

Protected but Accessible: Oxygen Activation by a Calixarene-stabilized Undecagold Cluster

Xi Chen¹ and Hannu Häkkinen^{1,2,*}

¹ *Department of Chemistry, Nanoscience Center, University of Jyväskylä, FI-40014 Jyväskylä, Finland*

² *Department of Physics, Nanoscience Center, University of Jyväskylä, FI-40014 Jyväskylä, Finland*

Ref. 10b with full author list

J. Enkovaara, C. Rostgaard, J. J. Mortensen, J. Chen, M. Dulak, L. Ferrighi, J. Gavnholt, C. Glinsvad, V. Haikola, H. Hansen, H. Kristoffersen, M. Kuisma, A. Larsen, L. Lehtovaara, M. Ljungberg, O. Lopez- Acevedo, P. Moses, J. Ojanen, T. Olsen, V. Petzold, N. Romero, J. Stausholm-Moller, M. Strange, G. Tritsaris, M. Vanin, M. Walter, B. Hammer, H. Hakkinen, G. Madsen, R. Nieminen, J. Norskov, M. Puska, T. Rantala, J. Schiotz, K. Thygesen and K. W. Jacobsen, *J.Phys.:Condens.Matter* **2010** 22 253202.

Total energies of structures 1 – 4 in Hartrees and electron volts

Structure 1	-182.9842 Hartree	-4979.00 eV
Structure 2	-196.3102 Hartree	-5341.60 eV
Structure 3	-183.3980 Hartree	-4990.26 eV
Structure 4	-184.2227 Hartree	-5012.70 eV

Coordinates of structure 1

Au	21.360197728980683	20.032664924817794	23.732971483238536
Au	21.434660745573900	18.126713476508552	25.694057374308819
Au	18.925903490578900	20.695928755071886	22.615216637889610
Au	23.437848078950921	20.420788412270742	21.789348121050953
Au	22.631348586471926	17.592384157789692	22.803447364425384
Au	21.029653221471232	19.015155680528149	20.994625858358184
Au	21.243695795191957	22.224798532880648	21.999486409189018
Au	21.518913976223430	22.130798113019576	25.400696064010635
Au	18.896826197394017	19.492619873214402	25.420495859593970
Au	23.697965380741277	20.128708649021927	25.199722679188383
Au	19.641772589584892	17.808977777255148	23.212545510585834
C	21.150867231161417	12.016344716320631	25.146015258321597
C	22.375264762445120	11.477447533616779	25.560302048763450
C	22.359759550893969	10.468852736381900	26.534159524831878
C	21.167998359362787	9.972501333213748	27.078767656195073
C	19.961425389638681	10.499433878410095	26.585633347346910
C	19.929227327882913	11.513362894357567	25.622995221006487
C	23.665950887656571	11.926342467478145	24.897026977878866
C	23.781433975943624	11.359923429582528	23.488880205308110
C	23.663509791034695	12.163799244366665	22.330364427358354
C	23.654565116161564	11.546458908049107	21.060947483412583
C	23.829117464436855	10.155218111764745	20.987096696130951
C	23.986029620542809	9.338164388409544	22.105419409447521
C	23.953596500820534	9.980730593942024	23.349033807144554
O	23.484801153914219	13.535286011397144	22.541213238048282
C	24.315075003191346	14.424128033845493	21.815640006715164
C	23.406607622419880	12.237639564905923	19.725482089066780
C	22.065897889673543	11.912249974461353	19.098230805541217
C	21.965569573348240	11.185379327351937	17.909619642585273
C	20.732151611335290	10.905567241015536	17.298270996668538
C	19.575145529929578	11.355719873600981	17.949874569176210
C	19.629019321891601	12.080342758364752	19.149838165567019
C	20.884568482667646	12.379941581476713	19.695970066428398
C	18.370735179872433	12.505429156765230	19.886662237624648
C	18.214515258185617	11.775646151617885	21.216028241906663
C	18.373115705764025	12.356082524451654	22.496202970827962
C	18.379621131859373	11.523945565332566	23.635705466983321
C	18.187893047139113	10.144045874840659	23.478341956297623
C	17.988554402296050	9.543947640863740	22.234871700621543
C	17.999843055067160	10.396177182669282	21.126262196790009
O	18.642749556160048	13.715741613327593	22.697646020323518
C	17.714751368666285	14.669840523039834	22.197701268223469
C	18.630186131302178	12.041264149332010	25.044106603659188
C	17.803057499840264	8.032158897141091	22.040917385963422
C	18.902280936355250	7.497398442204043	21.096448285233542

C	20.699290800485695	10.129478820784330	15.969744980208780
C	21.494094329997484	10.907587121552906	14.897249017809628
O	20.968218686303825	13.080577541253392	20.878261965687333
C	20.935254239871210	14.508070526431792	20.739928773523275
C	24.184367262332017	7.817374847041521	22.007486357617044
C	23.151339054073038	7.089343249144500	22.894097711613320
C	21.148542717973779	8.871799972372266	28.152942147352103
C	20.308419114029480	9.334978315609614	29.361185825417611
O	21.135649356799014	13.027657195045913	24.208149038061286
C	21.219151433710394	14.327300542621263	24.810723309091792
C	17.894084141964324	7.251709709531010	23.361639014053928
C	16.420272189715575	7.762048576182663	21.410782692650070
C	21.337592005174930	8.736421207293285	16.163385438860359
C	19.269312678787841	9.922294543670116	15.449204996314052
C	24.019977787644567	7.302054175725974	20.568457255455129
C	25.604888489112824	7.459560505475901	22.493698548794043
C	20.524625231879728	7.589496078800021	27.559585600789106
C	22.555589674369447	8.522683647675716	28.663988213100801
H	16.686129581661085	14.280142644099010	22.265697196403728
H	17.920064299457273	14.945059752495013	21.149854277713874
H	18.220859692826703	9.532000802085776	24.380340283404287
H	17.891860378170449	9.975605072680088	20.123634573999809
H	18.873276604462959	7.375334209797831	23.846822066132312
H	17.754590112152066	6.178762857424594	23.162820577630740
H	17.115918127735000	7.560769102467694	24.074036925708064
H	15.611284225372939	8.113741432835180	22.067628648689411
H	16.280441182524836	6.683798134903167	21.242774060942164
H	16.312517738539970	8.272763235967373	20.444341518628633
H	18.880283153134524	7.993656090985757	20.117335913754815
H	18.769711855429446	6.417781461105914	20.930152967319305
H	19.899292576798228	7.661686635384928	21.528066021733295
H	17.500991273724541	12.280085109289526	19.250756027005000
H	18.377876934892434	13.589116945591964	20.026009385776991
H	18.591291620800661	11.140156704355764	17.529700569561992
H	22.892712119357128	10.842514870120292	17.443281354842810
H	21.777530514056245	14.875456389402558	20.135278315371099
H	20.993770022416950	14.926406195552822	21.747028970221116
H	20.006107026931257	14.855723507199684	20.260579746860298
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H	22.375712198721224	8.807956097994538	16.513666594158245
H	21.339713321820252	8.180685156975120	15.213284047635046
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H	18.757666392665335	10.876777244260355	15.259927520759845
H	18.661026573380802	9.338653762559382	16.154521996929887
H	22.540403722095288	11.059675476846042	15.193897739993492
H	21.051451839555501	11.897791824702146	14.718413900599661

H	21.492629724613028	10.356710195922185	13.944226191586811
H	17.798620549921967	11.723686114026840	25.691512884306256
H	18.633431269910158	13.135206472847452	25.035780355888203
H	23.911495643242858	14.672295531872697	20.821383473658088
H	25.315924585098273	13.984586488763131	21.684509349679441
H	23.803220921663200	9.712982329108469	19.990348247286153
H	24.045734355762288	9.393095575992055	24.265788871371129
H	23.020964867927091	7.524937864196303	20.166496296811495
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H	24.767796743480083	7.737086874294626	19.889854301141224
H	26.366709994371412	7.938588072201624	21.861910007921768
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H	21.166430361881510	15.069415531289099	24.005878402754739
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H	21.095401662684981	7.250548654636130	26.683478787575762
H	19.487003579166021	7.756655289371102	27.241385690141826
H	20.524246328667559	6.777900736706549	28.303814946890629
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H	20.734038931187143	10.243948594775466	29.809871237751842
H	20.284704460731540	8.549348076226559	30.131673169722966
H	24.195981888461180	11.925908601990681	19.023906170709775
H	23.487897845329776	13.322558706960129	19.810590229580676
C	25.411209519400927	15.759665643966351	24.156380234362693
C	24.658903231029559	15.873842912985632	25.334362311834774
C	25.185993311149417	15.457609383780232	26.557824267626067
C	26.479380786496986	14.937458274360965	26.622564329084113
C	27.254245979315904	14.867216699830996	25.461235669990899
C	26.725862730105447	15.273823048765175	24.235770542229609
H	23.655004502612570	16.308149049017668	25.296466616325958
H	24.575886684251017	15.539219026690846	27.459761953154221
H	26.890073155567165	14.592563369205260	27.572808159624653
H	28.277227034962937	14.489569618371091	25.506750250277381
H	27.351133747713149	15.220767599959064	23.345530043800704
P	24.524274375793688	16.136686011092220	22.585952819189650

C	25.745135661160333	16.680157765578226	21.290846979475965
C	25.516151738079913	17.894548242052625	20.631167145385877
C	26.320741881278643	18.304194346592123	19.566134440030137
C	27.375009594607302	17.502642519632488	19.127536565014992
C	27.629294836512162	16.296146751108488	19.786369387458770
C	26.822582782004325	15.885685646182875	20.850520734142975
H	24.691591106261836	18.549794900946434	20.955943295843831
H	26.108218364729428	19.256870524520618	19.076895227080069
H	27.975738382514251	17.809103928018420	18.269717316696866
H	28.457659260332921	15.660251488349322	19.467414712936311
H	27.045676113488486	14.927578701378714	21.318896908218232
C	16.257266703233107	17.078737647439286	22.521479519404206
C	15.792682587337737	18.242432736541179	23.159110451118490
C	14.596961431113719	18.843177104477160	22.765885924881509
C	13.849025354180210	18.305407824482995	21.713189944856673
C	14.317082661567408	17.169883514525765	21.051737936632833
C	15.509891578922606	16.560984452602092	21.450315744255068
H	16.387047616441556	18.684420939956471	23.962474675623053
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H	12.913264950889294	18.774107237983745	21.403969803305422
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H	15.846121904477998	15.683160427182312	20.901699898276089
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C	17.279535380295869	15.664197039489633	24.819410124901388
C	18.132917648904023	15.806985145296643	25.919386648091095
C	17.840559172039484	15.160064794929099	27.122920754189845
C	16.694141153055696	14.374289060260352	27.234270557648404
C	15.805946677343021	14.275837389487572	26.158884931495713
C	16.096827220073337	14.919059757476782	24.956677460775719
H	19.032190953836583	16.424826938472915	25.828584843859694
H	18.525814361170564	15.259967083292134	27.966488741876756
H	16.480587789223591	13.836367383722894	28.156944388873903
H	14.896412343565297	13.682479213541031	26.266566362407236
H	15.401059609526442	14.833625515347867	24.118920517556479
C	27.380315508784093	20.804107796511886	32.858499284711925
C	27.454312717786504	21.814231093852555	31.885639155736499
C	27.904314050597989	23.084465218957927	32.280038649616344
C	28.302932496944205	23.360514422055122	33.594276561204197
C	28.226525821061362	22.313586763123499	34.526964838927498
C	27.771934803657029	21.035801908853564	34.190547492737032
C	27.121755422502396	21.505147872965210	30.431338480640449
C	28.246314194285610	20.714311466658511	29.765188633214539
C	28.075200250248603	19.475951688497368	29.105533925331684
C	29.195416276237417	18.626392812434716	28.955615120173043
C	30.476597157035460	19.128204801210615	29.209255494446921
C	30.696300936795780	20.436159177459462	29.645981352523240

C	29.553407788928766	21.178825650762448	29.958346929550352
O	26.859697352333736	18.920392295274585	28.697292421327671
C	25.809407145897595	19.582658733048625	27.980272608221288
C	29.051566238257525	17.152577174899619	28.593625998902972
C	29.656626681259702	16.257621580209545	29.660798750414681
C	30.885244201732302	15.619351803890179	29.451437151053739
C	31.511484158481029	14.835679663521184	30.433695731444359
C	30.876983749004864	14.749729570458589	31.680496485015784
C	29.655340635838872	15.384090993639134	31.945155183235840
C	29.030217485709695	16.100515162788380	30.909513681951701
C	29.034028909685826	15.358768236262843	33.331952801582489
C	29.373452261734386	16.625872991044272	34.111682684614919
C	28.393625535236119	17.557357951250712	34.506151634123540
C	28.758797425570542	18.826397135934450	34.983483742236039
C	30.117616482354595	19.092189200122323	35.199571689578519
C	31.115384776964696	18.144222715610098	34.950470193952818
C	30.711583195070315	16.932417177784700	34.373578264182420
O	27.033827665189499	17.264935186215364	34.360911049181503
C	26.538612596747601	16.305744404565150	35.289725084547207
C	27.734058329657159	19.922632487619680	35.229170624136792
C	32.598176369965053	18.385729893355027	35.272791175641792
C	33.454687227715546	18.227596424424508	33.998945144388593
C	32.872982139082254	14.169238503305507	30.165291106539843
C	32.964389214400093	13.657858836912192	28.714145530077325
O	27.809525313331754	16.699124309044684	31.159262791049787
C	26.680606635906333	15.916558207975235	30.726581703980926
C	32.096789212514750	21.037331314022019	29.836304761458287
C	32.261317214782849	21.559628437786959	31.279035053948558
C	28.839572515556615	24.732047641819442	34.036373318769868
C	27.926326875605902	25.318553294624913	35.134465173078617
O	26.977103520732030	19.539817621636004	32.476548128429997
C	25.577231221270022	19.314499630010420	32.664180580434945
C	32.847151074858488	19.791922736690296	35.839663965246643
C	33.061412177426689	17.350715256676192	36.321897097667538
C	33.989389754607856	15.210506136475686	30.404916099620173
C	33.122236989073933	12.971685589842417	31.101716709093093
C	33.207746268019612	20.008127798682459	29.572875962954161
C	32.274963220066049	22.210358282954711	28.847171690870972
C	30.268778483281022	24.565097472905279	34.598622812545507
C	28.901291999326496	25.738289538387150	32.877399864982031
H	26.568636698225010	16.682553014506460	36.329829582607324
H	27.112526250652017	15.362434408212218	35.266890024004987
H	30.382516778866975	20.081433966223280	35.573937290085532
H	31.466037007283298	16.197782302482036	34.083148893555673
H	32.560004033931790	20.576371946527118	35.125006945550169
H	33.916347929693117	19.917314188731421	36.059980299966021

H	32.294133848263002	19.957948312012039	36.774709473717017
H	32.491220537023139	17.454650873795366	37.256129715571802
H	34.127697437314389	17.492241454301741	36.553789220516144
H	32.928903230320955	16.323113892825571	35.957223059802637
H	33.343112946346245	17.233678509418059	33.545992343212028
H	34.518552312430508	18.369249624649022	34.240231500850399
H	33.171481681607027	18.971645595973946	33.242117860909339
H	29.403312321572329	14.475259835562746	33.875406573985174
H	27.946352229472147	15.268401998530496	33.239665799499349
H	31.330628427200296	14.166460255548522	32.483197110589316
H	31.357173214444668	15.745797349814763	28.475238794635789
H	26.498102793935740	16.047606964508123	29.648453920532443
H	25.810938787482961	16.257395505703983	31.298202311168847
H	26.838228688090823	14.848308140593961	30.941894509949400
H	33.959624751633442	15.584034215392947	31.438608810491690
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H	23.556804367918481	27.476098264850428	13.389249936627660
H	23.064137259985014	28.219215596909528	11.849730784560123
H	19.933644048274388	16.647530863248559	14.347048418954024
H	21.399333583876775	17.151153017233241	15.189403006382538
C	29.878076723750301	18.022440987818428	13.958049966011263
C	30.273423571980999	17.113091264365877	14.949734314740262
C	31.311259925307152	16.212420668808800	14.708369810797222
C	31.959398394633588	16.207803933390053	13.472253508213967
C	31.568882490057309	17.107596644870885	12.477484199400852
C	30.532653350717442	18.011971450538415	12.716367686003849
H	29.742450756673346	17.110109645998911	15.902181986224640
H	31.605888272076246	15.506614543761284	15.486063931092463
H	32.764827181142408	15.497924200255415	13.277928922956217
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H	30.234077437900396	18.695918052044366	11.920181342994944
C	29.134860572630842	20.787695501332415	14.670565519339210
C	28.772986584102316	21.414885364267793	15.870227205059848

C	29.255734340952859	22.690854738054650	16.168243766932115
C	30.102159012319522	23.346068915014030	15.272038325544230
C	30.468688289066606	22.723686390278839	14.075328452861854
C	29.988896558058201	21.448591006660504	13.775348086254560
H	28.114776268109630	20.885456801524555	16.560270301073178
H	28.970711226428456	23.170958225102002	17.105613642746331
H	30.482451489842333	24.341235015478173	15.505813560002405
H	31.131008698540317	23.233352339335138	13.373698871252842
H	30.297274651453705	20.967662116686672	12.845337674203481
C	18.813402759314837	18.563141936284037	18.262368542002903
C	17.886994630099863	18.945537034094041	19.244389570652441
C	16.525756197875332	19.019942837834986	18.943523200964879
C	16.071573808166228	18.700313066191388	17.663785466865733
C	16.985305504903501	18.316250585485005	16.678846068544338
C	18.348735708976680	18.251973881411637	16.971603557090834
H	18.242193667885495	19.207431247597022	20.246759794320528
H	15.821714131154927	19.325050958683068	19.718824931195229
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H	16.640207336020879	18.080534685015031	15.671007964611587
H	19.047148089209102	17.980421995355989	16.181325729391247
P	20.592731138695576	18.675439791326855	18.703534300904749
C	21.441232579507314	17.136132795305500	18.181868785813812
C	22.827366176810624	17.094719358431608	18.405083239433452
C	23.574469071885062	15.984283186075560	18.017760905339454
C	22.941202611770560	14.896286695952798	17.408740115277904
C	21.560718508629837	14.918245852375790	17.209329484645291
C	20.810716627090578	16.032739921485355	17.595272176917344
H	23.320020947087102	17.936880574043609	18.893984255930498
H	24.653097616355886	15.975876098901203	18.184229811514225
H	23.522334925053325	14.026663733869817	17.100801804884849
H	21.063690897926556	14.059943967183004	16.755745494410661
H	19.731929842056736	16.039207114273498	17.442277200243790
O	27.684632831000599	18.608789610330753	15.561794898910136

Coordinates of structure 2

C	20.331521698892356	15.367594910058715	28.063739858720989
S	20.171234021593200	15.615599722033959	26.316676943720740
C	19.194518356878778	15.073451804056267	28.812191651309281
C	21.605620494730211	15.161347560363090	28.671578437782529
C	19.270914908698099	14.459110415571688	30.088109342767080
C	21.715637136766350	14.554828664881768	29.902519140621866
C	20.562395530865736	14.147731564135480	30.629412807088212
C	18.115319571044324	14.095279091185674	30.834277484737829
C	20.647448318493343	13.443776902521787	31.857242869998778
C	18.230508865306302	13.426824445451917	32.036406479460780
C	19.504560919205005	13.087011637980577	32.546940107620344
H	18.210467782651293	15.259535590670101	28.380456182012381
H	22.499861001375812	15.444518404545805	28.114775890535832
H	22.693610751627517	14.358613077671713	30.342845841435828
H	17.127434834193664	14.341629019031506	30.440454574689294
H	21.637754028422982	13.201915205421139	32.245734336868438
H	17.332605309916325	13.150510121658098	32.591897345659142
H	19.580657326637194	12.540098620337911	33.487966523408112
C	14.764190342209705	21.269094427578075	20.324134317916812
S	15.614511041498771	19.933702568736457	21.096236929625718
C	13.596978321786271	20.947989318824099	19.629692851681117
C	15.136953415436405	22.644279653722183	20.402083212010016
C	12.782898055294687	21.931558619450215	19.024667672486668
C	14.358804142721718	23.625641340631415	19.825183827914046
C	13.163039823174884	23.313531798224034	19.120708893462350
C	11.600913321419384	21.598038923966044	18.305278938226969
C	12.342009442798066	24.296018545125676	18.510108342269728
C	10.829090039517865	22.576799083904731	17.714814652703293
C	11.198084646423197	23.939851940567404	17.820627280974335
H	13.296822218549666	19.901365156849316	19.550150436220882
H	16.058909703744444	22.904913778913560	20.925147751162864
H	14.664577740141633	24.672007621844784	19.898841119867932
H	11.320980472695830	20.545230489484226	18.223978224407592
H	12.634195901219313	25.345654451771217	18.590626675424428
H	9.929285130676755	22.303242964986598	17.160005162596438
H	10.574387596818845	24.704057727312083	17.354358582917865
C	25.648766155460923	21.187239589920313	20.203898517923104
S	24.449093761954785	19.946867470988739	19.863728910407978
C	26.774142154732818	21.227497262526622	19.381647453302808
C	25.535391973379813	22.152806700027607	21.244159365149866
C	27.775082716625054	22.213376912461072	19.534967458453011
C	26.492860839799935	23.128235359394271	21.413951448338999
C	27.633475576126401	23.201829722412462	20.568628211748909
C	28.919945778681193	22.272013689662238	18.691683704330515
C	28.626199435242345	24.205319650024851	20.699143330326056

C	29.863350582498470	23.267637952200822	18.841141969831668
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H	24.666734148764178	22.108769809548040	21.900380777679057
H	26.375751871271842	23.873038208182493	22.205625513149894
H	29.043932270053421	21.509254169917391	17.919456242894420
H	28.506773292442727	24.956771914439702	21.481292864518064
H	30.728003253846726	23.297404231645555	18.175850371243353
H	30.465716946951886	25.035310272032543	19.955996219097884
Au	20.525009153289211	17.535291375218598	24.987223691857118
Au	17.901769273255237	19.991673587741893	21.709562602426210
Au	22.606919854146550	19.713981892011471	21.328131832485457
Au	20.316845939578041	19.105557921865913	22.734275769479854
Au	21.804029887261986	16.803097175749961	22.005136646622056
Au	19.990133864090183	18.296434701522156	20.088003120436820
Au	20.283428785370447	21.278615061861569	20.801147952913098
Au	20.318122914839481	20.984532771212304	24.693683374097830
Au	18.055091702632858	19.014999089063778	24.521174217427646
Au	22.784561128698016	19.197482936579792	24.204796061482710
Au	18.489056981055921	16.917316141500137	22.399700037290277
C	20.114072569808354	10.986903281045091	24.175013231003486
C	21.328007141407280	10.445643952475649	24.614857237254164
C	21.291685458889717	9.446646896501305	25.596861883975382
C	20.085768407626325	8.969377446192770	26.126097192731532
C	18.892005937404814	9.507298245994813	25.617137017340180
C	18.881587067394609	10.511372760849484	24.646156532432919
C	22.629645420677715	10.883271604163456	23.968675283171457
C	22.754450462255036	10.325365631976869	22.559751064480491
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C	21.035152117536448	10.924192946654999	18.177278856730400
C	20.929473862049530	10.184636777555367	16.997492060623564
C	19.696971856977328	9.922191456180547	16.377934038043595
C	18.544076618591799	10.408467655133885	17.009247822341187
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H	17.796140863771356	6.464912591883633	22.822292770830249
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H	21.513140480999660	10.034180013170396	14.292721260733556
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C	25.138478849309081	16.999030919669174	18.401094762443996
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C	26.531511720509528	15.074140118929238	18.781115315725760
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C	24.055224800644545	16.257417606543207	10.522280350291179
C	23.963202235468177	17.709319486792204	10.072308652229941
C	24.451250921298403	18.785146781726304	10.839033383858640
C	24.130957551157163	20.109802960210445	10.499679323623386
C	23.411478023678320	20.339784017145643	9.317790252991824
C	23.004686262848178	19.306242326096285	8.469978130976610

C	23.279171571685740	17.997986524661140	8.889581102369133
O	25.202826589047085	18.550803530655031	11.999266546262968
C	26.528037924071114	18.093273041533084	11.750730533778325
P	27.449530954077094	18.081785918919241	13.369377942022236
C	24.493265905497267	21.289381297340199	11.392423864037406
C	22.288677080133002	19.550580487731306	7.131959037429771
C	21.023422078097120	18.673076868292895	7.037499530672621
C	20.109067833403454	13.269123508043144	9.198003433538021
C	19.503253387734894	12.102380001266669	10.007114445883133
O	22.554811776549759	16.997156520845689	12.807415788338236
C	23.375988895735762	16.355309563787365	13.800559912836743
C	17.429762236940693	19.786041757042081	10.612012662101778
C	18.121038821008469	20.834771313183001	9.714874553325503
C	21.219660825855605	25.182442760986138	11.259155264267092
C	22.343556724654587	26.230999274449221	11.401491747743648
O	22.912456876767745	20.168998185918703	13.478887961304972
C	23.736638991248373	20.283444388605194	14.646680968341952
C	21.863870778548154	21.017060686996771	6.950726680267387
C	23.247779156689599	19.178217482815569	5.979756097834985
C	18.987682079436350	13.979061271457866	8.407536504977788
C	21.104173368965252	12.675240766010647	8.187578094497512
C	17.060922091710918	18.577659930439513	9.735902836456951
C	16.124364086877861	20.395217704769916	11.169110999778274
C	20.919958750735365	24.952321183102484	9.761479557276314
C	19.951461949557849	25.751065566449192	11.915608322946953
H	27.061020667957088	18.753168913258591	11.040692145998126
H	26.548292695336254	17.067669263573070	11.341917781534546
H	23.157563211056569	21.372223142745160	9.077328824643827
H	22.916302863992144	17.152483663569157	8.301583629633313
H	21.174029286399669	21.341650040118953	7.743168652772050
H	21.345397388371264	21.133294466417770	5.987841674455658
H	22.726860762425325	21.697977230735695	6.943945913650845
H	24.136463732534743	19.825734316909450	5.987102643746960
H	22.745043490487753	19.298709926377047	5.008062468328626
H	23.587283752026266	18.136612891345539	6.062732346454427
H	21.258855461674539	17.601796700581193	7.080999328613367
H	20.505054262866484	18.858582001269294	6.085018609542162
H	20.326662634689594	18.896613147462020	7.857192325160119
H	24.538619211346369	15.653402907906653	9.738894720746877
H	24.675328750654334	16.183887910237875	11.422846729492989
H	22.655786024823250	14.416549739144935	9.080099498305680
H	19.048661506500739	14.456383828736923	11.443694964735046
H	22.751905790879732	15.905941817502518	14.585971221329816
H	24.033384316001598	17.119344429975371	14.227508197788437
H	24.001261485552941	15.564775715872663	13.352841553032995
H	19.401710832509142	14.779413038712876	7.777180940602117

H	18.245380057080013	14.432916234831341	9.078437214248835
H	18.465295948188839	13.265440026766965	7.751847825855371
H	20.589245047150285	11.942292521430998	7.549710286951063
H	21.934676018132837	12.158238631513864	8.689719922907349
H	21.525965945444369	13.445295470299213	7.526279060884461
H	18.719001202259172	12.444048903595688	10.695592376413668
H	20.274544904310222	11.593788405789484	10.603289297502840
H	19.052609975248512	11.361895342699597	9.328932962007306
H	25.075989543395430	22.020993327165939	10.811210588685071
H	25.134119547327174	20.934116194585801	12.208223633516747
H	19.519575891323541	19.711236910213746	16.409292881558386
H	21.190075450923352	19.308772044475823	16.910636765598134
H	18.404687405519919	17.275427129362061	11.377044005446487
H	18.735392389694240	21.429581459087057	12.396565622333043
H	17.950484898992084	18.100889373232331	9.300189716023045
H	16.417481452677460	18.905404249221768	8.906977415640814
H	16.506680081885534	17.815979740317506	10.302462446095381
H	15.576896342724831	19.666261903453758	11.783775261625388
H	15.467243438175259	20.709718063133025	10.343629386475644
H	16.329102416071652	21.274496612780780	11.795134127455029
H	18.349455263872013	21.756434768623482	10.266103790632535
H	17.467814855750891	21.102455286740362	8.870552619719525
H	19.065222507968521	20.446904481143587	9.308878516189610
H	19.719407935321492	21.924749042985159	14.857662103451226
H	21.058499541395335	20.843541859394417	15.227127887888944
H	19.992585875198326	23.643996380423772	13.249683134129633
H	23.434070278993971	23.683481190595863	10.654904110985704
H	24.623856685281943	20.909435924640221	14.452949461521891
H	24.064127418525242	19.270450474573263	14.902346169555155
H	23.182021890844961	20.724099829608491	15.490822616002031
H	20.112751422204902	24.216507311885241	9.637022925474371
H	21.802050641442396	24.576761747855972	9.225079918906612
H	20.604755767713925	25.891951657068727	9.283174563667332
H	19.696238655011690	26.713419413473577	11.449256821982278
H	20.093241178641794	25.929221385608223	12.990987734700632
H	19.087911507574081	25.083165805689490	11.785637070317000
H	23.278667743909821	25.890151392222720	10.938510491710476
H	22.549623362767107	26.443356709765265	12.460310049162215
H	22.053205677381083	27.173436268852345	10.913947802331075
H	18.952782003819436	15.639484825518371	13.465884520664805
H	20.449193472031517	16.134822689026471	14.255417788782418
C	28.891095030480603	17.012310785090069	13.021562677691438
C	29.282722482271815	16.138031896060419	14.046984414021221
C	30.356656225712520	15.267111304221293	13.858560628297401
C	31.043474511785586	15.255738661781542	12.642460418783648
C	30.651351170279742	16.115634671988115	11.613062500882881

C	29.580584046758055	16.991852515298884	11.799154649906384
H	28.724499199787029	16.142555688593568	14.983901307581085
H	30.653833647320411	14.590629903803768	14.661710007921302
H	31.877828397662849	14.569269579635224	12.490642697753385
H	31.174196605043463	16.099285797536112	10.656360923530091
H	29.280283572135772	17.643524534225524	10.975947690953868
C	28.056836794433021	19.791201805421839	13.606311402598918
C	27.617436162592025	20.465023828888285	14.753526255719262
C	28.014043250591737	21.782709877297666	14.990745883371517
C	28.858511621670942	22.431570209530648	14.088009154792836
C	29.315144824635333	21.758405586727275	12.950890540302103
C	28.915035049037222	20.444164169915418	12.708316659542049
H	26.964337694993095	19.939636031117132	15.452303646538555
H	27.667946679319684	22.301392517810385	15.885589466505467
H	29.168379327955041	23.460362403655413	14.275907741296484
H	29.988583970971177	22.259042583690601	12.253631854136041
H	29.293574157935897	19.926937359649951	11.825166207543534
C	17.792796090581643	17.597259570039760	17.356548877420469
C	16.821745283973030	17.853723724949436	18.331905384882315
C	15.466947754926293	17.864779912232464	17.992081145993087
C	15.068883296725673	17.615296240519861	16.679591620535319
C	16.031111662573494	17.352538787758188	15.700007851917228
C	17.383588297793615	17.346727300892088	16.034121672833294
H	17.118453476444692	18.082827814869333	19.356764070450016
H	14.734881228466371	18.091690385059312	18.765924318162298
H	14.010400849600757	17.638612437363896	16.414371407317379
H	15.730891882760252	17.158895503606931	14.669004340623514
H	18.118856367387117	17.156440055223253	15.255687293378417
P	19.562719106000465	17.712543544965659	17.813393046994776
C	20.331586555503542	16.130908166147826	17.295800255927720
C	21.722491116735135	16.028419892592350	17.439522642667665
C	22.398019061746826	14.890004794647968	17.003252062744757
C	21.687589262293926	13.834534051049664	16.424118615188799
C	20.299925721028288	13.915626983991361	16.305412347390345
C	19.622812450664536	15.058010063013413	16.740142119181147
H	22.283647588168229	16.847256132308527	17.889565868615637
H	23.482021806197178	14.837860744660921	17.113101988335799
H	22.211380243354373	12.942803126480150	16.078046706281889
H	19.740112125999921	13.080610908149469	15.882114877549203
H	18.539274049536925	15.113412139569677	16.641977555338222
O	26.653328046032694	17.594528404625692	14.553576439850474

Coordinates of structure 3

Au	19.738775480068401	18.477242799199189	22.195286613790099
Au	19.889222133993936	16.804710218451856	24.295492763513963
Au	17.282695560922669	19.194001776043311	21.116724947810486
Au	22.055068062408758	19.008383149422929	20.728376619266953
Au	21.262771933639105	16.219330124804898	21.518149978335060
Au	19.492663290782900	17.794355052031314	19.503261110163947
Au	19.701451776730188	20.671968989722767	20.419100142011047
Au	19.801604565713561	20.521245371472272	23.931048148281512
Au	17.403588141803226	18.300755090289634	23.909643212713103
Au	22.203537905554530	18.489749157058380	23.671042074951849
Au	18.013049716352857	16.302787035876150	21.723567223757374
O	19.903342626733913	15.795524919577533	26.181593770587394
O	19.519373970942489	14.524354037197314	26.280739743410731
C	19.646885015023930	10.489658628290426	23.677956059848476
C	20.868506134819114	9.958116829589850	24.110918971265338
C	20.847634890438364	8.946573134498125	25.082905529997809
C	19.648734589578304	8.441242211679947	25.604432848173651
C	18.447366503978202	8.964956858163911	25.095933217294096
C	18.421374091711431	9.984149139808563	24.139173926780774
C	22.158795531398869	10.421930583282759	23.458786297251439
C	22.274222385743030	9.870921111053418	22.045287084610671
C	22.142333591152756	10.672835705075348	20.886906380325275
C	22.142973463253941	10.059019853293686	19.615359671545207
C	22.336607231724482	8.671343523722351	19.539999602163970
C	22.498232764550202	7.854991125452532	20.658217948302315
C	22.457152516680264	8.494048441570746	21.902595186585550
O	21.941300166091061	12.039079835302044	21.096892742183979
C	22.737375693656059	12.941718003771939	20.353497541143536
C	21.885961102142392	10.740693806538998	18.275709541344099
C	20.546254393466270	10.402611557418178	17.648478711829487
C	20.448901627434207	9.672797202478336	16.461089721275837
C	19.215482222806312	9.397832407967948	15.845037895404481
C	18.059622715342318	9.859180352785948	16.488991663765326
C	18.109675058587751	10.581695829654288	17.690374159273404
C	19.364376265996796	10.873267844940885	18.242880896726387
C	16.843783416357216	11.011355815323942	18.410922383523737
C	16.670449717050698	10.278833161527320	19.737211577524103
C	16.840902456808116	10.852427598401434	21.017650950583675
C	16.851832908414341	10.021783684263985	22.156861119481874
C	16.637485556954061	8.646269807593736	21.997183457708157
C	16.416971021246749	8.051797011261913	20.754010536827479
C	16.433775603735256	8.903649789377337	19.645945279181895
O	17.107284899782726	12.215169291051426	21.210687003764008
C	16.144549640315038	13.147170915558046	20.743765349506468
C	17.128994401629864	10.533574453057872	23.562212878685727

C	16.219613507620355	6.540742242025943	20.562781251400025
C	17.341779962405909	5.992661896501294	19.654023055625146
C	19.178343149761655	8.618027646406105	14.519493467588143
C	19.963728179792284	9.396435637181646	13.441038312186668
O	19.456390738080600	11.560856480348662	19.432278159137734
C	19.421401654743931	12.988715096160279	19.320730298806886
C	22.696664214597160	6.334897529812183	20.555562882998078
C	21.641054551071420	5.609523434581461	21.417398988694565
C	19.604344946838360	7.340817427720556	26.679456882888775
C	18.787070915605078	7.832578644663807	27.894121628603475
O	19.633899719211659	11.500846944366858	22.739939785411664
C	19.735473953116244	12.799290847653669	23.348332648023113
C	16.273207674272243	5.774265160063575	21.893507273348249
C	14.851316622130510	6.272722363917610	19.901324751012258
C	19.831269356508376	7.233048001005478	14.718943469949261
C	17.746413824359500	8.404913059169965	14.004979052085181
C	22.553691260904877	5.831373279096907	19.111078371624195
C	24.106334111176466	5.967798505483077	21.066220691934443
C	18.934372530673656	6.079722179320750	26.093814793973383
C	21.004299279050745	6.949695846240266	27.178260596048887
H	15.127948813200513	12.732670220253045	20.841330033359249
H	16.310591487731465	13.434469645538822	19.692056579119363
H	16.670395293419375	8.033476784748935	22.898107461463603
H	16.314700889608797	8.486910918928501	18.643064435190194
H	17.247627567519267	5.889465130952632	22.388476308394473
H	16.118810896236958	4.702058090546696	21.707409063954184
H	15.491511190684960	6.106288547636276	22.591516292797952
H	14.033609166283437	6.643581781162171	20.535434167267450
H	14.705234121463628	5.192849301826184	19.745045873182747
H	14.766001369562494	6.767990857246063	18.924516677995619
H	17.338782210633362	6.473661708867584	18.666754700955071
H	17.222486609030248	4.909038380107281	19.504162714886061
H	18.327729005541578	6.167384642274922	20.106431892741568
H	15.982503390638836	10.789805080842170	17.760725076215074
H	16.856575346314742	12.096115722124944	18.547582215544892
H	17.077977762873413	9.654924471610062	16.059667516932034
H	21.374343526602672	9.320288786939200	15.998143444844667
H	20.254776607336158	13.364723992559755	18.709541940325188
H	19.498552251250910	13.380333092925355	20.337216464160349
H	18.485427758075812	13.345534576350408	18.863094118314059
H	19.280102612431570	6.643733412079972	15.465490942510316
H	20.870343094904150	7.318093887578200	15.063421894767382
H	19.836923788708013	6.671795275293248	13.772262505412849
H	17.770179947761967	7.829287805752552	13.069181276655613
H	17.243580674392700	9.358717575143737	13.791630839824226
H	17.131046114017376	7.844676862993452	14.723180155328038

H	21.014905083415432	9.538641407109074	13.726446862393862
H	19.522850982854951	10.389088079379190	13.272138240537133
H	19.946077365569700	8.850437859414727	12.485640468736827
H	16.298480099378288	10.240691747852978	24.221752069659271
H	17.159434540162611	11.627399715953711	23.548685602118692
H	22.285283503904115	13.215445755975367	19.386790271698612
H	23.728565198292326	12.506194852153399	20.159685336321608
H	22.320983628799734	8.230080817261600	18.542897871870782
H	22.549404556229121	7.908002915664157	22.820649069207711
H	21.563361229134117	6.067272560801532	18.695237721619971
H	22.678523197572467	4.739684302239864	19.086205757401327
H	23.316777542400128	6.264874812617491	18.449236393294576
H	24.881819151887623	6.455342130044327	20.457953727763755
H	24.264794561083793	4.880003718977314	21.015885815968517
H	24.250980559188772	6.282802914094382	22.108309484636418
H	21.725817862444984	5.877716997131918	22.478355028100523
H	21.764268491699880	4.519159348853976	21.335022040136266
H	20.624974946204301	5.866217732264243	21.088077706652495
H	23.007773186917792	10.055957581802781	24.055851453673387
H	22.223633554963474	11.514451212081813	23.440537031667400
H	21.803692144603211	8.556286679646067	25.436133381161614
H	17.492302920685351	8.580127177131645	25.462722048506066
H	18.922784084162693	12.967939323176926	24.067263704712097
H	19.680491344882903	13.540634016013156	22.543333575892959
H	20.686914311050138	12.916062028640042	23.886352169438389
H	19.512469557234496	5.691602952317483	25.242942024205814
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H	15.796010188860656	20.819951808419788	27.700755080692925
H	16.850229678354783	20.866695721808309	29.923865543247850
H	18.103752895306748	18.883646009711075	30.766441919454220
H	18.307574453789147	16.849279565342513	29.328248395096427
H	17.307436539672121	16.809465615739771	27.084245024987087

P	15.727565884146413	18.649326853932173	25.568499513593952
C	14.713773513867451	20.147203851745907	25.202494577111143
C	13.731884674250594	20.663230410426603	26.066109408556962
C	12.917404750422756	21.721388287720817	25.658863432509936
C	13.077968656701024	22.291621198306654	24.392196061898840
C	14.062592985095160	21.798536529981991	23.533630361555936
C	14.872314734029947	20.731944774936082	23.934653799971390
H	13.577123970209092	20.230606397724500	27.053123088762252
H	12.152312937391553	22.102374592169646	26.338066680455221
H	12.441298249839711	23.121141642369338	24.078691991268020
H	14.205281119066280	22.239082073912058	22.544654767738983
H	15.634365774070602	20.337193198313994	23.251734301901465
C	21.960579845971321	20.912570962793787	12.449918839302926
C	20.747090963306611	21.473268350345034	12.874378619686567
C	20.346060936947055	22.698559159351543	12.321864225914471
C	21.101348427144355	23.362206608940735	11.347207579089048
C	22.285616891072539	22.740222687545554	10.917078164289856
C	22.730741607780512	21.523224123135520	11.443674847640855
C	19.866502561345335	20.725848293168525	13.859148981276622
C	19.142533134326261	19.567814606134998	13.179011016937631
C	19.345425876314053	18.214421550395638	13.520905331440925
C	18.934050370214536	17.201872607710580	12.629311211882696
C	18.171824929939302	17.554417646604488	11.509007037690084
C	17.811540819767711	18.875208126154703	11.225915673947100
C	18.336317665014036	19.859053596335968	12.072352103510948
O	20.031622511547557	17.813707144680876	14.666190567100056
C	19.721569159816557	18.404157990504775	15.934315664579204
C	19.329542923501972	15.743468483395427	12.814598114141260
C	20.126403000519414	15.194522431884135	11.645841186842031
C	19.574976166318180	14.274860467950399	10.745163376053053
C	20.289521592669619	13.774192670698717	9.643312364912140
C	21.582923975551424	14.272375679056056	9.437395342187870
C	22.171007454151361	15.202713719524048	10.304866404174000
C	21.446316814506527	15.625562722692734	11.428909205062297
C	23.544489028512555	15.794871111079145	10.035041571767806
C	23.454653826426846	17.246732607193309	9.579674823574690
C	23.933828406125926	18.324409039191988	10.350254515077831
C	23.620527062933611	19.648220267118738	10.003611745661621
C	22.919557900336475	19.878973349300374	8.811989680632314
C	22.519040607264728	18.844315851285899	7.962828799292731
C	22.784708527527769	17.535393784835026	8.387620345453408
O	24.674408432208448	18.098915478426047	11.520551693533109
C	25.996890669804980	17.631344711568680	11.288618878806371
P	26.910457785756403	17.588628025487118	12.909423560658601
C	23.968541632013302	20.831182887926879	10.896368341451735
C	21.824385488993620	19.098381659581211	6.616834451466387

C	20.549483751353844	18.237696578657726	6.489184891381973
C	19.639726940349686	12.757628562090112	8.688238962007059
C	19.014892754480194	11.592234158153428	9.483374682467220
O	22.027285615208317	16.529274726463722	12.295864783542360
C	22.816762452335510	15.907852967098647	13.325618059423112
C	16.918415323750732	19.263250834331394	10.036564618398064
C	17.623748916888466	20.319388123168295	9.158173998410694
C	20.663680185226095	24.697866447966721	10.721369800751619
C	21.795809094812519	25.738198677406796	10.863609806741206
O	22.364676619396537	19.692280287107316	12.962007251745575
C	23.219634886467489	19.792990896818246	14.106932507177669
C	21.411409874622091	20.569400500425825	6.444160689428741
C	22.802015637345850	18.723929526510055	5.480700561817699
C	18.533016426121069	13.464786425126354	7.874382588714204
C	20.654552250835984	12.158844515226301	7.700921716154073
C	16.580472526110640	18.055680727131481	9.147005638095406
C	15.592897916056184	19.851737153946960	10.567022964856195
C	20.358452492387070	24.477287494161754	9.223681440271106
C	19.403680966769919	25.274541524643585	11.388069319057786
H	26.540469053336789	18.282825790838583	10.578044044157682
H	26.015637952390346	16.604446338724568	10.882462256801288
H	22.680113581249895	20.912271607703072	8.560972946804611
H	22.429984083641724	16.690994882986359	7.792786886275154
H	20.731014325667648	20.895726816271456	7.244343671247107
H	20.887323393982836	20.692519176620781	5.485244290450821
H	22.278303761945327	21.245655098403414	6.436608606204389
H	23.714855808161030	19.334592186197874	5.533581571931807
H	22.334604212183628	18.888316897422943	4.498157984913590
H	23.100108636435909	17.668279510824910	5.543041344431119
H	20.761886789823382	17.160965700905376	6.530660859862444
H	20.056871861318438	18.441398263554746	5.526946898047267
H	19.837169536181090	18.469316865820854	7.292743222773916
H	24.046211248940057	15.190525969109711	9.263214063077459
H	24.150013328536851	15.727878743357472	10.945359541078654
H	22.168563237721269	13.933397405302836	8.581260077087032
H	18.552645412142656	13.934067537507133	10.927111274222073
H	22.172849944359260	15.487586029374045	14.110603927656362
H	23.468552768462480	16.680164537943377	13.744450696366082
H	23.448726211929593	15.102927012372426	12.915622903317869
H	18.948754558835208	14.299084366261937	7.291536421580746
H	17.748324865691433	13.870411408340056	8.528162166785791
H	18.061966662187846	12.758737387737844	7.173044838710416
H	20.153429409043227	11.413539192721512	7.067048010264385
H	21.480868853598931	11.657628463530836	8.224800133531737
H	21.081255339427411	12.920826647831969	7.034076430936050
H	18.231213954530833	11.934719359218507	10.171375232293022

H	19.774722026214118	11.064843675842551	10.076962104263055
H	18.554503946432582	10.869134683263713	8.793390880265893
H	24.544630021585128	21.565891157134821	10.313786064183935
H	24.612963255216290	20.486034675610490	11.713479236025806
H	18.962192614883392	19.195089323432068	15.854946251678411
H	20.643392932897683	18.835660904928929	16.352723674507249
H	17.873886503463108	16.747298526819009	10.838735243978835
H	18.168225483900802	20.912395347026905	11.839110252228830
H	17.482821518642709	17.590250334094979	8.725140490207723
H	15.945370796888353	18.377823872021875	8.309131629037266
H	16.027626891787502	17.284365197608228	9.701757247673006
H	15.056220716610740	19.113952761143914	11.180364706877556
H	14.938879071627996	20.142683220923221	9.730398749533538
H	15.766095420098312	20.740918289996767	11.188506453329426
H	17.858741309511483	21.233992991672395	9.719093393112335
H	16.976542643305486	20.602607575424539	8.314206189183839
H	18.565785475269333	19.925870401303818	8.751984728920634
H	19.139795505078695	21.429259520526603	14.291818616210337
H	20.481814037489034	20.356098932809445	14.684503610632754
H	19.408298576901878	23.130238737113064	12.674425134680600
H	22.889432548517458	23.213400889520514	10.138505540454881
H	24.125304821618265	20.382187750968519	13.886748091550412
H	23.515456323138419	18.771410491603124	14.367669696030205
H	22.699624143300206	20.264983613337154	14.956174069332258
H	19.546861127384197	23.746845400783815	9.091074275772611
H	21.239593583547471	24.099774551903359	8.686302567069799
H	20.052814518663645	25.421854361924908	8.748179081960256
H	19.145871792601433	26.236263108998401	10.921253236804027
H	19.555618293020800	25.457621475607457	12.461546452865607
H	18.534691954551612	24.611291310613709	11.272213587454550
H	22.708906863258655	25.424462763983762	10.340621815072510
H	22.051085283884195	25.897894065814423	11.920477592644650
H	21.484553437562308	26.703750807235121	10.438411065009623
H	18.425887829101477	15.123902672185002	12.930431852990976
H	19.903631407402425	15.643490358525474	13.740915857883831
C	28.337567293286885	16.513093003389145	12.521983509682212
C	28.716582373742110	15.596995721763165	13.513777819087155
C	29.782613892380851	14.724143764361056	13.291899887793893
C	30.470150243651712	14.750740711051471	12.076794592543061
C	30.091782799525330	15.654939773307198	11.081203814789601
C	29.030949127665234	16.534842043347755	11.301429163652221
H	28.151555118518520	15.565970545648302	14.447178346688093
H	30.074502806433554	14.018175983002026	14.070110818596131
H	31.299155303366327	14.063508435789442	11.903169155084743
H	30.623450613627242	15.673772283221629	10.128987333542035
H	28.745081781479417	17.230587890618537	10.510297651995604

C	27.559991882454842	19.274198434206689	13.198913530067076
C	27.227669281312309	19.885664237594984	14.415992007708546
C	27.710509461634796	21.161350461246172	14.714664719117742
C	28.529057066834916	21.832460822341396	13.803819249803359
C	28.864097239883694	21.226646071460895	12.589542685295227
C	28.382012611985456	19.953007664873418	12.286814660177551
H	26.591856542811179	19.342906056250577	15.117355497063102
H	27.452466173041966	21.632671281732055	15.664425968730900
H	28.909451312466803	22.827471324890098	14.040593119788813
H	29.507409538014066	21.745974506719282	11.877771659429504
H	28.663230849557237	19.491276505342054	11.338583415568047
C	17.285549470989299	17.070943694350767	16.825750902661124
C	16.340570712517241	17.399382661864404	17.809574188574405
C	14.978188308054859	17.426238150616232	17.501678319422837
C	14.543051875795078	17.113850956900436	16.213639802158450
C	15.477332575727232	16.782404448200065	15.227664690727350
C	16.839541661961764	16.766127781621485	15.527056622665228
H	16.673383136547866	17.662312293875342	18.819941833701321
H	14.259574594017334	17.691201362010016	18.277925330841729
H	13.478793646215507	17.133440746971303	15.971949937014365
H	15.145958858097918	16.546098153954059	14.215141518990563
H	17.552173503486994	16.535222811486566	14.737502961105445
P	19.064003469619102	17.205448351546064	17.257563696311653
C	19.889126020462548	15.647868180623652	16.762592909545891
C	21.276442716410372	15.593556623029185	16.973841293326792
C	22.011436710130468	14.479304410663680	16.573474593430561
C	21.363644756444135	13.396646818883760	15.970622453774443
C	19.979492808415834	13.424572862911411	15.795966032201955
C	19.242862033032427	14.545064789854687	16.189010426010192
H	21.783323762196531	16.430438174589057	17.456649182610072
H	23.091233215704928	14.461485811707963	16.728997422658519
H	21.932163640340537	12.521130471933033	15.654988622738321
H	19.469976759995422	12.565088063318665	15.356952982694049
H	18.161548163207687	14.555577684490407	16.050137256967311
O	26.112834006407290	17.089227931783817	14.087927445243190

Coordinates of structure 4

Au	19.212204112994471	17.998069691037902	21.619105258239802
Au	19.404673008624503	16.296292298853221	23.716701847956259
Au	16.789432620835370	18.732081674827285	20.688710953141115
Au	21.507778630209334	18.614468064625413	20.308844890502979
Au	20.808881917694617	15.790208996744145	20.997329356444276
Au	18.994981208558290	17.328580794397354	18.933622793599945
Au	19.183430788778040	20.262948922369969	19.919673012915954
Au	19.292377410753264	20.064516835485712	23.389409631054008
Au	17.004790839491193	17.895433658528763	23.477120542738447
Au	21.690681002272953	18.002377338983074	23.126652184564943
Au	17.482840634643807	15.813481891918803	21.294675493663064
O	19.469983930456621	15.312727836831243	25.663173552438892
O	19.455328390409690	13.991459335522721	25.730375489935966
O	14.891499344939419	19.699270464065837	20.216221725114220
O	14.151108517547033	19.299100204053332	19.196995632994177
O	23.364982424155340	19.559707582614042	19.688725405205069
O	24.011248191300972	19.135028411798586	18.619116240043525
C	19.117792694955970	10.001965420440497	23.140844496398575
C	20.341718692526392	9.463697530280694	23.556138703036101
C	20.325543489911261	8.456320406196795	24.530477553614080
C	19.133769881260104	7.963389148868671	25.077319407168346
C	17.927370439940027	8.489839697467515	24.584110128680233
C	17.896441785026052	9.501383542588256	23.619595353331508
C	21.634308734390682	9.913844505225967	22.897975049706158
C	21.752730649687788	9.352299888032741	21.488689825545222
C	21.631343164004726	10.157735458611842	20.332061839675756
C	21.619490699398316	9.542282110536911	19.062206648726704
C	21.795935857196479	8.151119771219506	18.985121110178419
C	21.956778662638271	7.331956672081415	20.101725314841893
C	21.925762253549177	7.973125567163388	21.346077534608551
O	21.443656416692455	11.529183609691550	20.546937566704241
C	22.265575463846165	12.432290095194722	19.832667549729646
C	21.368222999430017	10.237560283155043	17.730030321626661
C	20.027677293960007	9.912278285209780	17.100970650172535
C	19.929938587458423	9.182632763022198	15.913338457132166
C	18.698507428382726	8.898442935696092	15.299268949760997
C	17.539574355886341	9.347513464149472	15.948207060464757
C	17.590513531750332	10.076344493265131	17.146238198905312
C	18.844255825578166	10.378011213837270	17.695077141624324
C	16.332260844731262	10.502537169871648	17.882477069255209
C	16.176940154044519	9.771291741404120	19.211736546699086
C	16.337711306615294	10.346750327551332	20.493491107816983
C	16.347992580944332	9.515998720289840	21.632386927258686
C	16.162685448258124	8.135616707426879	21.472178350905796
C	15.959812158368486	7.538799239789599	20.227839798201771

C	15.965282161864819	8.391983075867216	19.120045787604752
O	16.604526172909978	11.709073368024058	20.694838874870847
C	15.659773682864433	12.648347258192150	20.208188968405846
C	16.598186309961473	10.031447277315186	23.041458793823164
C	15.776632107556180	6.027592296456749	20.031136313236789
C	16.871414115025438	5.497952628635433	19.078822594553781
C	18.669972875184797	8.122227183238222	13.970685596901056
C	19.469082763858431	8.900333702799948	12.901891126264214
O	18.923454906801602	11.077399860253795	18.880487514113465
C	18.897494467855484	12.503017904186395	18.746803338118827
C	22.153236719969474	5.810250898341047	20.002964248759980
C	21.118202008767572	5.083933256480893	20.888996479387998
C	19.115814895289333	6.867556063219130	26.155440618527354
C	18.274289548724980	7.329254349150520	27.364103902217746
O	19.101682126035534	11.017111202238116	22.206705953107488
C	19.181208795237310	12.309529107634630	22.827925241132778
C	15.878400492088591	5.247059633633024	21.350766088248410
C	14.389557700844435	5.756998316690651	19.410541686811484
C	19.312848575326470	6.731483695168697	14.165217253435269
C	17.242508595320906	7.912133493286515	13.444595181069063
C	21.989313184615813	5.295302119428590	18.563581610328100
C	23.571467996646110	5.446588973782365	20.491606815780603
C	18.491348273674880	5.583973016279971	25.564788890490064
C	20.525400868361565	6.525486747763093	26.664708655525853
H	14.637841247539276	12.241907411050851	20.273014636284802
H	15.854963898512983	12.940688808959504	19.161742251519296
H	16.202918525669741	7.521538168447437	22.372444366363567
H	15.856312233983246	7.970947846078527	18.117745201576515
H	16.856771989739837	5.382365924622906	21.833990757928341
H	15.749358896842885	4.172977377474792	21.152087907894224
H	15.098944404763042	5.547123113256228	22.065854023179533
H	13.586045728674277	6.109218792829567	20.073627176281253
H	14.248957398280377	4.678665480560731	19.243999616546809
H	14.274414592786833	6.267290733893119	18.444775369179233
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