

Spin and Structural Features in Oxygen Dissociation on Tetrahedral Ag₂₀ and Ag₁₉Au clusters

Pichugina D. A.*, Polynskaya Y. G., Kuz'menko N. E.
Chemistry Department, M. V. Lomonosov Moscow State University
*corresponding author: daria@phys.chem.msu.ru, +74959394765

Supporting information

Figure S1 Energy diagram of the reaction between anionic Ag₂₀⁻ clusters and oxygen molecule (energy in kJ/mol); facet-edge pathway is colored by blue line, vertex-edge pathway is colored by red line.

Figure S2 The Kohn-Sham MO diagrams of Ag₂₀ and O₂.

Figure S3 The Kohn-Sham MO diagrams of ³TS₁ and ¹TS₄ corresponding to the O-O bond rupture in Ag₂₀O₂ complexes

Table S1 Activation energies (in kJ/mol) of oxygen dissociation calculated relative to the energies of isolated Ag₂₀ cluster and O₂ molecule using TPSSh, M06L, mPBE, BLYP, OLYP, B3LYP.

Table S2 The Cartesian coordinates of reagents (R), transition states (TS), and products (P).

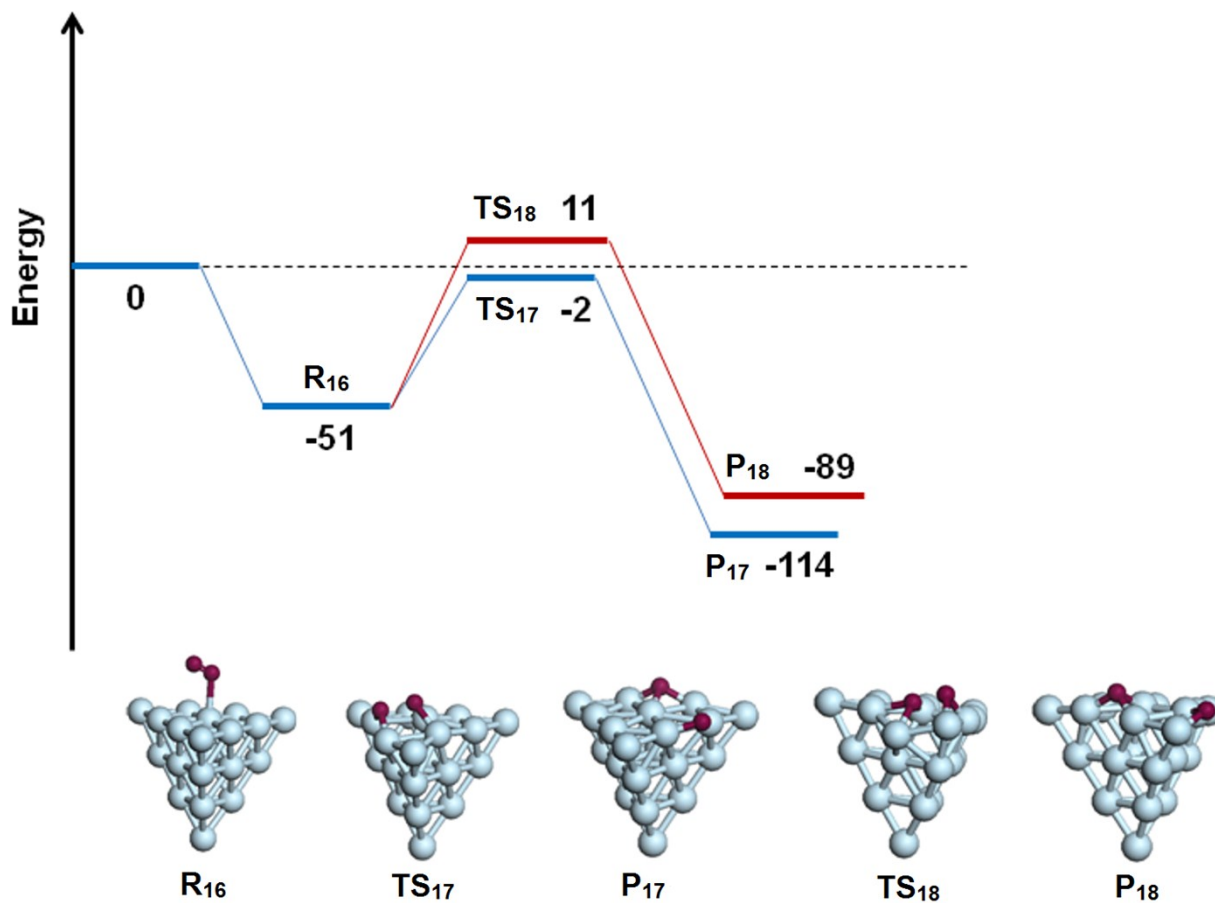


Figure S1 Energy diagram of the reaction between anionic Ag_{20}^- clusters and oxygen molecule (energy in kJ/mol); facet-edge pathway is colored by blue line, vertex-edge pathway is colored by red line.

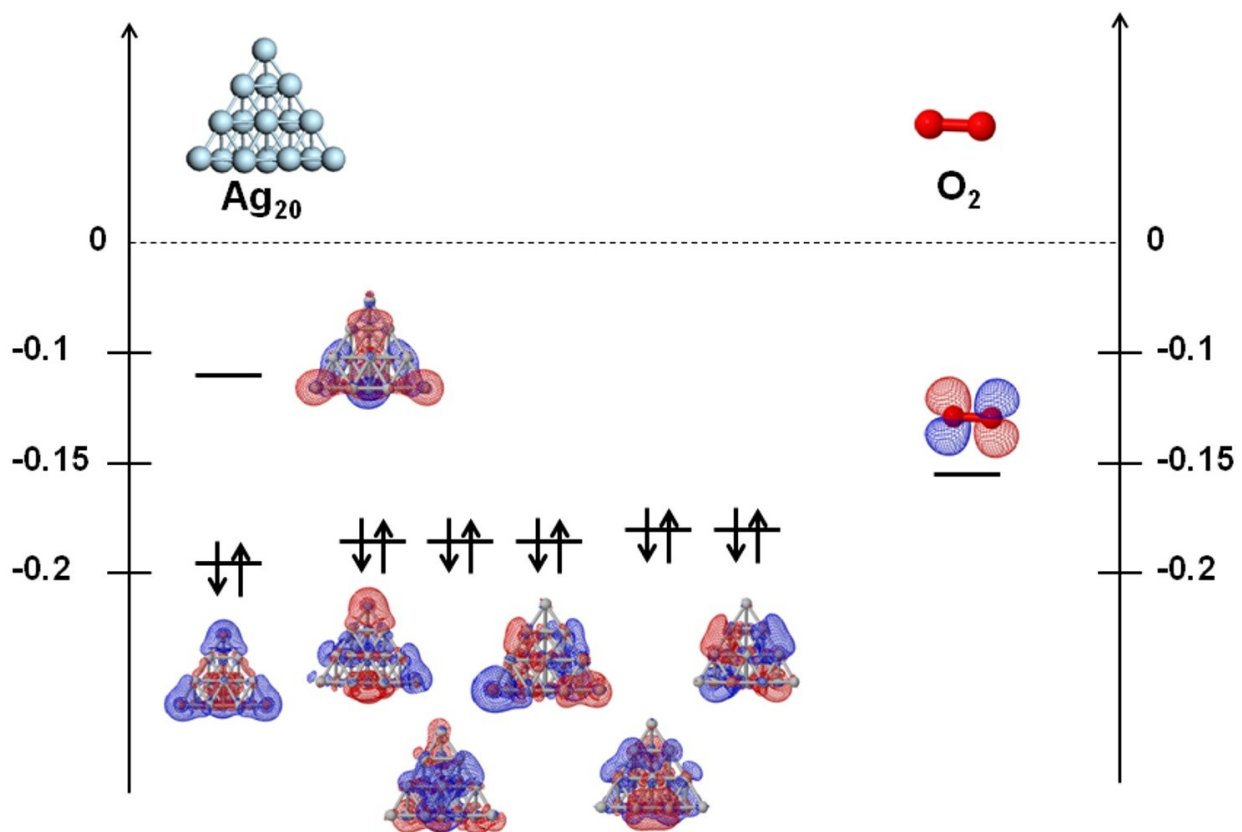


Figure S2 The Kohn-Sham MO diagrams of Ag₂₀ and O₂ (energy in a.u.).

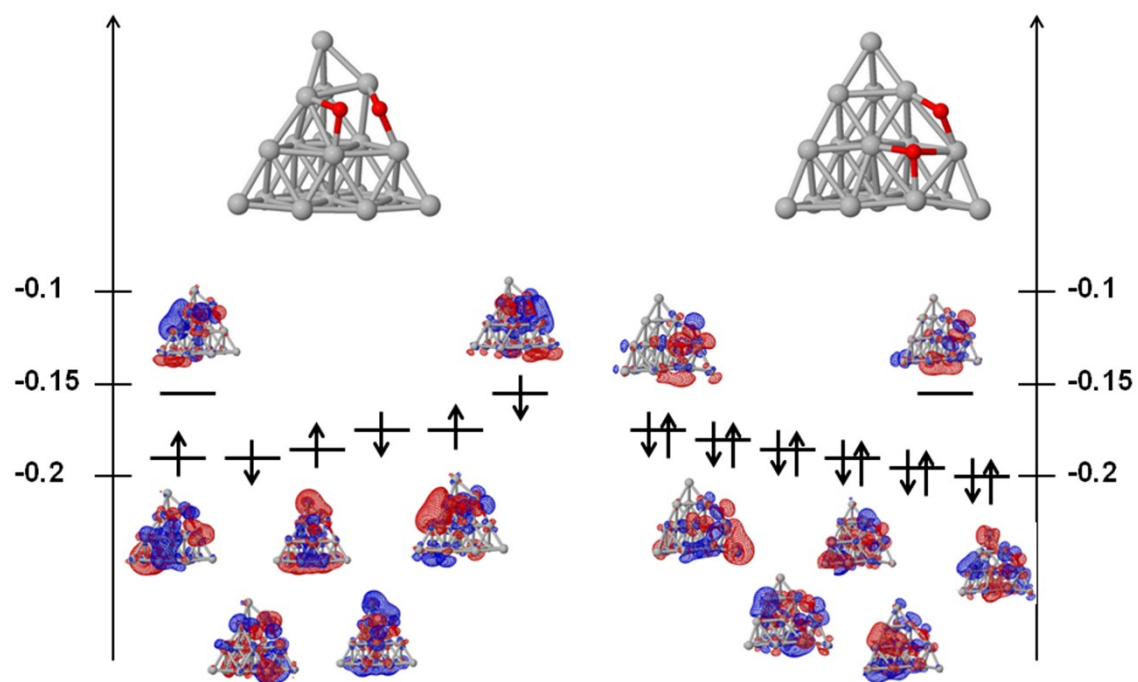


Figure S3 The Kohn-Sham MO diagrams of ${}^3\text{TS}_1$ (left column) and ${}^1\text{TS}_4$ (right column) corresponding to the O-O bond rupture in Ag_{20}O_2 complexes (energy in a.u.).

Table S1 Activation energies (in kJ/mol) of oxygen dissociation calculated relative to the energies of isolated Ag₂₀ cluster and O₂ molecule using TPSSh, M06L, mPBE, BLYP, OLYP, B3LYP.

Functional	³TS₁	¹TS₄
TPSSh	128	90
M06L	108	70
mPBE	119	107
BLYP	108	90
OLYP	174	165
B3LYP	70	54

Table S2 The Cartesian coordinates of reagents (R), transition states (TS), and products (P)

R₁

Atomic number	X	Y	Z
47	-2.10223177	-2.29293392	1.37612243
47	-3.37935573	-1.29331010	-1.04082232
47	-1.11361123	-3.11176334	-1.23037642
47	-3.58295387	-3.95525450	-0.28427023
47	0.44412061	-1.42781593	0.45116514
47	1.33063016	-2.18898949	-2.14147426
47	-0.87950352	-0.40338058	-2.06002474
47	-3.08581666	1.36502835	-1.76690763
47	-1.90804983	0.44955274	0.64860385
47	-0.58972110	-0.58460383	2.94652309
47	-0.51213456	2.33781120	-2.71714931
47	1.63730589	0.60785516	-2.90801737
47	3.76455239	-1.17611208	-3.01683341
47	2.90777096	-0.39061643	-0.50051489
47	2.00162313	0.38200601	2.02036892
47	0.89996626	1.18607213	4.46638568
47	-0.27350389	2.20246980	2.18050515
47	-1.50006086	3.15861092	-0.11231868
47	-2.70259417	4.02398711	-2.46167527
47	0.76225483	1.44754193	-0.33346920
8	4.28025401	0.14792173	2.97804367
8	4.59843936	-0.91876467	3.55633108

TS₁

Atomic number	X	Y	Z
47	-1.74266845	-2.24402941	1.56043300
47	-3.13395392	-1.46088677	-0.82911375
47	-0.81441818	-3.19451702	-1.11612560
47	-3.16607145	-4.09610290	0.05771795
47	0.77537881	-1.60351860	0.50152750
47	1.60539767	-2.14178332	-2.10894224
47	-0.64150758	-0.45834267	-1.79977835
47	-2.99395938	1.14927408	-1.72318939
47	-1.73676069	0.44755103	0.75393790
47	-0.05153031	-0.36581118	2.96877071
47	-0.49408625	2.24997699	-2.66207917
47	1.79504918	0.72208459	-2.71669323
47	3.98579549	-0.95440239	-2.93942683
47	3.12423518	-0.25867436	-0.42593907
47	2.12971878	1.39945160	2.41329506
47	0.61578061	1.81380131	4.67422116
47	-0.44839420	2.47519005	2.22916200

47	-1.59839320	3.14475477	-0.17775641
47	-2.81125770	3.79406520	-2.58563290
47	0.80344502	1.54724069	-0.18640962
8	3.03106487	-0.38747335	1.69652713
8	1.76713487	-1.57784834	2.41549637

P₁

Atomic number	X	Y	Z
47	-1.88274835	-2.56333354	1.42181058
47	-3.13126710	-1.48217415	-0.87124343
47	-0.74662167	-3.16149191	-1.08751905
47	-3.23691269	-4.19141143	-0.29038115
47	0.77769443	-1.35290768	0.75553397
47	1.67888629	-2.03482186	-1.86279641
47	-0.68100123	-0.45671317	-1.84776220
47	-3.01469828	1.14791191	-1.67595857
47	-1.72101206	0.37852838	0.77460727
47	-0.13357909	-0.11123175	3.31019405
47	-0.52615766	2.25241549	-2.68120719
47	1.75419547	0.66933437	-2.78250329
47	3.98285078	-0.96091025	-2.95954853
47	3.16087018	-0.13588744	-0.42806378
47	2.16453409	1.02601813	2.29271609
47	0.94895902	2.02689562	4.59396290
47	-0.35200983	2.47233647	2.19253147
47	-1.59162255	3.10689110	-0.15322861
47	-2.84472308	3.77791471	-2.55174545
47	0.76412101	1.46305465	-0.22765817
8	3.92528653	0.73913049	1.26486459
8	-0.24959273	-2.07016128	2.62152674

R₂

Atomic number	X	Y	Z
47	-1.00232327	-2.70439053	1.95544088
47	-2.79097891	-2.25705051	-0.34216979
47	-0.23045485	-3.58971596	-0.63031930
47	-2.37085700	-4.78392839	0.72367537
47	1.18496788	-1.40486062	0.61377239
47	1.82820725	-2.39598560	-2.02103734
47	-0.61485434	-0.97703373	-1.69981849
47	-3.11442757	0.35839778	-1.28623474
47	-1.52327132	-0.12542871	0.94507909
47	0.21576142	-0.47371739	3.13825107
47	-0.91930807	1.64889574	-2.73024440
47	1.50183499	0.30739194	-3.04068708
47	3.85971093	-1.10710526	-3.39002490
47	3.26342607	-0.20789051	-0.81002545
47	2.50073624	0.88311672	1.61462831

47	1.33347154	1.90333188	4.11712027
47	-0.95289260	2.04167056	2.54852366
47	-1.70733702	2.61452341	-0.11223825
47	-3.36003065	2.93752718	-2.28056598
47	0.85086918	1.41372573	-0.54010141
8	0.31758407	3.02588081	1.01177883
8	1.73016596	2.89264297	2.21519685

TS₂

Atomic number	X	Y	Z
47	-1.00232324	-2.70439061	1.95544091
47	-2.79097884	-2.25705049	-0.34216980
47	-0.23045484	-3.58971596	-0.63031927
47	-2.37085709	-4.78392823	0.72367540
47	1.18496791	-1.40486066	0.61377239
47	1.82820728	-2.39598571	-2.02103739
47	-0.61485432	-0.97703376	-1.69981849
47	-3.11442762	0.35839774	-1.28623478
47	-1.52327134	-0.12542872	0.94507908
47	0.21576143	-0.47371741	3.13825106
47	-0.91930807	1.64889573	-2.73024446
47	1.50183494	0.30739191	-3.04068709
47	3.85971082	-1.10710526	-3.39002496
47	3.26342604	-0.20789053	-0.81002543
47	2.50073629	0.88311672	1.61462826
47	1.33347153	1.90333189	4.11712032
47	-0.95289260	2.04167054	2.54852373
47	-1.70733705	2.61452350	-0.11223826
47	-3.36003054	2.93752711	-2.28056586
47	0.85086917	1.41372577	-0.54010143
8	0.31758406	3.02588077	1.01177887
8	1.73016594	2.89264303	2.21519684

P₂

Atomic number	X	Y	Z
47	-1.14714863	-2.63697525	1.99263321
47	-2.77694723	-2.25470955	-0.31342035
47	-0.17479759	-3.50798366	-0.50719467
47	-2.33071715	-4.79937268	0.68889381
47	1.06404933	-1.18911661	0.73241176
47	1.89074731	-2.27987081	-1.83268970
47	-0.61260127	-0.93356782	-1.64406545
47	-3.19677649	0.26090821	-1.36102127
47	-1.59566163	0.00456131	0.96435131
47	-0.04172694	-0.49440992	3.28990721
47	-1.01638960	1.56390909	-2.89285506
47	1.46292938	0.35570607	-3.05712333
47	3.90030680	-1.00576575	-3.26903626

47	3.15357038	0.02320873	-0.81311398
47	2.52151758	1.13124653	1.61341764
47	1.58422011	1.40969902	4.43551964
47	-0.09152848	2.10346485	2.34629173
47	-2.00832806	2.65225370	-0.46890592
47	-3.61140711	2.67106003	-2.66494741
47	0.73907134	1.57324830	-0.57301505
8	-0.26965391	3.19574560	0.56133755
8	3.41458468	1.39913096	3.45451584

R₃

Atomic number	X	Y	Z
47	-0.87180760	-3.03383970	1.56781818
47	-2.46474152	-2.39969577	-0.76698006
47	0.16106814	-3.61263570	-1.09099356
47	-1.97256717	-5.02844601	-0.01992510
47	1.34930607	-1.59794282	0.51559905
47	2.26475564	-2.11577500	-2.11967953
47	-0.30847009	-0.93806228	-1.91450702
47	-2.86777768	0.24101232	-1.49054395
47	-1.35281336	-0.32364530	0.83501334
47	0.24586998	-0.99839443	3.07354848
47	-0.66141089	1.80935967	-2.56851719
47	1.83989068	0.66422019	-2.87042894
47	4.32931538	-0.54720835	-3.10215016
47	3.43163939	0.03052891	-0.53723708
47	2.45115612	0.57032812	1.99382842
47	1.48542235	0.99081706	4.55842691
47	-0.10870285	1.76877605	2.43590265
47	-1.77663081	2.43260201	-0.00869045
47	-3.21529785	2.86206442	-2.33190061
47	0.87521753	1.26469662	-0.25361899
8	-1.65144330	3.35901525	2.03888892
8	-1.18197869	4.60222743	2.05614523

TS₃

Atomic number	X	Y	Z
47	-0.87273470	-2.93491216	1.62932964
47	-2.45995425	-2.41172881	-0.73461568
47	0.16243537	-3.60758585	-1.02203976
47	-1.95568219	-5.00656359	0.08302259
47	1.33003276	-1.52379748	0.52287998
47	2.26436507	-2.14000322	-2.09247731
47	-0.31049712	-0.96275062	-1.92984766
47	-2.89465269	0.20793240	-1.57248815
47	-1.37760705	-0.27358586	0.76833482
47	0.18574839	-0.76925607	3.04318418
47	-0.66431151	1.76560372	-2.70854165

47	1.85551463	0.60233089	-2.93254460
47	4.33337664	-0.61460560	-3.12027751
47	3.42174190	0.06485482	-0.55838397
47	2.36160442	0.75074721	1.93434001
47	1.17897366	1.52076062	4.39945959
47	-0.24245565	1.96011876	2.21521396
47	-1.82097656	2.46011319	-0.20015987
47	-3.24340370	2.80257562	-2.52584516
47	0.86539958	1.29365049	-0.37439968
8	-1.53262556	3.40034592	1.65172976
8	-0.58429172	3.41575853	3.52412516

P₃

Atomic number	X	Y	Z
47	-0.65008536	-2.88812177	2.01543751
47	-2.29475049	-2.35840560	-0.26693909
47	0.27476242	-3.47720563	-0.70489462
47	-1.73828711	-4.96405753	0.50836093
47	1.37344196	-1.33148756	0.80296025
47	2.33949900	-1.99709975	-1.79241400
47	-0.25413172	-0.78513568	-1.59088094
47	-2.76845965	0.24270242	-0.92411055
47	-1.34717265	-0.20471591	1.44715588
47	0.54927826	-0.84527252	3.46738498
47	-0.46495099	1.97290649	-2.40507343
47	1.90170078	0.68338983	-2.68920990
47	4.43303228	-0.49767219	-2.83155163
47	3.45916720	0.25652179	-0.35432051
47	2.58735130	0.87319337	2.17440787
47	1.85922631	1.24818463	4.82756619
47	0.07659288	1.91478232	2.88570867
47	-1.81761720	2.78056325	0.06807283
47	-3.49105857	2.34534774	-2.58336366
47	0.88058111	1.43410381	-0.02367244
8	-1.95437863	3.52448367	-1.86807059
8	-1.78820589	1.94386019	1.91905036

R₄

Atomic number	X	Y	Z
47	-1.79924494	-2.37540585	1.85872322
47	-3.01875451	-1.77020302	-0.68890229
47	-0.53323726	-3.18943433	-0.75803201
47	-2.86440199	-4.36752455	0.27082687
47	0.71625082	-1.53428707	1.11699517
47	1.88763784	-1.83351495	-1.42168044
47	-0.63205913	-0.55357872	-1.71801238
47	-3.13700824	0.83878525	-1.57512175
47	-1.69382333	0.24850516	0.83184422

47	-0.50791926	-0.33458220	3.32144708
47	-0.86774046	2.17407488	-2.68376456
47	1.54961445	0.85630699	-2.85026013
47	3.89080411	-0.62163264	-2.98799916
47	3.22837584	0.65150563	-0.64081077
47	1.88482642	0.93810227	2.13872838
47	0.85619854	1.76002900	4.55509597
47	-0.47173514	2.42228990	2.20672444
47	-1.94142300	2.95762930	-0.09024536
47	-3.30989971	3.48918765	-2.44820399
47	0.60074596	1.71288859	-0.31184613
8	3.48426485	-0.35092895	1.31479874
8	2.97797929	-1.65814264	0.98084993

TS₄

Atomic number	X	Y	Z
47	-1.81451468	-2.35600604	1.89379570
47	-2.98990934	-1.80005123	-0.69590034
47	-0.48016805	-3.19832599	-0.74057858
47	-2.76941364	-4.39739621	0.27335138
47	0.57920303	-1.28902028	1.07316462
47	1.87964185	-1.88068668	-1.63199870
47	-0.67472214	-0.55649888	-1.74629948
47	-3.16635674	0.82265247	-1.57608783
47	-1.83997535	0.29239135	0.87242107
47	-0.57300358	-0.27514250	3.36042351
47	-0.83073583	2.15266517	-2.63423363
47	1.56134217	0.80316187	-2.84496712
47	3.90228151	-0.54742467	-3.18027078
47	3.33541148	0.50094668	-0.69401822
47	1.94867655	0.90884678	2.37959254
47	0.74022923	1.82164075	4.65243674
47	-0.44637439	2.41422008	2.21507128
47	-1.84328122	2.95477384	-0.10372950
47	-3.27698264	3.45926688	-2.43193572
47	0.64949147	1.54590050	-0.24063672
8	3.58362074	0.17338841	1.36903798
8	2.52554000	-1.54930186	0.43136172

P₄

Atomic number	X	Y	Z
47	-1.64962999	-2.36289060	1.84204274
47	-2.99109651	-1.74809839	-0.68592626
47	-0.69991701	-3.39536891	-0.59464438
47	-3.07106731	-4.31720951	0.36687603
47	0.88012360	-1.31351466	0.90845954
47	2.09515725	-1.90650030	-1.87255085
47	-0.60183806	-0.56019943	-1.66582781

47	-3.10596555	0.84572579	-1.57227287
47	-1.63869810	0.29633640	0.84063883
47	-0.38912748	-0.39408950	3.29151665
47	-0.76054617	2.14103277	-2.54781250
47	1.60021261	0.75490239	-2.78010755
47	4.05173202	-0.56709545	-3.17943071
47	3.32899896	0.20348897	-0.61862470
47	1.89173112	1.03442012	2.52014712
47	0.59182808	1.70984990	4.81402801
47	-0.55287607	2.42370059	2.33269326
47	-1.82069707	2.96566077	-0.06251845
47	-3.20498469	3.46672694	-2.44500299
47	0.80270942	1.75176416	-0.15880390
8	2.85505929	1.65598566	0.79028619
8	1.36157429	-3.10135789	-0.34577273

R₅

Atomic number	X	Y	Z
47	-2.22778024	-2.30028044	1.34583667
47	-3.44907090	-1.23679063	-1.07418210
47	-1.23980478	-3.13597299	-1.22321304
47	-3.75676574	-3.89701397	-0.33267529
79	0.34222571	-1.48915121	0.45731588
47	1.25077942	-2.29247065	-2.10743332
47	-0.90857187	-0.42740490	-2.06352862
47	-3.05525997	1.41255810	-1.78850777
47	-1.93978880	0.45367233	0.63552697
47	-0.66548421	-0.64545424	2.94450747
47	-0.43483791	2.29838031	-2.70207959
47	1.65869683	0.49660180	-2.86648990
47	3.72400517	-1.36199770	-2.96490449
47	2.85617583	-0.58410252	-0.45142906
47	1.94668810	0.21982943	2.06868745
47	0.83801900	1.06338042	4.50526895
47	-0.26923666	2.13816396	2.20617827
47	-1.42179757	3.14686453	-0.10198891
47	-2.56679161	4.05779334	-2.46061196
47	0.78102174	1.36617382	-0.30548802
8	4.23850404	0.60660917	2.86452813
8	4.82221470	-0.32895136	3.46713799

TS₅

Atomic number	X	Y	Z
47	-1.75010927	-2.22413021	1.52154775
47	-3.15742597	-1.44919349	-0.83694354
47	-0.83948880	-3.21285912	-1.11124147
47	-3.20260500	-4.08801095	0.04392916
79	0.83257031	-1.76854804	0.51490313

47	1.61445006	-2.15460747	-2.10500863
47	-0.62328274	-0.46223831	-1.69132875
47	-2.99034185	1.15465739	-1.74654264
47	-1.82958977	0.50084570	0.77601932
47	-0.04346040	-0.33750249	2.88065178
47	-0.49853232	2.22691473	-2.64874737
47	1.78280976	0.70672980	-2.70187322
47	3.97678476	-0.96668216	-2.93163379
47	3.10158186	-0.25547242	-0.41029400
47	2.14241154	1.43504650	2.43289593
47	0.57775882	1.76013984	4.67515771
47	-0.46080123	2.49438449	2.23324503
47	-1.60214395	3.16522933	-0.18017180
47	-2.80080701	3.80022884	-2.59755349
47	0.78843520	1.54460062	-0.15350801
8	3.11934257	-0.31373675	1.71894744
8	1.86244190	-1.55579578	2.31754960

P₅

Atomic number	X	Y	Z
47	-1.81489128	-2.24320299	1.55269036
47	-3.12797190	-1.45655805	-0.86015783
47	-0.77106714	-3.15514325	-0.96392365
47	-3.17801576	-4.11441034	0.01178196
79	0.85612007	-1.53772022	0.58039182
47	1.65261327	-2.15680748	-1.98255703
47	-0.59465294	-0.41270653	-1.71206097
47	-2.99631465	1.15416473	-1.74195127
47	-1.75146306	0.47190829	0.74077501
47	-0.42784493	-0.37945320	3.13043596
47	-0.47871991	2.25509257	-2.65625048
47	1.75449303	0.66259879	-2.85292699
47	3.91967093	-1.13065542	-3.16530895
47	3.26653777	-0.24171584	-0.65738157
47	2.03947618	0.98874488	2.58737904
47	0.50216136	1.70681961	4.76601932
47	-0.40629831	2.41217278	2.23700755
47	-1.52409044	3.12117967	-0.19254023
47	-2.81804662	3.78250186	-2.57473722
47	0.96078671	1.65451268	-0.21315504
8	2.95638141	1.30494816	0.74157392
8	1.59697413	-1.21117578	2.45819474

TS₆

Atomic number	X	Y	Z
47	-1.00175102	-2.70183562	1.95129983
47	-2.79140920	-2.25841316	-0.33968849
47	-0.23027637	-3.59247618	-0.63075622

47	-2.37042318	-4.78336576	0.72839895
47	1.17869074	-1.39794699	0.61075869
47	1.83281623	-2.39806609	-2.01811757
47	-0.61764332	-0.97833770	-1.69471868
47	-3.12730189	0.34831762	-1.29113179
47	-1.52126510	-0.11880053	0.93927599
47	0.21168797	-0.47753835	3.13873336
47	-0.93588475	1.66316131	-2.72577088
47	1.51415258	0.31260161	-3.01438387
47	3.85820552	-1.10948779	-3.39655368
47	3.26282339	-0.19627178	-0.81114671
47	2.48687534	0.89750097	1.61351103
47	1.32634783	1.88711606	4.15421454
47	-0.91665065	2.05314120	2.52704951
47	-1.72796808	2.61948634	-0.12387019
47	-3.38852155	2.92308673	-2.29516788
79	0.83431543	1.41511154	-0.56609051
8	0.38462168	3.00104391	0.97150176
8	1.73855881	2.89197152	2.27265277

P₆

Atomic number	X	Y	Z
47	-1.12806051	-2.63928019	2.00099595
47	-2.76433703	-2.24424012	-0.29827930
47	-0.18195571	-3.52618157	-0.51872747
47	-2.33886751	-4.79152648	0.70108579
47	1.07048322	-1.23939560	0.72736586
47	1.90025328	-2.29149177	-1.83232334
47	-0.60284585	-0.94286425	-1.64244826
47	-3.17864982	0.26618840	-1.35192632
47	-1.55635259	0.01330768	0.96528582
47	-0.00120397	-0.49010751	3.27486717
47	-1.01606918	1.56222622	-2.90157368
47	1.47833696	0.35930625	-3.04291785
47	3.91706446	-1.01104514	-3.25979412
47	3.15279071	0.03234605	-0.81999208
47	2.41877688	1.15911812	1.57794075
47	1.59794789	1.41508041	4.45273612
47	-0.13883174	2.15314374	2.44365072
47	-2.01251593	2.68618950	-0.49404805
47	-3.60713290	2.66598090	-2.69016577
79	0.72444915	1.55289952	-0.60149868
8	-0.22323254	3.12966819	0.54999963
8	3.36587797	1.28808138	3.38445586

R₆

Atomic number	X	Y	Z
47	-1.76874243	-2.39701763	1.82884049
47	-3.04297380	-1.74639687	-0.69042751

47	-0.55507666	-3.12709388	-0.73317070
47	-2.90806331	-4.34762526	0.24414100
79	0.79499910	-1.65171466	1.27259397
47	1.81447693	-1.75595013	-1.37703556
47	-0.69302717	-0.54012696	-1.85518052
47	-3.15311836	0.86621523	-1.56006569
47	-1.56199365	0.19951620	0.76673984
47	-0.49438948	-0.33655722	3.33997897
47	-0.87660573	2.20431316	-2.71053440
47	1.55029056	0.87965164	-2.85784211
47	3.85277783	-0.65687563	-2.97629371
47	3.24956226	0.65314042	-0.63979124
47	1.83194995	0.95459102	2.12803575
47	0.81976938	1.79779769	4.55302908
47	-0.49985860	2.42793946	2.19490504
47	-1.93811288	2.94732615	-0.10339671
47	-3.32004933	3.51660754	-2.43764745
47	0.61350900	1.75543430	-0.35135720
8	3.49984042	-0.25917552	1.35097858
8	3.00352203	-1.59581940	1.04294423

TS₇

Atomic number	X	Y	Z
47	-1.81341715	-2.38256800	1.87437693
47	-3.02045715	-1.79482168	-0.70831162
47	-0.48937863	-3.17032239	-0.71335844
47	-2.80817651	-4.39421285	0.24455198
79	0.61777060	-1.36931914	1.19216749
47	1.87326681	-1.82764333	-1.61475472
47	-0.70049002	-0.56794029	-1.80161854
47	-3.17371476	0.83265842	-1.57130406
47	-1.78141554	0.25696666	0.84054576
47	-0.57513147	-0.26986519	3.38120207
47	-0.82359593	2.15448811	-2.63163377
47	1.55500270	0.79860144	-2.86579129
47	3.89968206	-0.56810368	-3.19690308
47	3.38179625	0.56549675	-0.75474795
47	1.95549286	0.92203664	2.39737031
47	0.71740150	1.83348112	4.66736266
47	-0.45092816	2.40765316	2.21483819
47	-1.82916309	2.93787253	-0.10163568
47	-3.26134865	3.47305211	-2.42178769
47	0.65618247	1.48863338	-0.23980701
8	3.56709661	0.19332669	1.29897032
8	2.50352558	-1.51946825	0.51026810

P₇

Atomic number	X	Y	Z
---------------	---	---	---

47	-1.10617553	-2.90979654	1.70237418
47	-2.65519369	-2.02545336	-0.46204452
47	-0.03222800	-3.33977169	-0.85750268
47	-2.34699621	-4.71599128	0.11094969
79	1.39726311	-1.51281356	0.69157963
47	2.10174305	-1.87151605	-1.98351472
47	-0.40065441	-0.63383640	-1.56996510
47	-2.97677420	0.58268750	-1.25018455
47	-1.37432124	0.00823397	1.07749292
47	0.19565321	-0.21097215	3.57125458
47	-0.79814264	2.08161776	-2.39872747
47	1.67946817	0.95698265	-2.74860086
47	4.09400011	-0.28463898	-3.28841447
47	3.45922678	0.23037409	-0.70665805
47	2.27986903	1.22520139	2.47385289
47	1.07917159	2.09440601	4.79770715
47	-0.32855897	2.31811300	2.41778378
47	-1.79575163	2.72598970	0.16759211
47	-3.32416543	3.21490891	-2.09246907
47	0.82804348	1.52251312	-0.08337771
8	3.20866098	-0.23059177	1.30764580
8	0.50660225	-2.09389608	2.73491439

R₇

Atomic number	X	Y	Z
47	-0.69598194	-2.82100809	1.74829136
47	-2.74462908	-2.18861501	-0.31215397
47	-0.21295810	-3.46738942	-0.98083898
47	-2.20935906	-4.78537241	0.44859244
79	1.26123412	-1.40187361	0.30238559
47	1.71638806	-2.07653731	-2.42224886
47	-0.77199695	-0.80122877	-1.83930514
47	-3.19228920	0.49159224	-1.01821286
47	-1.35337683	-0.14538209	0.98916815
47	0.55448561	-0.66188218	2.94174295
47	-1.16930214	1.94997611	-2.52971230
47	1.21501813	0.66577201	-3.27031157
47	3.58405211	-0.60883524	-3.87962453
47	3.21218431	-0.00330610	-1.17164302
47	2.61929676	0.82708068	1.39912235
47	-1.07664436	1.80923260	2.93253766
47	0.83653049	3.18854885	1.50330998
47	-1.66121485	2.63551775	0.28677925
47	-3.52965358	3.14491504	-1.72280128
47	0.78506022	1.39645266	-0.60850976
8	0.95258842	1.29691682	3.92724767
8	1.98324796	2.03993274	3.15738893

TS_8

Atomic number	X	Y	Z
47	-0.90679961	-2.63624835	1.64070640
47	-2.78366032	-2.11997889	-0.48459038
47	-0.20136405	-3.43353037	-1.00410549
47	-2.24827477	-4.70657173	0.38999502
79	1.18187691	-1.29523795	0.24781373
47	1.78214162	-2.09165356	-2.40264793
47	-0.75187445	-0.81186996	-1.98123125
47	-3.23523877	0.45509700	-1.38120779
47	-1.47421049	0.05139358	0.81700374
47	0.41235543	-0.56712730	2.85813499
47	-1.12537094	1.89004790	-2.80623688
47	1.31809749	0.63529058	-3.31341058
47	3.73039461	-0.66914630	-3.76634436
47	3.18497472	0.10152016	-1.14626624
47	2.49582367	0.91954151	1.40231652
47	0.21156967	2.13156094	4.77301201
47	-0.06326606	2.27291488	1.88801645
47	-1.86931156	2.68931786	-0.12199534
47	-3.59013804	3.05404390	-2.27748341
47	0.69592974	1.48256322	-0.70486305
8	1.43496571	0.47692304	4.34183075
8	1.80138177	2.17115005	3.03155412

 P_8

Atomic number	X	Y	Z
47	-0.11407683	-3.72250673	1.65696878
47	-1.50858787	-1.49263972	0.50993599
47	-0.02922741	-3.55583091	-1.20232803
47	-2.43972743	-4.02766805	0.16395607
79	1.40527891	-1.71757228	0.34451683
47	1.87631480	-1.99973486	-2.41876762
47	-0.86255436	-1.05075182	-2.23656795
47	-2.88046294	0.46388620	-0.76678219
47	-1.61933131	1.08994333	1.82099152
47	0.14097737	-1.13164307	2.77661517
47	-1.34026981	1.71608083	-2.83038220
47	1.19092484	0.74300725	-3.15668437
47	3.77703452	-0.27994315	-3.54452004
47	2.95307473	0.24983576	-0.99683713
47	2.21383040	0.59056428	1.62734666
47	0.57755725	1.51125955	3.64992704
47	0.51762498	3.06475892	1.25811622
47	-1.74746528	3.03746322	-0.28525471
47	-3.84905308	2.63779804	-2.15729262
47	0.14119447	0.92962392	-0.46838114
8	-1.08729632	0.28171384	3.85135173

8	2.14005931	2.48442545	2.63861545
---	------------	------------	------------

R₈

Atomic number	X	Y	Z
47	-2.03086910	-2.36918654	1.35063829
47	-3.31345330	-1.31858462	-1.03796239
47	-1.03383102	-3.12452002	-1.26844025
47	-3.49984126	-3.99951779	-0.32263028
47	0.53552720	-1.48012062	0.41479097
47	1.40414226	-2.16877839	-2.18177376
47	-0.81547749	-0.39508294	-2.03924716
47	-3.03597885	1.35558463	-1.73027230
47	-1.86766298	0.41547784	0.65860899
79	-0.53313662	-0.68093500	2.88447337
47	-0.46657945	2.35504806	-2.65224873
47	1.69081491	0.64041576	-2.88003055
47	3.83008323	-1.12755111	-3.03524002
47	2.98399814	-0.38387904	-0.50062033
47	2.06109048	0.30898837	2.04211583
47	0.89228033	0.99915450	4.51161107
47	-0.23189482	2.12848580	2.23990866
47	-1.44751100	3.13670863	-0.04063450
47	-2.66821149	4.02624948	-2.37339113
47	0.81940984	1.42817712	-0.28342086
8	4.27688920	-0.05513794	3.08621564
8	4.55371800	-1.17928044	3.56901671

TS₉

Atomic number	X	Y	Z
47	-1.71345447	-2.21950820	1.57329896
47	-3.13674743	-1.45030649	-0.80842754
47	-0.82289907	-3.19726305	-1.10884668
47	-3.16193690	-4.07277269	0.12137782
47	0.83539913	-1.67793848	0.47574094
47	1.60256486	-2.14362334	-2.13853129
47	-0.63690610	-0.45584005	-1.76206275
47	-2.99072341	1.15700342	-1.72202902
47	-1.78588858	0.48842067	0.76113918
79	-0.04942726	-0.35973938	2.85192881
47	-0.49870693	2.24227860	-2.66546842
47	1.79168836	0.71957464	-2.70887703
47	3.99128844	-0.94433142	-2.92816640
47	3.12421407	-0.24590956	-0.41548843
47	2.13969623	1.42661592	2.39318509
47	0.56788676	1.67994975	4.66054359
47	-0.45526905	2.49045470	2.22835634
47	-1.59299565	3.17753169	-0.18974940
47	-2.81093073	3.79039757	-2.60933480

47	0.79298540	1.55485905	-0.18392109
8	3.02715857	-0.39646649	1.71437723
8	1.78300385	-1.56338654	2.46095546

P₉

Atomic number	X	Y	Z
47	-1.89561677	-2.55716528	1.41122918
47	-3.13283762	-1.47959929	-0.87688792
47	-0.74218111	-3.16877926	-1.10362200
47	-3.23190478	-4.19339549	-0.30490122
47	0.76487948	-1.37792419	0.71132390
47	1.68106308	-2.03544525	-1.88183717
47	-0.67940959	-0.45924733	-1.84556451
47	-3.00864384	1.15361873	-1.66107470
47	-1.71779567	0.37866321	0.77826257
79	-0.08070010	-0.15513415	3.23721105
47	-0.53582727	2.24297404	-2.70454386
47	1.74512961	0.66256462	-2.81559084
47	3.97602293	-0.96643055	-2.99361403
47	3.17126230	-0.10602277	-0.46908016
47	2.18034833	0.97475499	2.26090798
47	0.88725001	1.94219833	4.59983019
47	-0.34915308	2.45471175	2.18045299
47	-1.56557318	3.12447093	-0.16746604
47	-2.84641988	3.77220335	-2.56313548
47	0.77070438	1.47922053	-0.25144152
8	3.93762976	0.80921752	1.21377002
8	-0.29317849	-2.09240684	2.69170979

TS₁₀

Atomic number	X	Y	Z
47	-1.02696283	-2.70919271	1.95998739
47	-2.78496209	-2.25577726	-0.34401239
47	-0.23163772	-3.59184160	-0.63194667
47	-2.37502090	-4.79179705	0.70674277
47	1.19988309	-1.45988828	0.63569445
47	1.83939771	-2.39129478	-2.00354663
47	-0.59898310	-0.96515282	-1.66906778
47	-3.11018111	0.35699143	-1.28317126
47	-1.53062412	-0.12069485	0.96067647
47	0.21892954	-0.48453379	3.13412575
47	-0.93838530	1.64553712	-2.74385063
47	1.51191348	0.31836126	-3.02189201
47	3.89148675	-1.07701984	-3.33982698
47	3.27488607	-0.22627045	-0.77587630
79	2.41372530	0.86575751	1.56318787
47	1.38447174	1.86647976	4.10384254
47	-0.92416406	2.04846421	2.54997073

47	-1.73315370	2.62273825	-0.10055596
47	-3.37490990	2.93276400	-2.28309522
47	0.81490561	1.46925453	-0.57771749
8	0.31359250	3.07379136	1.01337852
8	1.76579320	2.87332118	2.14695296

P₁₀

Atomic number	X	Y	Z
47	-1.17449353	-2.67038853	1.97370850
47	-2.79292839	-2.25761026	-0.32791115
47	-0.19615508	-3.52557452	-0.53311505
47	-2.36190523	-4.81660552	0.64970630
47	1.05591692	-1.25065412	0.72331471
47	1.88139928	-2.28722497	-1.84107590
47	-0.61938077	-0.93487296	-1.63925431
47	-3.19817191	0.26429427	-1.35641397
47	-1.59853978	-0.01131522	0.97156147
47	-0.04544074	-0.54839245	3.29307607
47	-1.01231322	1.57412156	-2.86607884
47	1.46343808	0.36452338	-3.03500069
47	3.90020658	-1.00792198	-3.26957493
47	3.17615291	0.00342315	-0.81947123
79	2.51021896	0.99526117	1.60249463
47	1.65309107	1.32191934	4.41587082
47	-0.08257439	2.06391191	2.38383473
47	-2.01706055	2.65179806	-0.44752170
47	-3.61133017	2.68175255	-2.64742259
47	0.74290387	1.55757814	-0.53795647
8	-0.28339692	3.16232942	0.59886240
8	3.47421551	1.28609507	3.32193912

R₉

Atomic number	X	Y	Z
47	-1.07163531	-2.50554458	2.06540716
47	-2.88141168	-2.00829165	-0.14403226
47	-0.56017438	-3.71006008	-0.55045008
47	-2.68752348	-4.51637844	1.03390725
47	1.14617309	-1.71272157	0.47641476
47	1.56452009	-2.80756054	-2.09279524
47	-0.73784075	-1.16128060	-1.80070229
47	-2.99470930	0.49338439	-1.31945375
47	-1.25099591	0.08409899	0.89479459
47	0.57979894	-0.47268992	2.97671704
47	-0.78757657	1.43395660	-2.96432426
47	1.44739608	-0.16588684	-3.32583450
47	3.66973692	-1.81505014	-3.61405210
47	3.28255038	-0.66420015	-1.13498595
79	2.74672056	0.45622947	1.29543177

47	2.33074039	1.53508185	3.77414387
47	0.46888426	2.19519390	1.76454567
47	-1.29704465	2.63153053	-0.35499363
47	-3.02136175	3.01196533	-2.49394789
47	1.01322521	1.06988493	-0.81755767
8	0.14537741	4.46759220	2.68124231
8	-0.75005368	4.66652732	3.53747041

R₁₀

Atomic number	X	Y	Z
47	-0.97995780	-2.71416504	1.59540388
47	-2.83260193	-2.06120705	-0.46335133
47	-0.32727786	-3.46877015	-1.11659017
47	-2.37960734	-4.70751936	0.30381779
47	1.16777555	-1.43350183	0.17404742
47	1.67103357	-2.15344113	-2.51432362
47	-0.78027373	-0.79186584	-1.97989575
47	-3.21488532	0.54463241	-1.32479934
47	-1.44601724	0.05193170	0.84268670
47	0.41585099	-0.69833766	2.80682697
47	-1.10545047	1.91039937	-2.81675718
47	1.28016617	0.60710948	-3.36422906
47	3.65403362	-0.75871258	-3.85805972
47	3.13765370	0.00793561	-1.23694403
79	2.55535445	0.68042489	1.34480789
47	0.08006862	1.34215213	4.63753868
47	0.00233788	2.20390618	1.92349645
47	-1.75052263	2.70960272	-0.12253134
47	-3.52556594	3.14414038	-2.22739666
47	0.73120937	1.42900407	-0.69837330
8	1.71327590	2.42295579	3.56851089
8	2.79779790	1.58590664	3.23924788

TS₁₁

Atomic number	X	Y	Z
47	-1.22415356	-2.73220310	1.55715387
47	-2.89285164	-2.20562558	-0.71361489
47	-0.29075435	-3.46838162	-1.10434312
47	-2.38471232	-4.81011451	0.13311939
47	0.96618619	-1.35955029	0.29510791
47	1.76264054	-2.05555864	-2.32179300
47	-0.78919203	-0.82634309	-2.05086839
47	-3.32213854	0.39387311	-1.59622081
47	-1.73517264	-0.04588000	0.71090988
47	-0.00928396	-0.60865621	2.85263807
47	-1.17207066	1.86369554	-2.91392183
47	1.31142603	0.67360143	-3.24826281
47	3.78584981	-0.56218239	-3.50027666

47	3.02033637	0.17825126	-0.94661450
79	2.11380170	0.87689131	1.55391600
47	1.09679250	1.61694978	4.23034443
47	-0.46517751	2.14850667	1.91691278
47	-2.10919699	2.62084885	-0.25957440
47	-3.67672418	2.99895044	-2.51551352
47	0.49745210	1.47512328	-0.66710995
8	2.56770409	2.23711676	5.33524468
8	2.94923891	1.59068514	3.25276663

P₁₁

Atomic number	X	Y	Z
47	-1.54237399	-2.66122009	1.82519608
47	-2.73404573	-2.33097938	-0.79481465
47	0.03367583	-2.99117290	-0.52868400
47	-1.94114551	-4.83365036	0.04847245
47	1.08120259	-1.50198107	1.80406824
47	1.67534867	-0.89099354	-0.99362891
47	-0.79726005	-0.89446136	-2.37966185
47	-3.26478767	0.26237859	-1.47337025
47	-1.08130482	-0.26340521	0.36083154
47	-1.23133105	-0.27669598	3.13266370
47	-1.32322806	1.87683429	-2.95781714
47	1.17368587	0.83685462	-3.46240956
47	3.27695011	-0.98679148	-3.22173822
47	3.36977087	1.28596275	-1.62336873
79	2.40599812	0.99102291	0.96877743
47	1.40083634	0.78895232	3.58930122
47	-0.10653860	2.17116699	1.73862461
47	-2.03299881	2.45159710	-0.19636261
47	-3.81579222	2.91707602	-2.20602697
47	0.64828600	1.91662249	-0.95208591
8	-0.48798680	1.67127095	3.81994377
8	2.92339485	-0.24624008	2.57196830

R₁₁

Atomic number	X	Y	Z
47	-1.37947640	-2.61373371	2.01059453
47	-2.96095682	-2.06015282	-0.45966821
47	-0.49851640	-3.43142759	-0.54706913
47	-2.68307075	-4.64191182	0.60467308
47	1.00859779	-1.41993725	0.96331305
47	1.66815347	-2.31678195	-1.81389787
47	-0.68389285	-0.76264748	-1.55954072
47	-3.16821971	0.54231788	-1.41297301
47	-1.72453055	0.03911673	1.04075714
47	-0.23004553	-0.51773529	3.37623875
47	-0.83884048	1.91270533	-2.46228955

47	1.60450285	0.49858757	-2.47805486
47	3.99782651	-0.94312447	-2.37891904
47	3.15301275	0.32376823	0.04778841
79	1.89477149	1.03941657	2.33015649
47	0.78440572	1.65563243	4.76875701
47	-0.69752909	2.24552735	2.46183721
47	-2.03998823	2.70574149	0.08830920
47	-3.37250829	3.14175189	-2.30751699
47	0.57178428	1.52551033	-0.06306975
8	4.02700809	-1.88126697	-0.09302137
8	2.97040655	-2.66926927	0.24137242

TS₁₂

Atomic number	X	Y	Z
47	-1.81132329	-2.35350911	1.88494349
47	-2.98821069	-1.79947156	-0.69467864
47	-0.47756715	-3.21033231	-0.77060897
47	-2.76423252	-4.39704506	0.27033406
47	0.58761798	-1.30324631	1.04168168
47	1.88687514	-1.87742856	-1.60353979
47	-0.66795173	-0.56028923	-1.73242714
47	-3.16455773	0.82027484	-1.57975152
47	-1.85250291	0.29894106	0.87550563
47	-0.55697159	-0.27829469	3.33628350
47	-0.82570812	2.16428348	-2.60006842
47	1.55770055	0.81196729	-2.83825646
47	3.88385161	-0.57369188	-3.20394054
47	3.35051132	0.50104323	-0.72787729
79	1.93675310	0.90868400	2.39385373
47	0.78458118	1.84491509	4.62450209
47	-0.44902127	2.42571358	2.20612763
47	-1.87894608	2.96135110	-0.08569272
47	-3.27260525	3.45690271	-2.44659081
47	0.64773749	1.55189544	-0.22807292
8	3.48437612	0.11478604	1.41215817
8	2.58959445	-1.50744861	0.46611549

P₁₂

Atomic number	X	Y	Z
47	-1.65080457	-2.34335302	1.87536490
47	-3.03231670	-1.78983972	-0.68895780
47	-0.73322908	-3.40061797	-0.57303666
47	-3.07834731	-4.32812888	0.42177080
47	0.92079716	-1.30077717	0.88758435
47	2.11100734	-1.81843144	-1.90454030
47	-0.65221912	-0.60078547	-1.67908737
47	-3.14423208	0.80214728	-1.60895901
47	-1.78900499	0.27308803	0.86335588
47	-0.35592505	-0.32248865	3.22075410

47	-0.83033442	2.12095143	-2.59377666
47	1.56930461	0.80910612	-2.76429113
47	4.07485565	-0.35196050	-3.06896918
47	3.20989852	0.27279326	-0.49289873
79	1.94385438	1.07051613	2.36694431
47	0.70493078	1.81995577	4.65272483
47	-0.54489741	2.43371818	2.25083404
47	-1.92094320	2.95165841	-0.08895484
47	-3.26678575	3.43363498	-2.49138326
47	0.61677216	1.58472456	-0.18062490
8	3.65060091	0.92410918	1.39897394
8	1.32181577	-3.05739049	-0.44100859

R₁₂

Atomic number	X	Y	Z
47	-2.10350852	-2.37484174	1.31746430
47	-3.32069105	-1.31650199	-1.09346067
47	-1.04001225	-3.12763227	-1.27048996
47	-3.53449493	-4.00110935	-0.41941478
47	0.46798942	-1.47180559	0.48531430
47	1.42239048	-2.17598816	-2.10090147
47	-0.79571032	-0.39491455	-2.02750933
47	-3.02073965	1.35831079	-1.75267065
47	-1.89063041	0.39325442	0.66839687
47	-0.65108366	-0.71728998	2.96554561
47	-0.42383783	2.36279893	-2.62472341
47	1.73742386	0.64478774	-2.80048657
47	3.86716020	-1.13687707	-2.91546282
47	2.95473097	-0.41003718	-0.40096913
47	2.00610176	0.30056900	2.10144001
79	0.80682561	1.03407252	4.47992943
47	-0.32166413	2.14632917	2.25365259
47	-1.48556884	3.12499827	-0.04044532
47	-2.63403515	4.02882028	-2.40257831
47	0.79457318	1.42271962	-0.22910286
8	4.31526544	-0.09613217	3.01365567
8	4.49267004	-1.11412167	3.71915078

TS₁₃

Atomic number	X	Y	Z
47	-1.73909890	-2.26071989	1.57187385
47	-3.12745456	-1.45712525	-0.80541487
47	-0.81566066	-3.19344750	-1.11866605
47	-3.16613287	-4.10000899	0.05522418
47	0.76563220	-1.59306803	0.49897277
47	1.60466058	-2.14191613	-2.10976946
47	-0.63705383	-0.45264167	-1.79676164
47	-2.99228792	1.15467172	-1.69622606

47	-1.71082121	0.43812348	0.76709186
47	-0.05956445	-0.39952506	2.99275500
47	-0.48591511	2.25670674	-2.65618861
47	1.80048609	0.72672059	-2.70999330
47	3.98317789	-0.95734338	-2.94930381
47	3.13011532	-0.26783773	-0.43122314
47	2.13938127	1.38986979	2.41833470
79	0.57253546	1.81744239	4.61096580
47	-0.47150573	2.50438499	2.21044437
47	-1.59214973	3.15113341	-0.18807758
47	-2.81365934	3.79650846	-2.58412703
47	0.81820903	1.55683393	-0.17621096
8	3.02615920	-0.39036492	1.69189876
8	1.77094748	-1.57839669	2.40440089

P₁₃

Atomic number	X	Y	Z
47	-1.86797871	-2.59256430	1.41626042
47	-3.12082545	-1.49283581	-0.85600462
47	-0.73427133	-3.17018572	-1.09608522
47	-3.22229707	-4.20976384	-0.30734327
47	0.79782989	-1.36139203	0.73787964
47	1.68400437	-2.04233059	-1.89004716
47	-0.67038702	-0.45742170	-1.83052479
47	-3.01628708	1.13757542	-1.65486461
47	-1.70837728	0.36309994	0.79273039
47	-0.11877297	-0.16240291	3.31173715
47	-0.52604364	2.25616368	-2.66118811
47	1.75083655	0.67862931	-2.77544507
47	3.97575367	-0.94972063	-2.99075904
47	3.15934215	-0.14981112	-0.44556922
47	2.21124220	1.06604459	2.30978625
79	0.89728491	1.99117523	4.54199957
47	-0.38628467	2.48591906	2.18687683
47	-1.60762168	3.09917152	-0.15259795
47	-2.86106188	3.77026941	-2.53949703
47	0.77061688	1.46272830	-0.20194025
8	3.93544100	0.69160644	1.25307964
8	-0.21672279	-2.09932033	2.59450832

R₁₃

Atomic number	X	Y	Z
47	-0.99427706	-2.68705964	1.96973562
47	-2.79036069	-2.25450635	-0.34519482
47	-0.23134537	-3.58339119	-0.61866552
47	-2.36646628	-4.76854038	0.75026113
47	1.19359434	-1.40137255	0.60753423
47	1.82729161	-2.39912987	-2.02375054

47	-0.61392814	-0.97636372	-1.70694947
47	-3.11018658	0.36332512	-1.28654492
47	-1.51077724	-0.12701470	0.93677360
47	0.22973655	-0.46874133	3.12635565
47	-0.90301186	1.66422009	-2.71145511
47	1.51052606	0.31804681	-3.03008747
47	3.84828591	-1.12093604	-3.41843104
47	3.28262115	-0.21924081	-0.83216155
47	2.57345128	0.85579008	1.59761178
79	1.27695441	1.90938675	4.03454399
47	-1.06116998	2.05087328	2.57640481
47	-1.70121932	2.61331081	-0.10751386
47	-3.34995127	2.94843960	-2.27423310
47	0.86550921	1.40384054	-0.51528937
8	0.29802936	2.98446178	1.05268276
8	1.72669506	2.89460111	2.21837282

TS₁₄

Atomic number	X	Y	Z
47	-0.99427711	-2.68705956	1.96973560
47	-2.79036061	-2.25450630	-0.34519484
47	-0.23134545	-3.58339117	-0.61866549
47	-2.36646627	-4.76854044	0.75026114
47	1.19359416	-1.40137249	0.60753424
47	1.82729153	-2.39912982	-2.02375046
47	-0.61392818	-0.97636365	-1.70694944
47	-3.11018666	0.36332521	-1.28654492
47	-1.51077731	-0.12701462	0.93677357
47	0.22973647	-0.46874125	3.12635573
47	-0.90301189	1.66422019	-2.71145508
47	1.51052598	0.31804689	-3.03008753
47	3.84828597	-1.12093590	-3.41843103
47	3.28262124	-0.21924074	-0.83216153
47	2.57345121	0.85579015	1.59761178
79	1.27695435	1.90938683	4.03454397
47	-1.06117005	2.05087319	2.57640489
47	-1.70121948	2.61331089	-0.10751388
47	-3.34995133	2.94843949	-2.27423322
47	0.86550914	1.40384071	-0.51528934
8	0.29802928	2.98446169	1.05268276
8	1.72669497	2.89460119	2.21837275

P₁₄

Atomic number	X	Y	Z
47	-1.21377551	-2.61175910	2.00168250
47	-2.79240007	-2.25629954	-0.33888294
47	-0.16532335	-3.47172421	-0.44844488
47	-2.33415755	-4.79335297	0.68740866

47	1.04597436	-1.10106291	0.77787822
47	1.89127235	-2.26769200	-1.78682310
47	-0.61226855	-0.91844742	-1.62576254
47	-3.20960776	0.24849273	-1.39748721
47	-1.63877119	0.01448670	0.96594076
47	-0.15101137	-0.51041068	3.34454054
47	-1.01692532	1.55393565	-2.92352480
47	1.45523567	0.33627850	-3.08777505
47	3.88341349	-1.04590420	-3.29178185
47	3.15918583	0.03893346	-0.85473623
47	2.62514468	1.23328343	1.52812480
79	1.58658963	1.31814104	4.32971360
47	-0.04883625	2.08783824	2.31127686
47	-2.02805769	2.63733224	-0.51221220
47	-3.61482277	2.65291367	-2.71964820
47	0.75053735	1.59317410	-0.61393158
8	-0.30402354	3.16976523	0.54554540
8	3.40979795	1.47602350	3.46952536

R₁₄

Atomic number	X	Y	Z
47	-1.14397799	-2.77476641	1.48888791
47	-2.93644172	-2.17384992	-0.68455757
47	-0.38832654	-3.49632244	-1.22293697
47	-2.45584542	-4.79225531	0.10532935
47	1.00858079	-1.44839187	0.16304682
47	1.63701011	-2.12170357	-2.51957976
47	-0.85941527	-0.83291412	-2.10490321
47	-3.33663553	0.44433903	-1.50226750
47	-1.62954230	-0.07408673	0.70249331
47	0.15868398	-0.70328664	2.78379465
47	-1.20387588	1.87882448	-2.90005300
47	1.22061322	0.62716728	-3.37680667
47	3.62502530	-0.67737900	-3.79480509
47	3.02719109	0.05121060	-1.16665009
47	2.27085486	0.74513428	1.41102339
79	1.42516517	1.42244237	3.96923673
47	-0.26556284	2.07915919	1.91406817
47	-1.96856341	2.61554544	-0.20181701
47	-3.65539294	3.07134602	-2.35372305
47	0.57314954	1.42034815	-0.73397795
8	3.09908685	3.24059181	5.56102303
8	2.73471415	1.99962742	5.51323723

TS₁₅

Atomic number	X	Y	Z
47	-1.18402653	-2.73056347	1.55788512
47	-2.88222908	-2.19704774	-0.68456893

47	-0.29843156	-3.47341618	-1.12166795
47	-2.37415631	-4.80592951	0.14564654
47	0.97466520	-1.36011107	0.28154749
47	1.73760745	-2.06901431	-2.35668929
47	-0.79861381	-0.83462712	-2.07011577
47	-3.31281314	0.40800083	-1.56878257
47	-1.69871629	-0.04045016	0.70830395
47	0.00313879	-0.58476163	2.86539193
47	-1.17933949	1.85412793	-2.93014777
47	1.28677643	0.65511761	-3.28248141
47	3.75206706	-0.59042340	-3.56683241
47	3.01869180	0.15951235	-1.00206728
47	2.15653720	0.87968019	1.53994594
79	1.06247948	1.59342837	4.17705542
47	-0.44757958	2.14236711	1.93964087
47	-2.07074809	2.63222939	-0.26235234
47	-3.66604624	3.00620679	-2.50577872
47	0.50664483	1.47023096	-0.67960591
8	2.48675438	2.23058668	5.36254823
8	2.92733739	1.65485584	3.45312430

P₁₅

Atomic number	X	Y	Z
47	-1.23710969	-2.71205270	1.72124643
47	-2.88922927	-2.21946289	-0.63934098
47	-0.21387994	-3.34073262	-0.81284058
47	-2.33026254	-4.79683102	0.20026709
47	0.92973958	-1.04478244	0.65709719
47	1.77818189	-1.95958141	-2.03603580
47	-0.78457433	-0.77621787	-1.88745732
47	-3.33235061	0.41129367	-1.48645325
47	-1.79601237	-0.07213537	0.82076466
47	-0.52217472	-0.58898298	3.23104563
47	-1.22089650	1.87277707	-2.87656025
47	1.23176360	0.66428445	-3.27744705
47	3.67131422	-0.64240857	-3.61876353
47	3.08573210	0.30470325	-1.10977256
47	2.51926647	1.42279859	1.26356821
79	1.61550298	1.30784848	3.84075531
47	-0.30131714	2.07283665	1.96445207
47	-2.04238146	2.60521736	-0.14349958
47	-3.66166594	3.07437577	-2.32100346
47	0.53480235	1.57863605	-0.68748028
8	-0.33003695	1.39578982	4.19115377
8	3.42716254	1.18656298	3.16054161

R₁₅

Atomic number	X	Y	Z
---------------	---	---	---

47	-1.75419242	-2.39880514	1.82154332
47	-3.04905278	-1.75032175	-0.69007580
47	-0.55341550	-3.11033778	-0.74723142
47	-2.89255968	-4.35131708	0.23801962
79	0.81210896	-1.65986869	1.26899538
47	1.79904052	-1.72499127	-1.39917345
47	-0.71665734	-0.53138381	-1.88738654
47	-3.17797435	0.86090179	-1.55825881
47	-1.55155363	0.19369608	0.74864269
47	-0.48517735	-0.33200891	3.32404215
47	-0.91812568	2.21492984	-2.72772776
47	1.51781433	0.90508489	-2.88759492
47	3.82427473	-0.62375005	-3.01468589
47	3.23188121	0.68430660	-0.67490309
47	1.82315660	0.96874046	2.08722969
47	0.83103640	1.80742614	4.52398564
47	-0.51149773	2.43138906	2.17827155
47	-1.96571050	2.94455577	-0.11000848
47	-3.37036592	3.50996449	-2.43067107
47	0.59300124	1.77790704	-0.37990913
8	3.49912316	-0.23816945	1.31163833
8	3.01484586	-1.57794589	1.00525803

TS₁₆

Atomic number	X	Y	Z
47	-1.84069224	-2.35617144	1.90478415
47	-2.96907389	-1.80757072	-0.70540492
47	-0.46912058	-3.21685759	-0.73000587
47	-2.77378652	-4.40071680	0.27554879
47	0.55967829	-1.31072044	1.09856001
47	1.88698302	-1.92614605	-1.63595223
47	-0.64644699	-0.56844037	-1.73232444
47	-3.13940832	0.81481901	-1.59550535
47	-1.83187510	0.29213237	0.86885633
47	-0.59243209	-0.27639322	3.37212088
47	-0.82377234	2.16024644	-2.62530885
47	1.53799542	0.82403334	-2.85685525
79	3.82658068	-0.54679005	-3.18674393
47	3.40231578	0.52329976	-0.71684360
47	1.93788985	0.90103331	2.39666723
47	0.72532647	1.81591463	4.66479787
47	-0.44074737	2.40905072	2.21633396
47	-1.81967190	2.95610496	-0.10512126
47	-3.26662692	3.46468308	-2.42726076
47	0.67981267	1.53644617	-0.23593321
8	3.56190434	0.19086519	1.34826603
8	2.49516829	-1.47882182	0.40732457

P₁₆

Atomic number	X	Y	Z
47	-0.64338276	-3.33120971	1.24694841
47	-2.16734881	-2.69733046	-1.03384153
47	0.43979871	-3.94171210	-1.27892913
47	-1.75159748	-5.35109178	-0.28566184
47	1.62473037	-1.80150701	0.24748113
47	2.56493375	-2.57186303	-2.33681525
47	0.04561082	-1.22490927	-2.11815401
47	-2.58255031	-0.11508107	-1.85316564
47	-1.01480529	-0.54177107	0.49549967
47	0.42502805	-1.39881299	2.80307696
47	-0.32398289	1.39519985	-3.04261757
47	2.15576348	0.21169754	-3.27561008
47	4.60049433	-1.21666623	-3.62925077
47	3.87903279	-0.41527485	-1.14679057
47	2.69889418	0.22855655	2.12160739
79	1.46168959	0.43179732	4.53907850
47	0.17371779	1.43363675	2.35878633
47	-1.54826484	2.17505401	-0.63684397
47	-2.98939103	2.40582971	-2.91616797
47	1.35661916	1.23752684	-0.67314570
8	3.42246658	0.95215740	0.32868001
8	0.01328604	2.57928968	0.64895199

R₁₆

Atomic number	X	Y	Z
47	-2.33300084	-2.10968369	1.55873500
47	-3.44191023	-1.22422013	-0.98271263
47	-1.23633871	-3.12201690	-0.93529702
47	-3.78183655	-3.82395283	-0.07421981
47	0.28757573	-1.38746927	0.72436652
47	1.28814316	-2.32695039	-1.75131371
47	-0.86467493	-0.47591704	-1.90883345
47	-3.01711681	1.37324788	-1.84996799
47	-2.00512859	0.57570074	0.68369859
47	-0.85995119	-0.35629085	3.11234140
47	-0.36487290	2.20644716	-2.71091930
47	1.73715608	0.40220879	-2.65092343
47	3.78044655	-1.45682519	-2.58711143
47	2.86977433	-0.50020047	-0.11785915
47	1.77861412	0.48535239	2.24986445
47	0.64940035	1.44565683	4.59193972
47	-0.41648497	2.37864402	2.20161576
47	-1.46135755	3.21584409	-0.21838288
47	-2.50891576	3.97299839	-2.67481223
47	0.74831498	1.42253732	-0.21288947

8	5.08551504	-0.82911976	0.95630560
8	5.37272055	-1.94598111	1.44935620

TS₁₇

Atomic number	X	Y	Z
47	-1.83073996	-2.22433516	1.58145749
47	-3.14728913	-1.45047845	-0.84935874
47	-0.81258375	-3.16995943	-1.06451204
47	-3.19073862	-4.09917991	-0.03878002
47	0.81069858	-1.60072328	0.56490212
47	1.59179159	-2.13925068	-2.06265783
47	-0.64825522	-0.45416960	-1.75870865
47	-2.99023302	1.15212587	-1.74554099
47	-1.77593186	0.44109069	0.79815046
47	-0.11972504	-0.44148007	2.97765803
47	-0.50534279	2.24118680	-2.68552581
47	1.78153977	0.71320476	-2.71702634
47	3.94773604	-0.98808170	-2.96754453
47	3.12978989	-0.22333488	-0.43265048
47	2.09522991	1.29347008	2.40695464
47	0.57327495	1.76109593	4.65042573
47	-0.43178876	2.48276181	2.21123639
47	-1.57986451	3.13116483	-0.19399154
47	-2.81163154	3.81644174	-2.59505725
47	0.79514502	1.52758367	-0.18165856
8	3.26200348	-0.29990031	1.66213427
8	1.85691470	-1.46923294	2.44009450

P₁₇

Atomic number	X	Y	Z
47	-1.91108084	-2.57040759	1.41119478
47	-3.14994980	-1.48001345	-0.88260708
47	-0.76878512	-3.16533249	-1.09572604
47	-3.26406871	-4.19070159	-0.30910327
47	0.75516629	-1.36428865	0.75686632
47	1.66244656	-2.04326404	-1.85920032
47	-0.69384714	-0.45870642	-1.84822359
47	-3.02397958	1.15125284	-1.68144814
47	-1.74038814	0.37329509	0.77232832
47	-0.16037696	-0.12486332	3.31016913
47	-0.52914939	2.25160994	-2.67614363
47	1.74692368	0.66253191	-2.77314938
47	3.97227588	-0.97281028	-2.94644180
47	3.14431069	-0.15025347	-0.41588702
47	2.14290562	1.01122600	2.30233938
47	0.92296940	2.00735431	4.60288392
47	-0.37094427	2.46174061	2.19883605
47	-1.60157333	3.10307529	-0.14984619
47	-2.84446053	3.78293659	-2.55101693

47	0.75052117	1.45441427	-0.21987486
8	3.90592397	0.72608884	1.27772721
8	-0.28137586	-2.08202157	2.61750267

TS₁₈

Atomic number	X	Y	Z
47	-0.95678564	-2.67446145	1.95759912
47	-2.76038486	-2.22726315	-0.33029637
47	-0.22648338	-3.60282860	-0.65457079
47	-2.35438248	-4.76651847	0.71114728
47	1.20221801	-1.41652609	0.63430216
47	1.82001847	-2.41505630	-2.04279252
47	-0.60817043	-0.98824796	-1.71643419
47	-3.07942927	0.38043290	-1.28432095
47	-1.46600298	-0.06838253	0.93868900
47	0.21751815	-0.42725487	3.13691241
47	-0.90533932	1.65477977	-2.71716286
47	1.50913375	0.31639962	-3.03855319
47	3.83884763	-1.13088895	-3.44491926
47	3.26971671	-0.25064633	-0.83522409
47	2.56370143	0.88358462	1.58020149
47	1.19998894	2.02985613	3.94839130
47	-1.29825438	2.03853676	2.71793347
47	-1.67329268	2.66684589	-0.05388618
47	-3.31646547	2.94729566	-2.28253967
47	0.84415050	1.38824089	-0.52199231
8	0.26875635	2.75073176	1.16748561
8	1.91094078	2.91136953	2.13002991

P₁₈

Atomic number	X	Y	Z
47	-1.16765081	-2.64962952	1.97869222
47	-2.78647735	-2.25696413	-0.33355037
47	-0.18264001	-3.50751490	-0.51968867
47	-2.34367995	-4.80625014	0.65928025
47	1.05074341	-1.19372428	0.73648299
47	1.88844870	-2.27430691	-1.83115234
47	-0.61564693	-0.92901295	-1.64754936
47	-3.20116944	0.26420306	-1.37059405
47	-1.61147584	-0.00410520	0.96073631
47	-0.06839919	-0.51445994	3.29250503
47	-1.01406443	1.57439699	-2.88634586
47	1.46550255	0.36680426	-3.04646911
47	3.90353990	-0.99452915	-3.25415443
47	3.14687989	0.02392479	-0.79699294
47	2.50675654	1.12393040	1.63038408
47	1.55634983	1.38322782	4.45041233
47	-0.11161831	2.08579022	2.35728503

47	-2.01593451	2.65173277	-0.46229262
47	-3.60955829	2.68031657	-2.66547282
47	0.73136032	1.57296301	-0.55995059
8	-0.28199723	3.18984336	0.57893782
8	3.39087183	1.38227659	3.47691971
