863911	0.42703818063712	-1.60674307343523
Au	-0.81293961540773	-0.21170037640247	0.41000821171522
Au	4.37538320575883	4.01651523035477	-1.15123593644289
Au	-1.17322092779706	2.50985483977448	0.65300104766730
Au	1.76046746599872	-0.90736755839808	-0.35683584265560
Au	3.42655159244752	-2.27232601273309	-2.14246415943051
Au	-2.08538238056407	-1.97100434227467	-2.29658369328787
Au	0.74606885741171	1.57305114808498	2.96123994577417
Au	-1.86179232792644	-0.61918825205180	3.68818619646212
Au	-3.21899456639047	-2.49562304682697	1.02317859678346
Au	4.42841010257703	-1.47736184951393	0.34755073320531
Au	1.47885163258778	-4.80404437313302	-2.09061112280933
Au	-0.23527967950778	-2.89136471927142	0.02014489621477

Au	0.78154152078353	-1.49106778238738	2.26286373963796
Au	3.77347192159293	-2.10942650223730	3.40526490698017
S	-2.61832807391112	-2.83992631104743	3.29885718541598
S	-0.16561798824598	-1.68538895374984	-3.67161786587781
S	-1.18047189794329	1.55872326290144	4.35874257653285
S	-0.43940494110767	-5.20306970177735	-0.74893131613192
S	1.66597891237730	-2.05569841731932	4.47890603891632
S	-4.12572058124235	-2.43353394106433	-1.17345478227598
S	3.41970399816642	-4.34177974983044	-3.39381661589821
S	5.82631364471953	-2.09257453647799	2.20694596562755
S	3.60197775711837	5.91015959944345	0.05694117951805
S	5.23284486788635	2.23538296445716	-2.46010749829951
S	0.69245624124981	2.78196253804859	-2.34454832140835
S	2.83454978894275	1.71515755671693	1.83599298068539
S	-0.94756930125421	4.91306661735746	0.97899797468485
Au	-2.44250575886320	1.04535834856383	-1.43950694931707
Au	-3.29246784910394	0.70026230135825	1.23345773699200
S	-3.43754365388451	1.45518047035661	-3.62814691501144
S	-5.35153623575703	0.69356765159014	2.53395455426391
Au	-5.57353211457637	1.19305153615787	-2.65671895725097
Au	-6.55368838810934	0.80660386341051	0.50489551274102
S	-7.67079892313888	0.89736145343557	-1.58805747680597
C	-4.34428913972863	-4.23799126458566	-1.53255809440411
H	-5.17321063533365	-4.60944420350905	-0.91252056707113
H	-4.60117943221213	-4.34221606444815	-2.59672349933686
H	-3.42610389268935	-4.79807704618355	-1.31167411890145
C	-4.26882236557562	-2.85067207159357	4.13641468479452
H	-4.79738795999170	-3.76793770187843	3.83772864179662
H	-4.09569914336577	-2.85999119451988	5.22250768882649
H	-4.85723390495765	-1.96642092598315	3.85788105618291
C	-0.42743036433452	1.23248205611392	6.01898974283029
H	0.10516346485179	2.14107271150073	6.33590242659011
H	-1.24348589707237	1.01768103877213	6.72395235465837
H	0.26626366589680	0.38249143312305	5.97544467800235
C	6.59519040909236	-0.48457107190096	2.70663795035629
H	7.01045210060535	-0.60226772594216	3.71773463701781
H	7.40648215660670	-0.26361304693746	1.99818306180643
H	5.85484672614242	0.32554493000101	2.69554785258428
C	1.19312489468735	-3.83135180230515	4.68577819904812
H	1.72446341545325	-4.23279959757903	5.56038842379113
H	0.10714697689273	-3.86759472512656	4.85496110536274
H	1.44655173441346	-4.41611102593660	3.79256140689329
C	2.74915955638331	-3.90285964465987	-5.05982655862146
H	3.55364786389230	-3.41392072220485	-5.62843579983440
H	2.45213403920140	-4.83311502482099	-5.56491392743331
H	1.88631413677126	-3.23078429327047	-4.96807552526750

C	-0.93370114843393	-1.26332502393844	-5.30432200391232
H	-0.13512216247199	-0.91871433167754	-5.97780412969210
H	-1.39056270797806	-2.17846794839784	-5.70874401104555
H	-1.69615917908512	-0.48080800966920	-5.19073426706723
C	-8.05488201109504	-0.88141784515698	-1.92826798445427
H	-8.88673191274432	-1.17833202649558	-1.27399785744666
H	-8.36378989648920	-0.96383544621448	-2.98001845125982
H	-7.17904156681451	-1.51509783170629	-1.74058817001285
C	-1.83920030944225	5.54117085386966	-0.51438658856428
H	-2.90417000378681	5.29328064035783	-0.39191330223239
H	-1.71617007649268	6.63317892798055	-0.56350275457865
H	-1.45143602467170	5.07250301042434	-1.42881199793958
C	3.54707186599771	3.26766284006521	2.53924272632591
H	3.86316643764805	3.05148191307974	3.57011722124152
H	4.42068052487246	3.54944820427765	1.93174754895947
H	2.81358737336295	4.08587112715520	2.53544498327908
C	1.93052713869983	3.28143251327388	-3.61923810857134
H	1.38460201151696	3.45525408818507	-4.55844169829975
H	2.41162859090906	4.21424264050170	-3.28876913689479
H	2.69059599913762	2.50469143229572	-3.77193156685237
C	6.86324642614229	1.83039361064184	-1.68865336438930
H	7.24244138558539	0.92001102250560	-2.17412647093862
H	7.55212453750303	2.66729404190964	-1.87488030537311
H	6.76038647717928	1.65735211493605	-0.61004120835937
C	0.20255914582240	-6.18590424398712	0.67970937253656
H	-0.56759177858396	-6.17658499234447	1.46502416418567
H	0.37724658891810	-7.21761560375471	0.34280838464961
H	1.13465944475200	-5.75667807017162	1.06801925205381
C	3.51870737131379	7.24143175008071	-1.22282529028842
H	3.06487888847194	8.12718396397316	-0.75585495726416
H	4.54575254592499	7.47345962367524	-1.53709743620298
H	2.92312468018521	6.93143921943461	-2.09022435464988
C	-5.41043132578191	2.41129098123391	3.21650949089112
H	-6.40791403766230	2.57893722548794	3.64739254665472
H	-4.64521623083632	2.48126458939470	4.00317049875473
H	-5.20638376467255	3.15464048362157	2.43641469046769
C	-3.24191324310589	3.27934976564109	-3.85010884796833
H	-2.16872901978022	3.48393750732349	-3.97755149700776
H	-3.79091697556746	3.58073457735379	-4.75384855262814
H	-3.62299616629328	3.82809225072822	-2.97987714489068

Frequencies calculated at PBE/LANL2DZ level of theory

ISO1

Frequencies --	9.0029	10.6749	13.0875
Frequencies --	14.3107	15.7448	17.4632
Frequencies --	18.0338	18.6919	20.8480

Frequencies --	21.0783	22.2203	22.7942
Frequencies --	23.3570	23.9818	27.4021
Frequencies --	27.9818	29.7506	30.2596
Frequencies --	31.2508	31.5741	32.1420
Frequencies --	33.2721	34.9876	35.5372
Frequencies --	36.8090	37.5624	40.2463
Frequencies --	41.2015	41.8624	42.2750
Frequencies --	43.3927	44.6963	45.5455
Frequencies --	46.1258	47.6115	49.1571
Frequencies --	49.8411	49.9394	50.8913
Frequencies --	51.5408	52.2981	53.3061
Frequencies --	54.0730	55.7572	57.1711
Frequencies --	57.6359	58.8514	58.9288
Frequencies --	60.5043	61.4398	61.6109
Frequencies --	62.0511	63.1038	64.3781
Frequencies --	64.6620	65.3124	66.3464
Frequencies --	66.6364	67.2194	68.2081
Frequencies --	70.6886	71.4729	71.7452
Frequencies --	74.0927	74.4474	76.9585
Frequencies --	78.2202	81.7377	88.0692
Frequencies --	88.8103	90.9150	93.4486
Frequencies --	98.0243	99.6958	108.3336
Frequencies --	109.5194	118.6296	127.7708
Frequencies --	134.9680	136.1412	139.0020
Frequencies --	139.8618	140.5693	141.1408
Frequencies --	141.2214	143.0742	144.2064
Frequencies --	145.2538	145.4345	147.2294
Frequencies --	149.1269	151.4986	151.6152
Frequencies --	151.9665	156.3515	157.0206
Frequencies --	159.3720	160.0617	160.1689
Frequencies --	160.6272	161.4755	162.5729
Frequencies --	163.0919	164.2786	165.5149
Frequencies --	167.4592	168.7693	169.3984
Frequencies --	170.5372	171.6317	174.0934
Frequencies --	177.2116	177.5927	180.3187
Frequencies --	181.7816	183.4141	183.8735
Frequencies --	184.1323	185.9851	186.1457
Frequencies --	188.0964	188.9781	190.1854
Frequencies --	191.0661	191.5085	195.5403
Frequencies --	196.2543	197.7454	198.5548
Frequencies --	202.0936	209.3074	212.4705
Frequencies --	251.2283	254.6475	257.6688
Frequencies --	258.4894	258.7673	262.3777
Frequencies --	265.2956	268.8010	269.5223
Frequencies --	270.2280	270.5333	271.8087
Frequencies --	279.0846	281.2732	281.6779

Frequencies --	282.5363	285.0871	292.9700
Frequencies --	310.7838	312.8703	313.0144
Frequencies --	314.0976	314.5989	315.6833
Frequencies --	316.6682	317.7636	318.3774
Frequencies --	320.3929	320.4695	321.8604
Frequencies --	321.9885	325.5287	327.4495
Frequencies --	331.2101	333.8624	334.2595
Frequencies --	669.0282	670.6623	670.9559
Frequencies --	671.1503	671.8954	672.4113
Frequencies --	672.5667	674.0261	674.4012
Frequencies --	674.4610	674.9009	675.5301
Frequencies --	675.5541	675.6312	675.9239
Frequencies --	677.8698	677.9034	680.8802
Frequencies --	950.3026	950.7314	951.6205
Frequencies --	952.4780	952.6190	953.5591
Frequencies --	953.9463	954.1455	954.4092
Frequencies --	955.0378	955.0687	955.1594
Frequencies --	956.1244	956.2206	956.3377
Frequencies --	957.5901	958.4623	958.7782
Frequencies --	958.9751	959.6250	959.7995
Frequencies --	960.9787	961.0268	961.2018
Frequencies --	961.6652	962.4189	962.4958
Frequencies --	963.3805	963.9198	964.0519
Frequencies --	966.4189	966.4768	966.7685
Frequencies --	968.4833	968.6173	969.9862
Frequencies --	1311.6695	1318.4758	1319.1494
Frequencies --	1320.0064	1320.8725	1322.8966
Frequencies --	1323.1564	1323.6479	1324.7782
Frequencies --	1324.9362	1325.2084	1325.3782
Frequencies --	1326.0138	1326.3719	1326.3794
Frequencies --	1326.6532	1326.8931	1327.3334
Frequencies --	1427.9633	1429.1089	1429.5057
Frequencies --	1434.4789	1434.9967	1436.7845
Frequencies --	1437.2225	1438.5430	1438.6627
Frequencies --	1439.1388	1441.1788	1441.6205
Frequencies --	1442.2314	1442.3417	1445.6147
Frequencies --	1445.7849	1445.8236	1446.0954
Frequencies --	1446.3019	1446.5804	1447.1230
Frequencies --	1447.3108	1447.7075	1449.5681
Frequencies --	1450.5794	1451.2528	1452.0115
Frequencies --	1452.2826	1453.8516	1454.1547
Frequencies --	1454.2678	1454.9196	1457.7354
Frequencies --	1458.6086	1464.4376	1465.2236
Frequencies --	2977.6010	2980.5044	2983.3139
Frequencies --	2990.8093	2995.8198	2995.9324
Frequencies --	2997.3991	2998.7150	3000.1867

Frequencies --	3000.7085	3006.1790	3006.4425
Frequencies --	3006.4591	3006.8373	3008.5979
Frequencies --	3009.2461	3009.4559	3009.6015
Frequencies --	3071.3014	3072.4225	3074.3945
Frequencies --	3087.9329	3089.5417	3090.5622
Frequencies --	3091.9235	3092.0932	3092.2746
Frequencies --	3092.8812	3093.0623	3093.8463
Frequencies --	3095.0682	3095.8805	3097.0420
Frequencies --	3098.2728	3099.0914	3099.2657
Frequencies --	3099.7128	3099.9096	3100.0364
Frequencies --	3100.0791	3100.4454	3101.3935
Frequencies --	3101.6859	3101.7932	3102.0057
Frequencies --	3107.7528	3111.4692	3112.1458
Frequencies --	3112.2698	3116.1533	3116.5211
Frequencies --	3117.0080	3117.7144	3118.2688

ISO2

Frequencies --	2.6101	8.4080	11.8929
Frequencies --	14.6103	15.7154	16.5362
Frequencies --	19.5992	20.8260	21.9102
Frequencies --	23.4959	24.7627	26.9075
Frequencies --	27.3398	28.0554	28.6383
Frequencies --	29.3134	30.1932	31.1137
Frequencies --	31.5448	32.7050	33.1913
Frequencies --	34.0407	34.8364	36.1291
Frequencies --	37.1907	38.2498	38.8992
Frequencies --	41.0425	42.2386	42.5773
Frequencies --	43.1386	44.9534	45.4696
Frequencies --	46.9273	47.3780	48.9224
Frequencies --	49.3340	50.2108	52.2328
Frequencies --	53.4793	54.7895	55.3129
Frequencies --	56.1800	58.1019	58.5359
Frequencies --	59.3603	61.1344	61.9477
Frequencies --	62.9277	63.5919	64.6201
Frequencies --	64.9044	66.0257	66.9267
Frequencies --	67.7020	70.8677	72.0846
Frequencies --	72.3433	73.0569	74.2007
Frequencies --	74.4553	78.2671	79.7906
Frequencies --	80.0119	81.9402	83.0241
Frequencies --	83.3509	84.5016	88.0212
Frequencies --	90.3434	91.0538	92.1997
Frequencies --	95.7698	97.4879	99.4315
Frequencies --	100.6914	119.9484	124.5948
Frequencies --	126.0911	126.5110	128.8306
Frequencies --	133.7152	136.5015	137.2863
Frequencies --	137.4437	138.8597	140.9934
Frequencies --	141.9059	142.8251	144.1230

Frequencies --	144.4225	145.1419	145.3517
Frequencies --	146.6217	147.7668	150.9912
Frequencies --	152.1656	153.4026	155.1747
Frequencies --	156.9328	158.8106	159.5475
Frequencies --	160.7129	162.6873	163.5476
Frequencies --	166.2964	167.1871	167.9821
Frequencies --	170.3890	171.5286	173.4870
Frequencies --	173.7354	174.6449	176.0713
Frequencies --	177.8055	178.1501	180.3556
Frequencies --	183.8950	184.8680	186.0006
Frequencies --	191.6211	193.1382	193.5156
Frequencies --	196.7501	197.0230	198.4785
Frequencies --	198.7541	200.5385	201.7665
Frequencies --	203.7351	206.7354	218.3490
Frequencies --	233.4229	238.6769	243.8589
Frequencies --	246.7263	247.3475	249.2791
Frequencies --	253.7303	255.8212	262.9042
Frequencies --	263.5709	267.4395	270.3042
Frequencies --	274.2910	275.2244	278.4356
Frequencies --	280.7059	281.6810	284.7645
Frequencies --	299.3561	300.6068	312.3035
Frequencies --	313.7558	316.7155	318.1357
Frequencies --	318.9232	319.4125	320.7632
Frequencies --	323.9820	324.4602	325.9239
Frequencies --	326.3082	327.0914	327.3212
Frequencies --	329.5122	331.7245	333.1350
Frequencies --	672.9840	673.2252	673.4673
Frequencies --	673.9082	673.9189	674.4243
Frequencies --	674.5243	674.5677	675.2111
Frequencies --	675.8248	677.5357	679.9029
Frequencies --	680.5531	681.9545	683.1984
Frequencies --	684.8935	686.0094	686.8300
Frequencies --	940.4547	944.4289	946.9276
Frequencies --	947.3316	948.1204	950.4100
Frequencies --	951.8793	954.5521	955.0737
Frequencies --	955.2422	955.7177	956.3066
Frequencies --	956.4742	956.9928	957.7207
Frequencies --	957.7626	957.9032	958.2571
Frequencies --	958.8589	959.5236	959.9380
Frequencies --	959.9898	961.3825	961.5461
Frequencies --	961.9554	962.1764	963.0443
Frequencies --	964.2352	964.8124	965.9358
Frequencies --	966.3433	967.6743	968.4772
Frequencies --	970.4147	971.8528	982.8644
Frequencies --	1315.4787	1316.4826	1316.8846
Frequencies --	1317.5452	1319.7499	1320.7676

Frequencies --	1320.9326	1321.6219	1323.7132
Frequencies --	1323.7966	1324.1294	1324.6455
Frequencies --	1325.2516	1325.5254	1326.0439
Frequencies --	1326.2638	1326.9936	1327.8940
Frequencies --	1431.8363	1433.4242	1434.0834
Frequencies --	1434.6335	1435.5303	1437.6507
Frequencies --	1438.0448	1439.2660	1439.5653
Frequencies --	1440.5925	1440.6795	1441.5977
Frequencies --	1441.7843	1443.9483	1444.4232
Frequencies --	1444.6865	1445.0753	1445.3381
Frequencies --	1445.7023	1447.3147	1447.8079
Frequencies --	1448.5954	1448.9977	1449.1562
Frequencies --	1450.1864	1451.1007	1451.1714
Frequencies --	1451.6398	1452.3267	1452.4643
Frequencies --	1452.6728	1454.0224	1455.7094
Frequencies --	1456.3278	1458.0718	1458.4508
Frequencies --	2984.0300	2987.1902	2988.6474
Frequencies --	2988.6664	2989.2083	2996.9908
Frequencies --	2998.1329	3000.1867	3000.6827
Frequencies --	3004.0854	3005.1829	3005.8342
Frequencies --	3006.0825	3006.7692	3010.0174
Frequencies --	3011.6724	3011.7419	3012.5745
Frequencies --	3077.7857	3080.2698	3080.8797
Frequencies --	3083.1961	3085.0867	3091.4095
Frequencies --	3093.1209	3093.4956	3093.9806
Frequencies --	3094.2843	3094.6293	3094.9994
Frequencies --	3095.5720	3095.8834	3097.5446
Frequencies --	3098.0581	3098.4856	3098.5459
Frequencies --	3098.6145	3099.9449	3100.6145
Frequencies --	3102.2184	3102.7150	3102.7854
Frequencies --	3102.8850	3103.9094	3105.3444
Frequencies --	3110.5149	3112.2958	3112.5482
Frequencies --	3115.1582	3119.4153	3121.7926
Frequencies --	3122.9939	3131.4011	3137.9721

ISO3

Frequencies --	4.7803	8.8295	10.8905
Frequencies --	11.1618	14.3491	15.8926
Frequencies --	16.7158	17.7501	18.9018
Frequencies --	20.4009	20.7800	21.7655
Frequencies --	22.9299	23.3675	24.1419
Frequencies --	26.2148	26.8490	28.4167
Frequencies --	29.3663	31.0868	31.8241
Frequencies --	32.9378	33.9537	34.3305
Frequencies --	37.0791	37.5740	38.0159
Frequencies --	38.5211	40.5174	40.8128
Frequencies --	41.8794	43.3745	44.2455

Frequencies --	45.6983	46.5972	47.5888
Frequencies --	48.2083	48.8550	49.5402
Frequencies --	50.6471	52.2873	53.7800
Frequencies --	55.3356	55.8152	56.5262
Frequencies --	57.6502	58.0122	59.4131
Frequencies --	60.4504	61.7347	62.4124
Frequencies --	62.9392	64.8465	65.2755
Frequencies --	66.5302	67.9593	69.9171
Frequencies --	70.7282	74.3654	74.7432
Frequencies --	76.0329	76.4084	81.7467
Frequencies --	84.0435	85.7291	86.7923
Frequencies --	87.8952	88.6188	89.7762
Frequencies --	91.0139	91.3998	91.8306
Frequencies --	93.1165	96.3146	107.9126
Frequencies --	113.0674	116.7610	117.2550
Frequencies --	124.5447	129.1067	129.6717
Frequencies --	134.9690	139.1962	140.0929
Frequencies --	140.8690	141.9963	143.1749
Frequencies --	143.9865	144.5836	146.3284
Frequencies --	146.9957	148.0218	148.6356
Frequencies --	149.6661	150.0803	150.8441
Frequencies --	152.3543	152.8114	153.3844
Frequencies --	155.4631	156.1704	157.3561
Frequencies --	159.9947	162.1815	164.6621
Frequencies --	164.8966	166.1310	166.9184
Frequencies --	167.7513	168.0250	169.7886
Frequencies --	170.1547	172.8910	175.8674
Frequencies --	177.1053	178.7279	180.2833
Frequencies --	182.2270	182.6536	183.7957
Frequencies --	186.0585	187.1032	188.5270
Frequencies --	190.1166	193.7431	194.3496
Frequencies --	195.6497	195.8654	196.9044
Frequencies --	198.2129	203.3169	209.8024
Frequencies --	231.8628	240.5019	243.2798
Frequencies --	247.1494	251.0009	253.3921
Frequencies --	253.9904	259.7155	265.2727
Frequencies --	268.7130	271.3347	273.5021
Frequencies --	274.0181	274.4011	278.1108
Frequencies --	279.6564	290.4846	292.7505
Frequencies --	296.1404	296.8773	297.1998
Frequencies --	299.9052	302.1763	303.7106
Frequencies --	316.6144	320.4914	320.8420
Frequencies --	322.3701	323.7349	327.1822
Frequencies --	329.4104	329.7938	329.8674
Frequencies --	334.1137	337.8603	340.6297
Frequencies --	669.7365	671.2648	671.7695

Frequencies --	672.6325	673.9058	674.8687
Frequencies --	675.0362	675.5985	676.1099
Frequencies --	676.3095	676.4596	676.7247
Frequencies --	676.9538	677.6544	678.6569
Frequencies --	679.1689	682.2403	682.7373
Frequencies --	945.3270	945.9806	948.3268
Frequencies --	948.8691	950.2056	951.0977
Frequencies --	951.3143	951.7921	951.8198
Frequencies --	952.5258	952.7531	954.5697
Frequencies --	954.9254	955.1886	955.5211
Frequencies --	955.6409	955.9404	956.9025
Frequencies --	957.5665	958.7909	959.1958
Frequencies --	959.5127	959.6439	960.4908
Frequencies --	961.1045	961.9149	962.3144
Frequencies --	962.8498	963.0433	963.2111
Frequencies --	965.1781	965.5666	966.1750
Frequencies --	968.7808	969.0728	969.9996
Frequencies --	1315.0353	1318.1670	1319.8526
Frequencies --	1320.0236	1321.5788	1321.8751
Frequencies --	1322.4648	1322.8572	1323.2276
Frequencies --	1323.3589	1323.7263	1324.1731
Frequencies --	1324.4581	1324.9963	1325.6255
Frequencies --	1325.9497	1326.5036	1326.7460
Frequencies --	1428.9103	1432.3813	1433.8924
Frequencies --	1434.8045	1436.4127	1437.1196
Frequencies --	1437.5480	1440.4316	1441.0498
Frequencies --	1442.9511	1443.3199	1443.9952
Frequencies --	1444.1816	1444.5987	1444.9687
Frequencies --	1445.2074	1445.2669	1445.8099
Frequencies --	1446.1834	1446.4612	1446.5404
Frequencies --	1446.9230	1450.0657	1451.4159
Frequencies --	1452.0597	1452.3026	1452.3179
Frequencies --	1452.3941	1452.7799	1453.6365
Frequencies --	1453.9030	1454.4160	1454.6562
Frequencies --	1455.1928	1457.0917	1457.9486
Frequencies --	2971.8905	2972.8865	2976.7755
Frequencies --	2989.6335	2989.6550	3002.3446
Frequencies --	3003.1500	3003.9365	3004.7741
Frequencies --	3004.9173	3005.9685	3006.1762
Frequencies --	3006.6958	3006.9829	3007.0281
Frequencies --	3007.0770	3007.3289	3008.7500
Frequencies --	3057.5819	3065.4694	3066.1027
Frequencies --	3084.1635	3084.6232	3085.5347
Frequencies --	3087.3083	3088.9658	3090.9665
Frequencies --	3092.1691	3092.7503	3093.1038
Frequencies --	3093.7567	3096.1537	3096.9351

Frequencies --	3097.2494	3097.8390	3098.0786
Frequencies --	3098.1045	3098.2672	3098.9555
Frequencies --	3099.0757	3101.6603	3107.9545
Frequencies --	3109.9755	3111.7766	3112.2921
Frequencies --	3114.1663	3114.2061	3114.6129
Frequencies --	3115.8953	3115.9331	3120.1186
Frequencies --	3122.1912	3122.8822	3123.0811

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