

Au_n⁻ structures (xyz format)

Au₁₄⁻

(1)

-1.3531730	-4.6918500	0.0000000
-2.7680609	-2.3763720	0.0000000
0.0000000	-2.3503800	0.0000000
2.7680609	-2.3763720	0.0000000
-4.0361878	0.0000000	0.0000000
-1.3457792	0.0000000	0.0000000
1.3457792	0.0000000	0.0000000
-2.7680609	2.3763720	0.0000000
0.0000000	2.3503800	0.0000000
4.0361878	0.0000000	0.0000000
2.7680609	2.3763720	0.0000000
-1.3531730	4.6918500	0.0000000
1.3531730	4.6918500	0.0000000
1.3531730	-4.6918500	0.0000000

(2)

-1.9399407	1.7071562	0.5567711
0.2425764	-1.4171877	-1.5155867
-2.4630036	-0.5965925	-1.0566404
2.4630036	0.5965925	-1.0566404
-1.3663504	-0.2038336	-3.4913679
-0.2425764	1.4171877	-1.5155867
-3.4138448	-0.4275982	1.4978609
3.4138448	0.4275982	1.4978609
1.9399407	-1.7071562	0.5567711
1.2633478	-0.4731952	2.9918145
0.7704219	1.3573041	1.0171484
-1.2633478	0.4731952	2.9918145
-0.7704219	-1.3573041	1.0171484
1.3663504	0.2038336	-3.4913679

(3)

5.4188505	1.5428127	0.0000000
4.0251533	-0.6968936	0.0000000
2.7428072	1.7590457	0.0000000
1.3429523	4.0675446	0.0000000
2.7115823	-3.0301809	0.0000000
1.3166689	-0.6695594	0.0000000
0.0142694	1.6976518	0.0000000
-0.0035770	-3.0726709	0.0000000
-1.3727593	-0.6544999	0.0000000
-1.3994094	4.0131685	0.0000000
-2.7682975	1.7083858	0.0000000
-2.6435063	-3.0686322	0.0000000
-4.0946086	-0.6039958	0.0000000
-5.2901259	-2.9921764	0.0000000

(4)

0.0000000	-3.7132709	0.0000000
-2.4289019	0.0000000	-1.4084095
2.4289019	0.0000000	-1.4084095
0.0000000	1.3550147	1.4538734
2.4289019	0.0000000	1.4084095
0.0000000	-1.3550147	-1.4538734
0.0000000	1.3550147	-1.4538734
2.3629985	2.3436306	0.0000000
-2.3629985	-2.3436306	0.0000000
2.3629985	-2.3436306	0.0000000
0.0000000	3.7132709	0.0000000
0.0000000	-1.3550147	1.4538734
-2.3629985	2.3436306	0.0000000
-2.4289019	0.0000000	1.4084095

Au₁₅⁻

(1)

2.9287755	1.4234984	1.1132398
0.4660565	2.4501806	0.8436842
4.3188831	0.7435294	-1.2345416
2.8220654	-1.1703115	0.0097874
1.6484988	0.9749134	-1.4749835
0.1098961	-1.2777510	-1.1749359
-2.0232055	3.3202365	0.2152667
-1.0213127	1.2025877	-1.3510222
-1.8347563	0.8092186	1.3968310
1.0104078	-3.0017929	0.7415589
-2.6668036	-1.1674417	-0.9600408
-3.6952323	1.2926245	-0.7094070
-1.3909430	-3.5868961	-0.5836145
0.7673321	-0.2021742	1.6530003
-1.4396620	-1.8104217	1.5151773

(2)

0.0000000	3.6664597	-0.1045550
-1.4717521	0.0000000	-2.7311063
-2.0158364	0.0000000	2.0291293
1.5234535	-1.3586476	-0.3284401
2.0158364	0.0000000	2.0291293
-1.5234535	1.3586476	-0.3284401
-1.5234535	-1.3586476	-0.3284401
0.0000000	-1.9516760	2.0156179
0.0000000	2.3378609	-2.5201876
0.0000000	1.9516760	2.0156179
0.0000000	-3.6664597	-0.1045550
1.5234535	1.3586476	-0.3284401
0.0000000	-2.3378609	-2.5201876
1.4717521	0.0000000	-2.7311063
0.0000000	0.0000000	3.9359636

(3)

0.7783122	1.4736035	0.0000000
-0.5563069	-1.2969380	1.3360530
0.7133410	0.8285652	2.7371484
-3.2811174	-0.8101928	-1.3270735
-1.7465742	-0.1390212	3.5641974
-1.6490576	1.4782714	1.3183881
3.0085019	0.5992288	1.4184232
-1.7465742	-0.1390212	-3.5641974
-0.5563069	-1.2969380	-1.3360530
0.7133410	0.8285652	-2.7371484
-1.6490576	1.4782714	-1.3183881
3.0085019	0.5992288	-1.4184232
1.7679524	-1.5506492	0.0000000
-3.2811174	-0.8101928	1.3270735
4.4761616	-1.2427812	0.0000000

(4)

1.4175987	1.4009884	1.9440072
0.0000000	1.5184246	-0.4417910
-1.4175987	-1.4009884	1.9440072
-2.7662614	-1.4313063	-0.3331256
-1.3308022	0.0000000	-2.4325874
2.7662614	-1.4313063	-0.3331256
2.7662614	1.4313063	-0.3331256
-4.0238750	0.0000000	-2.2891400
-2.7662614	1.4313063	-0.3331256
1.3308022	0.0000000	-2.4325874
4.0238750	0.0000000	-2.2891400
0.0000000	-1.5184246	-0.4417910
0.0000000	0.0000000	3.8835100
1.4175987	-1.4009884	1.9440072
-1.4175987	1.4009884	1.9440072

Au₁₆⁻

(1)

-1.3614307	-1.3614307	-1.3891778
1.3614307	1.3614307	-1.3891778
-0.9539033	0.9539033	-2.9481995
-1.3614307	1.3614307	1.3891778
-0.9073815	2.8696894	-0.9890422
-2.8696894	0.9073815	-0.9890422
0.9539033	-0.9539033	-2.9481995
-2.8696894	-0.9073815	0.9890422
0.9539033	0.9539033	2.9481995
2.8696894	0.9073815	0.9890422
-0.9539033	-0.9539033	2.9481995
1.3614307	-1.3614307	1.3891778
-0.9073815	-2.8696894	0.9890422
0.9073815	-2.8696894	-0.9890422
2.8696894	-0.9073815	-0.9890422

0.9073815	2.8696894	0.9890422
-----------	-----------	-----------

(2)

-0.8034898	1.1975081	2.0772828
2.2875113	0.9267522	-0.5250575
1.8994657	1.3444370	2.2366061
-0.5708942	-2.9579698	0.4542986
3.4026561	-0.8014202	1.3301672
0.8034898	-1.1975081	2.0772828
0.5708942	2.9579698	0.4542986
-1.8994657	-1.3444370	2.2366061
-0.4585452	-2.2127231	-2.1644297
1.3833750	-0.2874016	-2.8300924
-2.2875113	-0.9267522	-0.5250575
-1.3833750	0.2874016	-2.8300924
-3.4026561	0.8014202	1.3301672
-1.7679771	1.8610322	-0.5787752
0.4585452	2.2127231	-2.1644297
1.7679771	-1.8610322	-0.5787752

(3)

-2.9834876	-0.3501148	2.7168798
3.5372328	0.8523269	1.1431963
-2.8085287	-1.5032968	0.2518999
1.6735140	0.1616992	3.0574638
-2.1847867	-0.2023330	-2.0237880
-0.5072526	-1.3334584	1.9828784
-1.2886557	1.4843049	-3.9897346
-0.2515521	1.9109378	-1.5355668
-0.7947705	1.2999329	3.1406654
-0.2671899	-1.7813869	-0.7416700
2.2286979	-2.0661052	-1.9017999
-1.8186456	1.0754470	0.5598076
2.2121831	0.6301600	-1.2501405
0.8587270	1.6967077	0.9185900
0.4234999	-0.4425979	-3.1214882
1.9710145	-1.4322233	0.7928068

(4)

-1.0151460	-2.8389054	1.3840331
-0.6978883	1.8494977	3.9901956
1.3714770	-1.4041609	-2.3382753
-1.2145793	1.8768509	-1.3258373
1.4002954	1.2983849	2.3424247
1.3714770	-1.4041609	2.3382753
-1.2586499	-0.5112262	2.7520903
1.1847936	2.7122703	0.0000000
-1.2145793	1.8768509	1.3258373
-1.0151460	-2.8389054	-1.3840331
1.3827659	-2.7386665	0.0000000
-0.6978883	1.8494977	-3.9901956

1.4002954	1.2983849	-2.3424247
1.9647677	0.0006404	0.0000000
-1.7033453	-0.5151262	0.0000000
-1.2586499	-0.5112262	-2.7520903

Au₁₇⁻

(1)

0.0000000	-3.1591209	-0.3396855
0.0000000	0.0000000	2.7061257
1.3602477	-2.3047756	1.9150201
2.1644258	1.4330942	-0.5938636
2.7315017	0.0000000	1.6954932
2.1644258	-1.4330942	-0.5938636
-1.3602477	-2.3047756	1.9150201
2.2908417	0.0000000	-2.9314542
0.0000000	3.1591209	-0.3396855
-1.3602477	2.3047756	1.9150201
0.0000000	1.4195925	-2.4197293
-2.1644258	1.4330942	-0.5938636
0.0000000	-1.4195925	-2.4197293
-2.1644258	-1.4330942	-0.5938636
-2.7315017	0.0000000	1.6954932
1.3602477	2.3047756	1.9150201
-2.2908417	0.0000000	-2.9314542

(2)

0.0000000	3.0499801	0.2007627
-1.4771572	0.0000000	-2.9733961
0.0000000	2.2220255	-2.3829574
2.1345545	-1.5099418	-0.7711930
1.4771572	0.0000000	-2.9733961
2.1345545	1.5099418	-0.7711930
-2.1345545	1.5099418	-0.7711930
3.5673089	0.0000000	1.0099797
0.0000000	-3.0499801	0.2007627
-2.1345545	-1.5099418	-0.7711930
1.4026054	-1.4439278	1.8986377
-1.4026054	-1.4439278	1.8986377
1.4026054	1.4439278	1.8986377
-1.4026054	1.4439278	1.8986377
-3.5673089	0.0000000	1.0099797
0.0000000	-2.2220255	-2.3829574
0.0000000	0.0000000	3.7814433

(3)

1.6780974	-2.0853955	-0.0969397
0.1857396	0.8489222	3.0564982
2.7055715	-1.2689556	-2.5318894
3.4207381	0.1779584	-0.2974415
2.3015464	-0.5025004	2.0642313
-2.7807938	-2.3092053	1.4115525

-0.1473099	-1.7203931	2.0091099
1.4440636	1.1078297	-2.0019715
-0.9342526	2.7941360	1.5424386
-2.3836119	-0.8129753	-0.9166486
-0.1619820	3.0531732	-1.0567408
-2.6546802	1.9080594	-0.4264459
-0.0184415	-1.3645700	-2.3154217
-0.8441664	-3.0674110	-0.3654741
-2.1552698	0.2934634	1.7363360
1.5874802	1.9082060	0.7998897
-1.2427286	1.0396578	-2.6110829

(4)

2.3105970	-2.3105970	-0.3271829
-1.3640015	-1.3640015	2.2661409
1.3640015	-1.3640015	2.2661409
0.0000000	3.2145253	0.7639575
1.3640015	1.3640015	2.2661409
3.2145253	0.0000000	0.7639575
0.0000000	-3.2145253	0.7639575
2.3105970	2.3105970	-0.3271829
-2.3105970	2.3105970	-0.3271829
-3.2145253	0.0000000	0.7639575
0.0000000	2.0102502	-1.7908678
-2.0102502	0.0000000	-1.7908678
2.0102502	0.0000000	-1.7908678
0.0000000	-2.0102502	-1.7908678
-2.3105970	-2.3105970	-0.3271829
-1.3640015	1.3640015	2.2661409
0.0000000	0.0000000	-3.6481907

Au₁₈⁻

(1)

0.0000000	-1.5184236	1.3911964
0.0000000	1.5184236	1.3911964
1.3913810	0.0000000	3.3060629
1.6117469	0.0000000	-0.8204104
2.7637954	1.3978345	1.3165273
2.7637954	-1.3978345	1.3165273
-1.3913810	0.0000000	3.3060629
1.4772793	-2.7753522	-0.6446714
0.0000000	1.3368871	-2.6719029
-1.4772793	2.7753522	-0.6446714
0.0000000	4.0323722	-2.5486577
0.0000000	-1.3368871	-2.6719029
-1.6117469	0.0000000	-0.8204104
0.0000000	-4.0323722	-2.5486577
-1.4772793	-2.7753522	-0.6446714
-2.7637954	-1.3978345	1.3165273
-2.7637954	1.3978345	1.3165273
1.4772793	2.7753522	-0.6446714

(2)

0.0000000	-3.2075725	-0.0283754
0.0000000	0.0000000	2.8982286
1.3751578	-2.3339099	2.1873962
2.1057056	1.4123885	-0.3307316
2.7210305	0.0000000	1.9655795
2.1057056	-1.4123885	-0.3307316
-1.3751578	-2.3339099	2.1873962
2.1964499	0.0000000	-2.6878045
0.0000000	3.2075725	-0.0283754
-1.3751578	2.3339099	2.1873962
0.0000000	1.6053387	-2.1854588
-2.1057056	1.4123885	-0.3307316
0.0000000	-1.6053387	-2.1854588
-2.1057056	-1.4123885	-0.3307316
-2.7210305	0.0000000	1.9655795
1.3751578	2.3339099	2.1873962
-2.1964499	0.0000000	-2.6878045
0.0000000	0.0000000	-4.4527682

(3)

-0.0002036	2.0630560	1.7874684
2.4360450	-0.9727926	0.0000000
2.2062955	0.4728552	2.3506741
-1.2227013	-2.1282337	1.4038173
1.4150139	-2.1381341	2.3608001
-0.3612757	-0.2310187	3.2171271
2.1581899	1.8290670	0.0000000
-2.2767911	0.4861891	1.4048824
-1.2227013	-2.1282337	-1.4038173
1.4150139	-2.1381341	-2.3608001
-3.5352444	-1.5209530	0.0000000
-0.3612757	-0.2310187	-3.2171271
-1.9674951	2.8344314	0.0000000
-0.0002036	2.0630560	-1.7874684
2.2062955	0.4728552	-2.3506741
0.8437149	-3.3206889	0.0000000
-2.2767911	0.4861891	-1.4048824
0.5441144	4.1015085	0.0000000

(4)

-3.2417850	1.1444571	0.0000000
0.9182183	2.3884164	0.0000000
-1.4903719	2.7887185	1.3677253
0.7054398	-1.1417531	2.1240617
0.4999654	1.5437012	2.6943433
-1.8373047	0.1453984	2.1760557
-1.4903719	2.7887185	-1.3677253
-1.6229932	-2.6052370	2.2880093
2.4140908	-1.7677664	0.0000000

2.6733515	0.6890664	-1.4043519
-0.0903589	-2.7727468	0.0000000
0.7054398	-1.1417531	-2.1240617
-2.6217051	-1.4942438	0.0000000
-1.8373047	0.1453984	-2.1760557
0.4999654	1.5437012	-2.6943433
2.6733515	0.6890664	1.4043519
-1.6229932	-2.6052370	-2.2880093
4.7653659	-0.3379050	0.0000000

Au₁₉⁻

(1)

2.3273884	-4.0311549	1.4213537
2.3273884	4.0311549	1.4213537
-4.6547767	0.0000000	1.4213537
-0.8811173	1.5261400	-0.8860639
0.0000000	0.0000000	1.6636550
1.7622347	0.0000000	-0.8860639
-0.8811173	-1.5261400	-0.8860639
0.8008877	-1.3871781	-3.1291692
1.6115961	-2.7913663	-0.9221156
-0.0621225	2.7856955	1.4807217
-3.2231922	0.0000000	-0.9221156
2.4435443	-1.3390481	1.4807217
2.4435443	1.3390481	1.4807217
-1.6017753	0.0000000	-3.1291692
-2.3814219	-1.4466474	1.4807217
1.6115961	2.7913663	-0.9221156
0.8008877	1.3871781	-3.1291692
-0.0621225	-2.7856955	1.4807217
-2.3814219	1.4466474	1.4807217

(2)

-1.2507438	-1.2341410	-0.0004481
-0.1857855	1.3375084	-1.4257844
-2.9303015	0.4414817	-1.4601227
-0.1876366	1.3369203	1.4262851
-2.0267368	2.7456702	-0.0007011
-2.9318619	0.4410564	1.4573875
-1.1934423	-1.0678845	-2.7890741
-4.6854276	1.8741606	-0.0021084
-1.1960811	-1.0681608	2.7878667
0.6845696	-2.5934352	-4.0363679
2.5744667	1.7335471	1.4316621
2.5761536	1.7333445	-1.4296207
3.8411143	3.5743250	0.0016627
1.5668410	-0.3378169	2.8035002
1.6778531	-0.4951892	0.0007948
0.6810487	-2.5932211	4.0368770
0.7078260	-2.7452860	1.3417818
0.7090733	-2.7451908	-1.3413403

1.5690710 -0.3376888 -2.8022503

(3)

-1.0983665	1.8549143	3.5234793
0.9316547	2.1321327	1.6687185
-1.7469553	1.8612205	0.8616526
0.2827542	-0.4922898	2.8112764
-2.4431149	-0.3624894	2.4356132
2.8199234	0.0282035	1.8577393
0.2996715	2.5827955	-1.0409086
-2.6354125	-0.5738308	-0.3040136
-2.2349895	1.7027878	-1.8007455
-1.0547400	-2.4170019	1.1490964
0.2987924	-0.0743681	0.0233340
2.7844600	1.5910679	-0.4049407
1.6712871	-2.4532026	1.3062290
3.1194296	-1.1769550	-0.6629958
1.5501800	0.1629196	-2.4955313
-0.2489901	1.8850606	-3.6526781
-1.0449643	-0.7146825	-2.6136288
-1.9757780	-3.0710417	-1.3326301
0.7251582	-2.4652406	-1.3290660

(4)

3.1394159	3.1071051	0.0292131
-3.9733932	1.9688878	1.2335276
0.8912333	-4.3759246	1.9674242
-1.3661563	-1.1223164	-0.5470252
0.2335385	0.1385404	1.7017041
0.4283331	2.3570198	-0.4816486
1.6123534	-1.0324450	-1.2856045
-0.0684775	0.7508985	-2.6587026
2.4956952	1.4396725	-2.0847561
-2.5132105	-0.2056496	1.7944769
0.3106115	-3.3745624	-0.5649560
1.3500752	2.6276250	2.1044037
-1.3471570	2.4231961	1.6801416
-0.3485774	-2.0660720	-2.9320221
1.9795438	-1.9889333	1.3093628
-2.2057007	1.5123513	-0.8660049
-2.5135113	-0.2942901	-2.9899149
2.7966337	0.5129892	0.7069933
-0.9012496	-2.3780922	1.8833876