

## Supporting Information

# The Importance of Charge Redistribution during Electrochemical Reactions: A Density Functional Theory Study of Silver Orthophosphate ( $\text{Ag}_3\text{PO}_4$ )

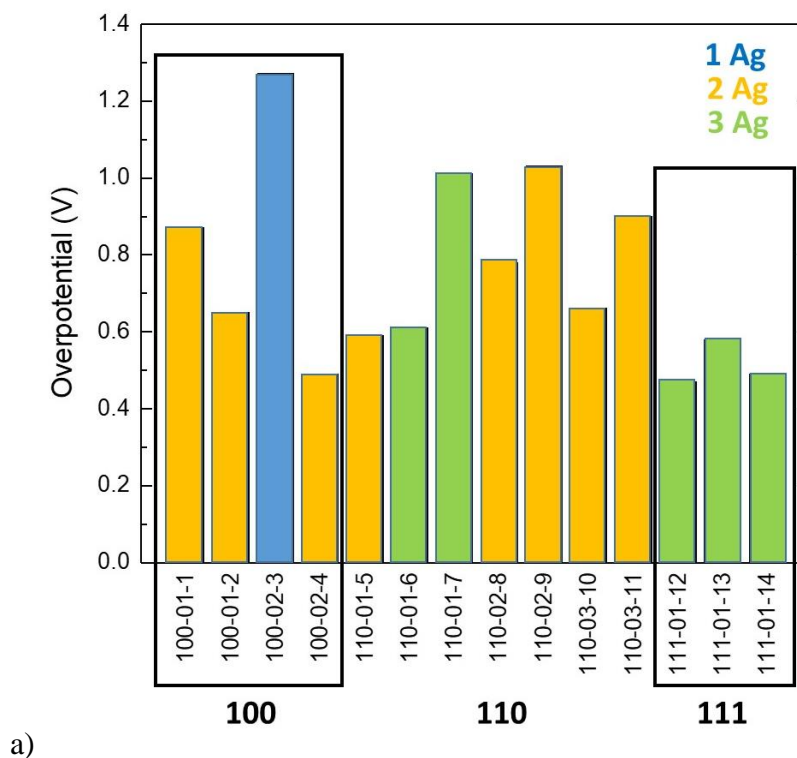
Xi Cao<sup>1</sup>, Xueqing Zhang<sup>2, 3\*</sup>, Rochan Sinha<sup>2</sup>, Shuxia Tao<sup>1\*</sup>, Anja Bieberle-Hütter<sup>2, 3\*</sup>

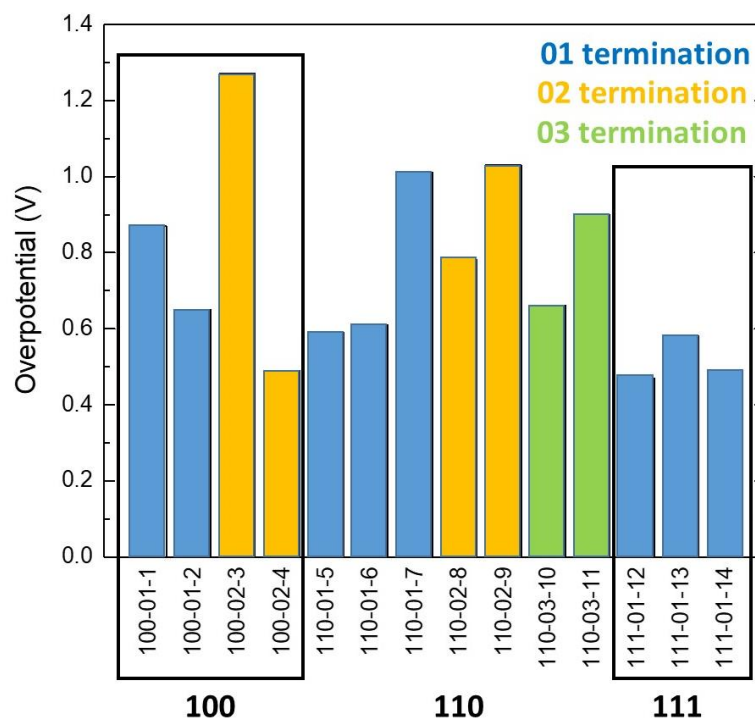
1. Center for Computational Energy Research, Department of Applied Physics, Eindhoven University of Technology, P.O. Box 513, 5600MB, Eindhoven, The Netherlands.

2. Electrochemical Materials and Interfaces, Dutch Institute for Fundamental Energy Research (DIFFER), De Zaale 20, 5612AJ, Eindhoven, The Netherlands.

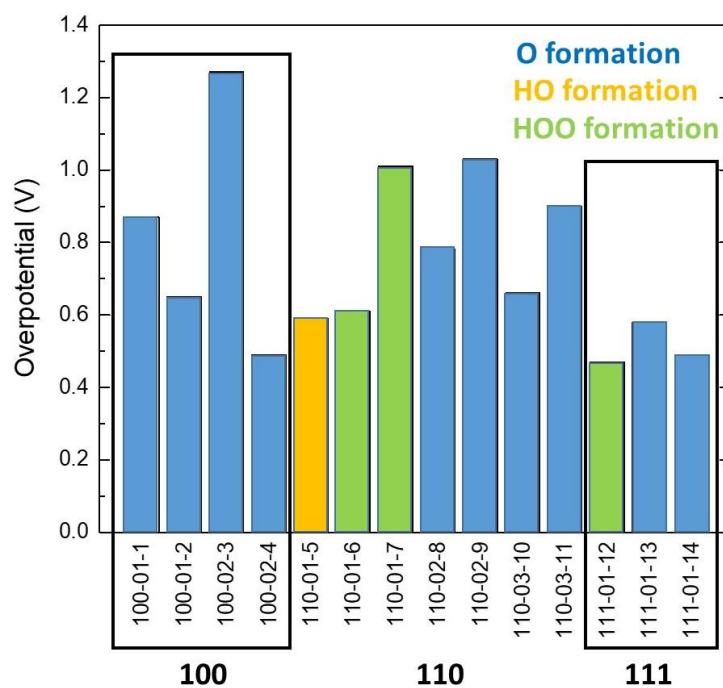
3. Center for Computational Energy Research, Dutch Institute for Fundamental Energy Research (DIFFER), De Zaale 20, 5612AJ, Eindhoven, The Netherlands.

Figure S1 shows the overpotential data of all 14 geometries sorted by number of Ag atoms involved in the adsorption of the intermediate species, different surface terminations, and different potential determining reaction steps. None of these ordering parameters unambiguously explains the trend in overpotential.





b)



c)

Figure S1. DFT calculated overpotentials of all 14 geometries sorted according to (a) the number of Ag atoms involved in the adsorption of the intermediate species, (b) different surface terminations, and (c) different potential determining reaction steps.

Fig. S2 shows the PDOS data of three selected structures, i.e. 100-02-03, 110-02-8 and 111-01-12, respectively. It is seen that the first PDOS peak from below Fermi level (occupied states) for 111-01-12 (overpotential = 0.47 V) shifts to above Fermi level (unoccupied states) for 110-02-8 (overpotential = 0.78 V) and even further for 100-02-3 (overpotential = 1.27 V). The more states in the Fermi level, the higher the overpotential.

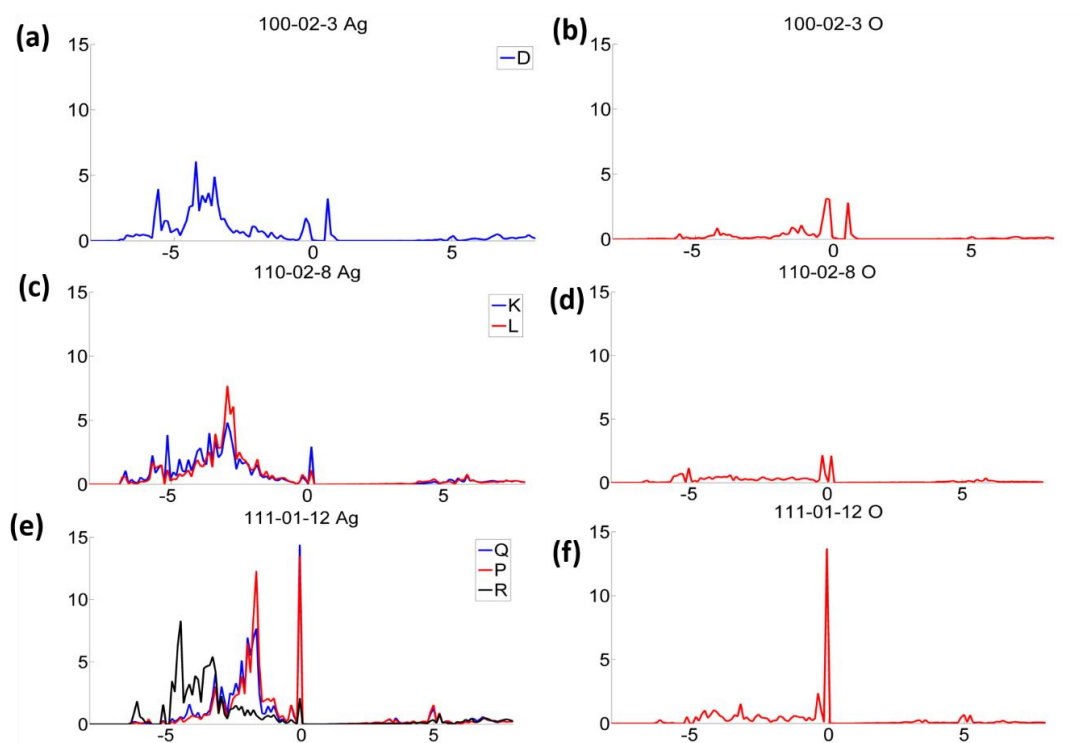


Figure S2. PDOS (partial density of states) of active Ag sites and  $O_{ad}$  on three selected structures of 100-02-03, 110-02-8 and 111-01-12, respectively.

Table S1 summarizes the 14 geometries with their calculated overpotentials, Bader charges for oxygen, charge redistribution, and potential determining step.

Table S1. The calculated overpotentials, Bader charges of oxygen (BC), charge redistributions (CR), and potential determining steps (PDS).

Geometry	Overpotential [V]	BC <sub>HO</sub>	BC <sub>O</sub>	BC <sub>HOO</sub>	CR <sub>O</sub> = BC <sub>HO</sub> - BC <sub>O</sub>	CR <sub>HOO</sub> = BC <sub>O</sub> - BC <sub>HOO</sub>	CR <sub>O</sub> - CR <sub>HOO</sub>	Potential determining step
111-01-12	0,47	7,061	6,7442	6,4519	0,3168	0,2923	0,0245	HOO formation
100-02-4	0,49	7,0195	6,6221	6,3772	0,3974	0,2449	0,1525	O formation
111-01-14	0,49	7,1936	6,7597	6,4427	0,4339	0,317	0,1169	O formation
111-01-13	0,58	7,2989	6,8156	6,4848	0,4833	0,3308	0,1525	O formation
110-01-5	0,59	6,9952	6,6957	6,4232	0,2995	0,2725	0,027	HO formation
110-01-6	0,61	7,4324	6,7749	6,5075	0,6575	0,2674	0,3901	HOO formation
100-01-2	0,65	6,9962	6,6208	6,3894	0,3754	0,2314	0,144	O formation
110-03-10	0,66	7,0673	6,5464	6,3386	0,5209	0,2078	0,3131	O formation
110-02-8	0,78	7,0328	6,6648	6,4047	0,368	0,2601	0,1079	O formation
100-01-1	0,87	7,003	6,6309	6,4236	0,3721	0,2073	0,1648	O formation
110-03-11	0,9	7,0827	6,6961	6,4575	0,3866	0,2386	0,148	O formation
110-01-7	1,01	7,1666	6,8136	6,5423	0,353	0,2713	0,0817	HOO formation
110-02-9	1,03	7,3063	6,5689	6,2418	0,7374	0,3271	0,4103	O formation
100-02-3	1,27	6,9425	6,5106	7,3293	0,4319	-0,8187	1,2506	O formation

In the following, the POSCAR data of the optimized geometries from Table 1 in the main manuscript are listed.

### 100-01-2

Bare Surface:

Ag3PO4

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6.0999009999958309 -0.0000071330448850 0.0000000000000000

0.0000000000000000 6.0999010000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 36.2119748865923228

O P Ag

36 9 26

Direct

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### Surface connecting OH<sub>ad</sub>:

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0.0000000000000000	0.0000000000000000	36.2119748865923228

O	P	Ag	H
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Direct

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Surface connecting  $O_{ad}$ :

Ag<sub>3</sub>PO<sub>4</sub>

1.000000000000000		
6.0999009999958309	-0.0000071330448850	0.0000000000000000
0.0000000000000000	6.0999010000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	36.2119748865923228

O    P    Ag

37    9    26

Direct

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0.5920123803347790	0.4885322327713690	0.6139302607095346
0.4061998677134327	0.6288091697343979	0.0235953593831954
0.4674872057137538	0.7557043260186063	0.1919088656654680
0.4593926290986750	0.7536389852487938	0.3625533911597079

0.4233657513447943	0.8028066339145664	0.5336797759050717
0.4714844688689785	0.5045471555376370	0.7211610353503047
0.3078100563341226	0.1555451509134861	0.0253234587955053
0.4618076918044705	0.2613900604555062	0.1949388249320705
0.4550135993025400	0.2644175354873128	0.3614654320997112
0.4363218100038427	0.2997296539817506	0.5305747118710685
0.6209949841926037	-0.0737563808200603	0.6967514207352754

Surface connecting OOH<sub>ad</sub>:

Ag<sub>3</sub>PO<sub>4</sub>

1.0000000000000000		
6.0999009999958309	-0.0000071330448850	0.0000000000000000
0.0000000000000000	6.0999010000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	36.2119748865923228

O	P	Ag	H
38	9	26	1

Direct

0.8217022970494993	0.0451620363733730	0.7736016988591797
0.8428356703693449	0.9140810355856548	0.7413392751042480
0.0663532742112635	0.6431212625790038	0.0395036241114830
0.0749837447721743	0.5982478259922792	0.2207615580000760
0.0905961276736983	0.5782193171538803	0.3908848253976855
0.0703184473088724	0.5903334881907547	0.5617685891567399
0.1508987823322802	0.6060218955833193	0.7195144942312660
0.7214673539707392	0.5807220721050942	0.0011345755665220
0.8134471804405556	0.5756657684463059	0.1657368750640361
0.8157910226140807	0.6068708232924053	0.3375598475228176
0.8057642630857096	0.6245412065786902	0.5068426420430666

0.8900084109207489 0.6208505705674928 0.6646538134345332  
0.0507741085020990 0.3239559018747254 0.9934851576840243  
0.1298887884887061 0.3023780068030528 0.1713557736206278  
0.1211835330245744 0.3185683769733127 0.3363080259376045  
0.1007987946624085 0.3257768731269873 0.5069521264017969  
0.0972912561738191 0.2722341867439084 0.6778544008647343  
0.8217477448976074 0.3124447213469043 0.0529054564143288  
0.8057731608597927 0.2794879414789360 0.2157525603724968  
0.7996019307382983 0.2782342328572773 0.3812864056790775  
0.7757109850235657 0.2981939790418517 0.5509602008613175  
0.7953139703769682 0.3889143202004816 0.7223973637559896  
0.6242197620523244 0.0736789705160145 0.1363759112849024  
0.6249419211014404 0.0959276507205329 0.2970126627601293  
0.6061036202729972 0.1157833808744700 0.4668636806441978  
0.6191632057261502 0.1507978377822713 0.6320112143328771  
0.3270056801165150 0.1232977941072768 0.0875073358518901  
0.2991440285145163 0.0946281021290744 0.2525509525580528  
0.2908011248451983 0.0785586647262692 0.4206414489527600  
0.2559493102875781 0.1038613128608537 0.5962618944939810  
0.3062742452634854 0.8040159970534086 0.1330303069534269  
0.3089603555725896 0.8255591787847431 0.3066045419002294  
0.3201261312178336 0.8116830040437695 0.4751734700690735  
0.3591509595154335 0.8538826588700607 0.6523319407621995  
0.5939013356360314 0.8016689636609420 0.0820054561043917  
0.5720383117852728 0.7752029152395186 0.2523979306061627  
0.5962795084898065 0.7926352404215306 0.4221018057477953  
0.5529793809153953 0.8170558645085345 0.5908383793035160  
0.9124367807711026 0.4625702542663662 0.0203966575533448

0.9570862068887221 0.4391865470067118 0.1930368262862516  
0.9536054841212745 0.4474373263756589 0.3616339659774244  
0.9350557789473524 0.4640725383132027 0.5319432041596852  
0.9750454836475901 0.4725070870958730 0.6963565547429152  
0.4691596506960782 0.9520518273560115 0.1091011488250906  
0.4493597446303761 0.9501162350129567 0.2768754819539123  
0.4500158687860268 0.9523245340515079 0.4464638605727607  
0.4414841836440571 0.9882937037271657 0.6181906291052037  
0.9045275292399152 0.9607362862089328 0.0498543335580483  
0.9495835358909550 0.9432930662741560 0.2245639599421363  
0.9465670393023111 0.9469279439741222 0.4099216054239232  
0.9241175747915454 0.9557544046876678 0.5762172378699979  
0.9683314918672428 0.9570236499216507 0.1386310671683301  
0.9557856760800039 0.9481411861862139 0.3102149942846182  
0.9475811405379713 0.9658703940989031 0.4940393995216854  
0.1207993397027785 0.9498183655231336 0.7006663919986196  
0.2874548606081507 0.4601249435577687 0.1095934184576323  
0.1411661297582204 0.4505577469473692 0.2774835478128446  
0.1261302053630112 0.4511258252146735 0.4478017674820380  
0.1108107386592311 0.4338619256228045 0.6189407253105352  
0.7949588088667725 0.4577580559834268 0.1080466871273941  
0.6379517969364383 0.4496277928678262 0.2794716987593385  
0.6278804100429282 0.4539573922492762 0.4456438357132966  
0.6008628885908086 0.4919916740990626 0.6166059773213465  
0.4064579855759397 0.6283515364664545 0.0235875462020478  
0.4664798434274213 0.7547412631862777 0.1918875899871536  
0.4567283179275400 0.7526831026188622 0.3626097198560213  
0.4270796851786353 0.7966328015249120 0.5331793332015617

0.4784965503041295	0.5045241251443675	0.7192288793464646
0.3060746164583584	0.1548514191225683	0.0255239596731253
0.4612622466708071	0.2603435891954934	0.1948337598387599
0.4536310697762538	0.2641295466147282	0.3615151916653250
0.4356630118867097	0.2929894880716488	0.5310939742277836
0.6128673847038402	0.9678710865960494	0.6960695268787476
0.8961380063434695	0.9510978394412426	0.7917688701821198

### 100-02-3

Bare Surface:

Ag<sub>3</sub>PO<sub>4</sub>

1.0000000000000000		
6.0999009999958309	-0.0000071330448850	0.0000000000000000
0.0000000000000000	6.0999010000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	32.5872412001630067

O P Ag

32 7 22

Direct

0.0285480028805707	0.5548713567452538	0.0957437377022665
0.1026650265226331	0.5815734480882994	0.2841872742985385
0.0763241004647347	0.6416502936969476	0.4672398566793822
0.0297982662285782	0.5986209785358708	0.6696377710435879
0.8720332467983221	0.5984734201726923	0.0231729489002928
0.8061825911362053	0.6306008066290276	0.2294012853623556
0.7788299714138971	0.5981972370712364	0.4118159622564908
0.8695648062346110	0.5523074591814322	0.5973998301294494
0.0538409881740938	0.2453336784736723	0.0443547937173817
0.0951262443144612	0.3263321563104297	0.2220436600037432



0.1019537473730507 0.3308631255083412 0.4147217286591567  
0.2177181280679214 0.3543595128063260 0.6163470337886926  
0.6786148684472075 0.3595637460545532 0.0766027748358862  
0.7991583852201373 0.2948293957527914 0.2771013081478422  
0.8050735327997049 0.3211373309516634 0.4701688575859914  
0.8440553997401473 0.2458039301635410 0.6497117749180158  
0.6520422036514908 0.0051036132432717 0.0119703409067897  
0.5757744702048624 0.1531428857400947 0.1836406313925199  
0.6181741106998667 0.1001760393130839 0.3703853952966215  
0.5823310549152236 0.0935286389935284 0.5696860812060303  
0.3071395313819724 0.0840712562440745 0.1243128317396578  
0.2996955498953485 0.0948541121961328 0.3191231981901483  
0.3147785826572208 0.1705279478750491 0.5106382994498557  
0.2477004936624793 0.0017953253456779 0.6812783790771251  
0.2677441288027723 0.8526650608482510 0.0401244386220202  
0.3100764606669648 0.8269830913883267 0.1862818314423704  
0.3070737263991882 0.8235084606492986 0.3791424139602275  
0.2540433763384050 0.8425635054227744 0.5580812063435948  
0.6318342371312862 0.8269603029807865 0.1358619476967700  
0.5799533681818717 0.7847468285256531 0.3191359198521296  
0.5747606462037742 0.8401428179568406 0.5076320966540493  
0.6314883585492398 0.8499452510217527 0.6511840526077909  
0.9078484157707156 0.4363212333951903 0.0606009126870744  
0.9466186441461826 0.4604590820689614 0.2531077660141459  
0.9418097261317382 0.4787589274171500 0.4407039328064876  
0.9898793240588648 0.4346465382116670 0.6326284912940190  
0.4561168443200371 0.9718795240797555 0.1579788620248783  
0.4497696831393831 0.9504089861962089 0.3469009483387609

0.4300869683423889	0.9862395302745468	0.5358629278473872
0.9692473498532328	0.9395156051689618	0.1212821086807813
0.9473768401409945	0.9485733878158149	0.2990231605862367
0.9512626815060590	0.9785272300595600	0.4786984775231351
0.9411531204558792	0.9303389171955774	0.6640748741173352
0.9579503382041366	0.9312321065325186	0.0284162539066543
0.9433699633126844	0.9673053803071694	0.2098831700529464
0.9516823232743064	0.9498251602027854	0.3880928433726739
0.9148642010323009	0.9428621995946491	0.5698877420919687
0.0945075261878799	0.4252642956145569	0.1562764928075179
0.1353872713792954	0.4494018582568916	0.3486837960037823
0.2815175622653769	0.4903015776313691	0.5410369622191151
0.6132573573939308	0.4737124713386883	0.1528463912038237
0.6357600289114685	0.4472185626202624	0.3453103867249782
0.8019466958949978	0.4213711322841810	0.5367857612305724
0.4994383912170320	0.6341789324870765	0.0145679165737836
0.4355109020632545	0.7414785473390129	0.2509649383669329
0.4526121650914152	0.7868106267099638	0.4436730411148563
0.4033250545559571	0.6293984031047385	0.6777971770600976
0.4642374970695215	0.1006393520185696	0.0598725374762483
0.4410542381408613	0.2341085855445657	0.2533023135189513
0.4496545581862424	0.2772862773279506	0.4409105231303113
0.4311857503301230	0.0972259893113341	0.6332089261306922

Surface connecting OH<sub>ad</sub> :

Ag<sub>3</sub>PO<sub>4</sub>

1.00000000000000

6.0999009999958309    -0.0000071330448850    0.0000000000000000

0.0000000000000000 6.0999010000000000 0.0000000000000000  
0.0000000000000000 0.0000000000000000 32.5872412001630067

O P Ag H

33 7 22 1

Direct

0.3548737543936820 0.5551654024100605 0.7541557774289984  
0.0251954832286390 0.5440387225760026 0.0953117736772506  
0.1114114233311600 0.5804316644037142 0.2826249649194053  
0.0832931430252001 0.6421473154923508 0.4665881386393490  
0.0124946570896674 0.5782552849437259 0.6685493000106478  
0.8539209491460548 0.5907223275906229 0.0244419115790222  
0.8149264511644818 0.6366160397217442 0.2278887851824377  
0.7904375337043378 0.6193150878162611 0.4101534861603137  
0.8709524495686157 0.5473399167633946 0.5951434261767697  
0.0478800272886834 0.2385810914686773 0.0429416344225680  
0.0947485827868651 0.3239529093525104 0.2211456379847304  
0.0998441839150040 0.3364708704651326 0.4125959517343378  
0.2194934062263108 0.3508895887999438 0.6137244456442451  
0.6774078701034261 0.3386965676829368 0.0782358316721996  
0.7970485464523220 0.3044542579065796 0.2759878996314098  
0.8007384805652582 0.3307611926741541 0.4671873278921924  
0.8500685964011692 0.2213328689933265 0.6438716540834184  
0.6430458175978740 -0.0015112922506007 0.0122445592861042  
0.5794243859479037 0.1496157537439053 0.1823413544962575  
0.6044630345066614 0.1226888408216454 0.3688900503340775  
0.5903479264776953 0.0882424760761231 0.5677220200388495  
0.3066474387690374 0.0768467197530666 0.1238099175933128  
0.2928695317046305 0.0936087708555976 0.3159778345187435

0.3221065819736028 0.1707024881912084 0.5088916758276125  
0.2520200461222293 0.9769315102891412 0.6788349317088173  
0.2580251496936864 0.8407391644227213 0.0419827095607384  
0.3132811075971921 0.8244680895339723 0.1860943764590779  
0.3122307592214338 0.8255001838228421 0.3762960297362026  
0.2595514048036234 0.8424587568841754 0.5557473306481167  
0.6320958745464063 0.8213146659172734 0.1350420610349882  
0.5950669242354307 0.8045646319850471 0.3179133101238255  
0.5796260168791532 0.8394417271954268 0.5048883000785780  
0.6148135336353830 0.8482794310400270 0.6556156137276412  
0.9004189950572121 0.4246061020389731 0.0608596156104789  
0.9500056529987313 0.4640239843812226 0.2521371576386270  
0.9442726972597181 0.4885329556529899 0.4392197803195721  
0.9896884723684012 0.4249231046268171 0.6304761272147292  
0.4584795541605380 0.9669548834881011 0.1575458000566296  
0.4491680811233206 0.9630153671487964 0.3449536817275807  
0.4373718349733849 0.9843285512732277 0.5338256234656854  
0.9714640874327088 0.9288259873966687 0.1229936040677336  
0.9458772324237467 0.9549130847757678 0.3033829423878948  
0.9582815739297763 0.9851422017838115 0.4817839784034003  
0.9391584541265982 0.9079436176018146 0.6631861613121499  
0.9486539931712978 0.9229801434206713 0.0292955260628265  
0.9481571382470027 0.9718304982858474 0.2128495970712184  
0.9479850410375480 0.9699781333856295 0.3924641392390253  
0.9250497769197334 0.9467652409247374 0.5703445532966858  
0.0938326971911617 0.4193889231137838 0.1557652048201520  
0.1353721511317190 0.4608460541192456 0.3473734134629123  
0.2834136103972673 0.4852904993398029 0.5423151707981058

0.6115190330895799	0.4726465738137547	0.1536846552335346
0.6345843479629562	0.4641811327648440	0.3445464488146245
0.8017005778882680	0.4257615085044731	0.5342732927663445
0.4848049422598643	0.6216242771071097	0.0145044740564488
0.4424015310354232	0.7413451588577887	0.2505976723480655
0.4490369972598763	0.7959097755383072	0.4412638932002469
0.4456792889466191	0.7219035257369619	0.7049791081128594
0.4605286153515845	0.0845843955221788	0.0608972455999836
0.4448840316413886	0.2401667605315190	0.2520277629753780
0.4466386128180819	0.2853777133301832	0.4401977237531672
0.4324402690597481	0.0996906100568020	0.6314434173656303
0.3789576140666508	0.6394255798542798	0.7792130184714686

### Surface connecting $O_{ad}$ :

Ag<sub>3</sub>PO<sub>4</sub>

1.0000000000000000		
6.0999009999958309	-0.0000071330448850	0.0000000000000000
0.0000000000000000	6.0999010000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	32.5872412001630067

O    P    Ag

33    7    22

Direct

0.3643238953422463	0.5960475346177674	0.7529343372323580
0.0250701713208266	0.5437815908728401	0.0955097047701653
0.1052736121483836	0.5808675123803082	0.2832831169107431
0.0792132097793037	0.6428155143938976	0.4669705434335383
0.0156119265459291	0.5787627678917404	0.6685561348965154
0.8555957517649677	0.5921370708310961	0.0245380586806363

0.8111405152580006 0.6324931755768082 0.2280500397004463  
0.7882383350367571 0.6145944549794322 0.4101347444652661  
0.8694708118979778 0.5494264280140535 0.5953092082673395  
0.0485300381907963 0.2391996325331361 0.0431576718760476  
0.0967692400165455 0.3247046320603090 0.2215716977239472  
0.1029917224302840 0.3376571119077761 0.4129863273001865  
0.2196666583713077 0.3543403334546730 0.6131412646879513  
0.6774105378045061 0.3401097319986848 0.0782664065346489  
0.7967981424931322 0.2987668340486042 0.2758380998359156  
0.8018916810878808 0.3272577161823151 0.4671821937746424  
0.8517168906620511 0.2221429837062789 0.6435951625418133  
0.6464872492723727 -0.0001972282931608 0.0124200541388531  
0.5793314698756729 0.1487614759777938 0.1825597198765757  
0.6109839885107227 0.1167015297151061 0.3686497729559317  
0.5906996999360863 0.0890360298835265 0.5676203332685811  
0.3070460330473242 0.0770880069809868 0.1238153216092774  
0.2936249314180434 0.0952940827623940 0.3169444822891437  
0.3219033758927202 0.1709928505689541 0.5089135812597723  
0.2502037868540203 -0.0133889162958624 0.6798512637468743  
0.2622194020542293 0.8423864870638216 0.0413829834531366  
0.3121634018648403 0.8246659173103429 0.1860640516515432  
0.3120617146332939 0.8265444203040083 0.3770526400846152  
0.2594546990971311 0.8436400341013350 0.5561822421859035  
0.6318600310301979 0.8210710347891813 0.1350947732073981  
0.5891755181866375 0.7993926673048629 0.3176989139978701  
0.5779946710386380 0.8381638759803238 0.5051003721158874  
0.6159539128651964 0.8481218013573818 0.6552451018571387  
0.9005583851184827 0.4252254718157204 0.0608846187739735

0.9480872532785763 0.4617720924889805 0.2523633448893243  
0.9440978087016699 0.4872344613034041 0.4392683147514468  
-0.0098159913537565 0.4265224008387037 0.6303374160991662  
0.4584308530949178 0.9669185203852582 0.1575497059493779  
0.4497648659422768 0.9604388289273289 0.3452013639901382  
0.4367438096942940 0.9849342555779983 0.5339303871787218  
0.9715506286442215 0.9280881087482576 0.1224291303189120  
0.9458075728530696 0.9516750689411736 0.3016720649649987  
0.9560310163076626 0.9846563872837140 0.4805665989201079  
0.9400576259997344 0.9083766721769494 0.6639843141401085  
0.9519625041376759 0.9237867596069301 0.0292745445038971  
0.9456216777853953 0.9693480355764696 0.2116377147749913  
0.9507740220129169 0.9653236115584249 0.3907047267415839  
0.9248522822080432 0.9482974751998903 0.5698830654171990  
0.0937766930947160 0.4186476706672218 0.1559865005492332  
0.1342125858142888 0.4577174547041121 0.3476457561197459  
0.2826051887285483 0.4867270710199414 0.5419154096294169  
0.6115009092207058 0.4717898343013447 0.1536914904658790  
0.6338589275006667 0.4605503393567091 0.3446527943894203  
0.8008495209717134 0.4259419413906721 0.5343608127098005  
0.4877486971477460 0.6267491329922543 0.0120594564847607  
0.4388220647337429 0.7405851176342897 0.2505536180767864  
0.4495819657498418 0.7927427914948252 0.4416263614790594  
0.4501023529910789 0.7404353914567300 0.7053386086948261  
0.4624983705050912 0.0861615480414809 0.0608354125237361  
0.4428648698327170 0.2384208451965596 0.2524612013921809  
0.4480146553752858 0.2825951036601445 0.4401409571185293  
0.4340159402711098 0.1048803497948659 0.6317304630550458

Surface connecting OOH<sub>ad</sub> :

Ag<sub>3</sub>PO<sub>4</sub>

1.000000000000000

6.0999009999958309 -0.0000071330448850 0.0000000000000000

0.0000000000000000 6.0999010000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 32.5872412001630067

O P Ag H

34 7 22 1

Direct

0.3262876913169198 0.6336895861545586 0.7931939468411124

0.3221704825233832 0.5379429953280584 0.7537641801974218

0.0243148522456380 0.5422273209897613 0.0955986273905791

0.1104564981754056 0.5801569769274054 0.2836737676983755

0.0845385796551958 0.6458924845540409 0.4677510985465108

0.0178473293437273 0.5749011779989335 0.6708409144368269

0.8543822949341834 0.5899501108219660 0.0244220946029628

0.8169580949134565 0.6377918711886530 0.2284104384386283

0.7915672553257621 0.6208600139415292 0.4113337448531482

0.8714258514200381 0.5434352251142226 0.5977361891942528

0.0474514023453577 0.2376992481334670 0.0430478160144623

0.0958694228682027 0.3246107415148382 0.2219465689185533

0.1005997805794883 0.3377394207254553 0.4141656086905868

0.2201441400818027 0.3456571145508704 0.6157839409758319

0.6761676090698197 0.3390068129908809 0.0780192266280146

0.7955149227609208 0.3053143003630153 0.2764326920133396

0.8014198393632882 0.3354152797999196 0.4689900899590044

0.8496595055088083 0.2191874289445428 0.6463409816082859



0.6422554943615789 -0.0026133262856497 0.0122175679806601  
0.5795617711400037 0.1499412438390174 0.1823672110258975  
0.6020417558021540 0.1249475306368380 0.3697528182177735  
0.5899146254233334 0.0822763172184104 0.5697156783198811  
0.3057564014759942 0.0759640574239748 0.1240409143459528  
0.2893222154689427 0.0947360033114527 0.3172240278435178  
0.3196043282898572 0.1675853338268278 0.5113243151194983  
0.2498476815952506 -0.0240297032018391 0.6811558058043011  
0.2568834019409944 0.8399804627311996 0.0421778115839758  
0.3152957957847415 0.8235862925369095 0.1863630871742674  
0.3113701846322363 0.8272732724998962 0.3776595363389636  
0.2595279360247086 0.8366845124483592 0.5577236637914590  
0.6321517138711609 0.8213806820529175 0.1350149544943271  
0.5921505019420781 0.8062317983947893 0.3188096481022590  
0.5780490527995772 0.8377780036406817 0.5064078804141788  
0.6167132443013632 0.8413067660609171 0.6569134227896716  
0.9002409697565201 0.4240710399054275 0.0609045969824233  
0.9500599987223612 0.4646163051941977 0.2528761935683613  
0.9455001226410651 0.4911737840219020 0.4405942692221081  
0.9913945759213427 0.4206270612527650 0.6328021356912381  
0.4588983422193382 0.9669927268264846 0.1576159055222176  
0.4465387450398057 0.9644353143341253 0.3460440487579845  
0.4359306090763265 0.9803845124320896 0.5357663862123756  
0.9715893593847121 0.9278908637089669 0.1233015812042029  
0.9436207936058050 0.9551764414558916 0.3042074399065635  
0.9539235845991233 0.9868474440409232 0.4828268954992984  
0.9391628483218001 0.9047800153096935 0.6649856928135683  
0.9477763978345495 0.9221427326775044 0.0293401893830585

0.9499815621455361	0.9725360930677527	0.2134857239939124
0.9459111743191254	0.9723362357018074	0.3934087776310974
0.9236284347325421	0.9393593200166090	0.5716923882304221
0.0927413553583002	0.4185203421977121	0.1562215245165351
0.1328398153595991	0.4618920804623823	0.3485146763469357
0.2843911816547880	0.4818244627362961	0.5441514650174815
0.6110828211833594	0.4726841354145158	0.1536960726420692
0.6326030439626439	0.4656504644148663	0.3453185101509327
0.8024925188888424	0.4237776321119316	0.5365543790348760
0.4843186604817962	0.6194435099559480	0.0155132769396317
0.4420690993547153	0.7432776582423715	0.2511087699889624
0.4498208921801762	0.7961576002300417	0.4424932519719552
0.4399718095064709	0.7044865355122660	0.7050085200326284
0.4594730374644592	0.0846412947020401	0.0608404410599704
0.4447252284275823	0.2405992558723239	0.2524722328522989
0.4467923194453655	0.2851202968943861	0.4420774580952275
0.4316470204440869	0.0917370971852529	0.6334264272240621
0.4781538934574641	0.6843272932812900	0.7966056480508776

## 110-02-8

Bare Surface:

Ag<sub>3</sub>PO<sub>4</sub>

1.00000000000000

6.099900999999840	-0.0000004516858560	0.0000000000000000
0.0000000000000000	8.6265610671518971	0.0000000000000010
0.0000000000000000	-0.0000000000000040	34.1294861280913295

O P Ag

48 12 34

Direct

0.5581658246898925	0.5246177595366660	0.0795206267124818
0.6266059662597413	0.0449936102245724	0.1972952395191472
0.5821529289459816	0.5403712341750908	0.3296722539205498
0.6303903829031937	0.0523838070440582	0.4511786853956768
0.5761133841713544	0.5484113728665282	0.5844550591198749
0.6758848238133799	0.0458710053498019	0.6984560851269982
0.6544615050214380	0.5530849746352589	0.0072421730808935
0.5701570122875038	0.0592579759074556	0.1229187129025477
0.6250350498879678	0.5623374209922440	0.2553222645527275
0.5870376684632107	0.0726221411143904	0.3767806932417281
0.6322372530804077	0.5656477841042075	0.5101544273381090
0.5595140385532884	0.0840717702210746	0.6274662448085920
0.3072449660509797	0.4074566549222995	0.0262028869032964
0.3225615464126956	0.8888942065155353	0.1643139064865077
0.2982645621160183	0.4165311821104002	0.2837955177028281
0.3272574219724726	0.9016268539568753	0.4161689243457009
0.3012814077671650	0.4227725232966454	0.5371681303175011
0.3361301806667427	0.9073003466017200	0.6714433800874109
0.3247726542876792	0.6984832064140735	0.0361930762888590
0.2952067133590596	0.1862499280095822	0.1699832106323324
0.3228446823654725	0.7123449784063822	0.2906509055874133
0.3029770168112193	0.1975009744546395	0.4223347819741883

0.3270051401476046 0.7198123747386820 0.5435200878329947  
0.3264949724677998 0.1974027875896597 0.6838034462853900  
0.0541056012621129 0.0785280157451446 0.0788660575851614  
0.1290900413449217 0.5593724948079427 0.1964087423944850  
0.0814876994213718 0.0745039412498066 0.3297551207559012  
0.1320612469939559 0.5667789721908448 0.4516053349657331  
0.0740018664300596 0.0635903179624175 0.5841642766491785  
0.1742610515468728 0.5613686109581244 0.6992033218276723  
0.1528050067352391 0.0473423101819158 0.0067181326214030  
0.0729235613908493 0.5443870991723146 0.1220342317212288  
0.1249768335950947 0.0470382730486427 0.2555694036221959  
0.0888898034342922 0.5452151408596176 0.3773262811773008  
0.1304917523716293 0.0489673046280849 0.5098600711689136  
0.0652587934369957 0.5268374122271636 0.6277326590307657  
0.8051858991350922 0.1942736680233033 0.0251894821294786  
0.8239107547015956 0.7141488965993554 0.1636181554203237  
0.7982720422418916 0.1956280841137058 0.2833616781338216  
0.8267288151990481 0.7156975620283121 0.4165576173296872  
0.7991953389062626 0.1898946322779716 0.5369974956629890  
0.8375713499005804 0.7020989132684596 0.6714075000709300  
0.8224447188199190 0.9033496029519744 0.0357303937567737  
0.7978378425332698 0.4170376541925456 0.1691314032686818  
0.8210259388413756 0.9003441357283593 0.2912453107924880  
0.8055585446773178 0.4202505409402763 0.4230223285439198  
0.8270776038601769 0.8921865033005617 0.5429705518305020  
0.8256190974533690 0.4117961302558262 0.6831618750169240  
0.4630893527405754 0.5478378304379965 0.0363933311271832  
0.4503450012687898 0.0457114832072480 0.1637677621684661

0.4544508924380934 0.5569339419855368 0.2896403651598826  
0.4596991752357685 0.0569801400456046 0.4169427208320457  
0.4562465822767284 0.5634544417619616 0.5436844759026720  
0.4762645968276049 0.0570867412180749 0.6712637469942498  
0.9607783162413479 0.0542527241636490 0.0356545911546113  
0.9530718134317625 0.5576400188621422 0.1628306574752327  
0.9536864807369486 0.0553332414446930 0.2897465245709678  
0.9612174994096662 0.5612484434801464 0.4174502230007526  
0.9542050330426979 0.0492310904562925 0.5433915860629605  
0.9773380069926216 0.5519003498372910 0.6713210728125337  
0.9689602537727633 0.6961978811378812 0.0658239518384708  
0.9519611759426110 0.1533520011828849 0.1875818374290614  
0.9553107829346245 0.6892191804694271 0.3244164214912686  
0.9612819169046877 0.1621272258405413 0.4433689401566854  
0.9539596947360351 0.6923357138829789 0.5801367650371571  
0.9812865505321025 0.1614408992699918 0.6923690723094220  
0.9636415188678452 0.4445081398436675 0.0150626975558972  
0.9485707528014686 0.9148901197259108 0.1270528779944995  
0.9564752868141871 0.4547795256507651 0.2631886651740075  
0.9600714887349437 0.9263948886432336 0.3827274824080076  
0.9574421857937919 0.4548396841506294 0.5195837884016737  
0.9813178624327882 0.9111298744330401 0.6412690400279293  
0.4618055573783896 0.1561469480273245 0.0146052789664798  
0.4501620042409777 0.6884128220953952 0.1276274748062788  
0.4551772278221418 0.1590169664803601 0.2628224444203079  
0.4611264048980382 0.6897799974616272 0.3826467243239040  
0.4563224395371177 0.1573267611995744 0.5194331908418528  
0.4828506348656079 0.6995034991731296 0.6413808850910017

0.4684144576492090	0.9073235729235050	0.0664196310670724
0.4543487107930673	0.4485096271994635	0.1873873953498456
0.4525490544535550	0.9259985149648761	0.3240411059772841
0.4624122883435363	0.4550641510890093	0.4437767414271369
0.4529416934541415	0.9186123223885546	0.5802115052622315
0.4808918360790365	0.4486515574896444	0.6924121765302150
0.5899543119846830	0.2919334100853656	0.1002129209615916
0.6740588468204706	0.8046023253076421	0.2270739781518199
0.6128870470736381	0.3067959994808791	0.3532671332453162
0.6802004528790194	0.8079159962996622	0.4799153456510670
0.5900623399734601	0.3157963548461500	0.6069270547283402
0.0901948823856925	0.3111103072568091	0.0994152635856716
0.1707675954270091	0.8011855064568061	0.2272246743994375
0.1116304324044336	0.3100980741184621	0.3530900312088787
0.1816993199767436	0.8094473653332067	0.4799648335698961
0.0903621934962848	0.2955986840299548	0.6067223456194061

Surface connecting  $\text{OH}_{\text{ad}}$  :

$\text{Ag}_3\text{PO}_4$

1.0000000000000000

6.0999009999999840 -0.000004516858560 0.0000000000000000

0.0000000000000000 8.6265610671518971 0.0000000000000010

0.0000000000000000 -0.0000000000000040 34.1294861280913295

O P Ag H

49 12 34 1

Direct

0.0761164780102731 0.0613805042119297 0.7495639585173389

0.5542541977286262 0.5193034683821505 0.0763347061941702

0.6305924017856294 0.0331104580340365 0.1944132167700542

0.5797687241609983 0.5389889807063090 0.3296720200115607

0.6230695628431433 0.0459514376509468 0.4500008684196627

0.5718816395067328 0.5429069963463743 0.5875438895846226

0.6596755899092515 0.0520475701714237 0.7028143777994954

0.6610715244168062 0.5557335931013968 0.0047625123245262

0.5683864781666412 0.0553358109469798 0.1203590630214309

0.6255196893774592 0.5619366653768347 0.2553608106848833

0.5877870662994913 0.0731549985874849 0.3758355113415158

0.6497707749021803 0.5824388336502846 0.5143204617773579

0.5799693580513307 0.0700557860117102 0.6292080528748555

0.3121732086218876 0.4068608460690419 0.0210196799195282

0.3209471595391275 0.8823835453879028 0.1613563474778484

0.2983025305325590 0.4152905189385336 0.2833019892986134

0.3190983313758833 0.9021081658094720 0.4134676554814995

0.3165631269740363 0.4276280951284198 0.5352961990295665

0.3333560707639165 0.9049231503307980 0.6722321650593497

0.3253963476911595 0.6963967688395462 0.0332694333883900

0.2993163180500762 0.1792310792020689 0.1689567487071689

0.3215246056160159 0.7112245552440728 0.2902468423853625

0.3021920615567430 0.1982222395513212 0.4209801989715457

0.3294587737914333 0.7221604783052453 0.5462432944358064  
0.3247592669418899 0.1997586420043354 0.6785283375377258  
0.0528591898981481 0.0775158544444877 0.0766668082004789  
0.1295834846044276 0.5608550654392584 0.1946604473973984  
0.0852353832496402 0.0746502003422096 0.3280961998809437  
0.1339715112125638 0.5739372909230208 0.4515716136312118  
0.1045937664730977 0.0920929121072546 0.5795191770984348  
0.1536057411872026 0.5731196618149004 0.7032743408158146  
0.1536545410494443 0.0432922309002668 0.0047545040327732  
0.0685439213389495 0.5391141111846162 0.1205415789963514  
0.1327115566604641 0.0405147144304488 0.2541908729646061  
0.0773457287303059 0.5422965008557658 0.3777776046239102  
0.1262242929556592 0.0512992110193314 0.5059215689111728  
0.0752180597607889 0.5470639859656351 0.6295563494024596  
0.8062203903662507 0.1925654182734976 0.0222727855958923  
0.8201671418441829 0.7110876304450403 0.1614566726059003  
0.8042189632284666 0.1915523248919866 0.2804133056023661  
0.8220710814637532 0.7172178649885690 0.4171810002938137  
0.8048706748691086 0.2036668393750483 0.5347012848108663  
0.8358899280215195 0.7201045871353795 0.6713867274255555  
0.8209351663348018 0.9018583781884575 0.0338525557725956  
0.7984614407813672 0.4143249062787785 0.1690037705531681  
0.8262842360998083 0.8970460513418368 0.2900167449908233  
0.8035127614123097 0.4224503249755246 0.4261725456634476  
0.8319757087922433 0.9106094157371754 0.5456250290858566  
0.8145588994711518 0.4278847633463682 0.6800535815385367  
0.4651424261966220 0.5462297821445067 0.0328788869104480  
0.4513817777574174 0.0377725029329215 0.1613929821585862



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0.4540806542034498 0.0555567314701978 0.4154221048260857  
0.4639767566758858 0.5684215530646167 0.5459650832156553  
0.4745773307261202 0.0564328603344329 0.6717557508918818  
0.9597491443364955 0.0523851349660065 0.0333636188260760  
0.9506583934009778 0.5556701384530951 0.1615394917793728  
0.9596298257256934 0.0519136403139010 0.2880594675183175  
0.9562166624370357 0.5635870398201632 0.4183636298269360  
0.9639762124385989 0.0652534471230432 0.5420350817431386  
0.9734621137232646 0.5682117648457260 0.6717215127955359  
0.9694409060488983 0.6924606577669282 0.0634249075420809  
0.9533046984220437 0.1485087678368927 0.1855731378391058  
0.9567238724847164 0.6906952046207313 0.3251057876618983  
0.9553013110208806 0.1676538534539573 0.4432198287244619  
0.9549504988537365 0.7260714102332132 0.5855538000733287  
0.9593919163431349 0.2462457719083401 0.7143109364344614  
0.9673401320167333 0.4429231646610073 0.0119880611023518  
0.9477768500696617 0.9115204686937974 0.1247005995069264  
0.9563827872348529 0.4556014331286417 0.2635487677179928  
0.9534092837100917 0.9306629778495580 0.3828286587479302  
0.9682664637265610 0.4716051860968689 0.5250080726165524  
0.9813586267164186 0.9003938353980873 0.7054116796504182  
0.4616705447342070 0.1543511996191296 0.0123650944429881  
0.4482455262397369 0.6828643540135935 0.1245598081781904  
0.4599008119244771 0.1561547049390473 0.2612903464705778  
0.4603880649165958 0.6899824092466743 0.3820842804069732  
0.4591257247060558 0.1607321342253951 0.5172247884427917  
0.4755038246130939 0.7056927314511823 0.6396248937956898

0.4657683668967523	0.9049088395309869	0.0639358981541509
0.4523533851289618	0.4456073536720014	0.1855962299446408
0.4571177678565713	0.9250183404734142	0.3227373574413566
0.4595402245416339	0.4593645339441784	0.4444662487438634
0.4446874331313809	0.9278846522341796	0.5805977233286834
0.4588542693621381	0.4479055003254429	0.6918441875000850
0.5791360182250100	0.2879810634217853	0.0977200763442137
0.6651979764650542	0.7988774459980417	0.2257667645574513
0.6055321015856943	0.3058130317456177	0.3524173015014789
0.6599394190543636	0.8157055585154519	0.4823592973973022
0.6020290134281573	0.3028420322793803	0.6067859936227370
0.0795205199527838	0.3080680809796774	0.0978566010939126
0.1634128523102023	0.7985827519642474	0.2254495061848704
0.1003566994016841	0.3083151077766415	0.3531021236009755
0.1606461428038193	0.8095734604283328	0.4808172903669483
0.1008027716653536	0.3121533739554689	0.6077570014091833
0.9716189366600144	0.0462122479654129	0.7709059765660187

Surface connecting  $O_{ad}$  :

Ag<sub>3</sub>PO<sub>4</sub>

1.0000000000000000

6.099900999999840 -0.000004516858560 0.0000000000000000

0.0000000000000000 8.6265610671518971 0.0000000000000010  
0.0000000000000000 -0.0000000000000040 34.1294861280913295

O P Ag

49 12 34

Direct

0.0822014182478656 0.0577850620823134 0.7415807502228504  
0.5539946923436024 0.5191303847199791 0.0763590051313862  
0.6305843682158949 0.0329541765792329 0.1944197030625692  
0.5799906728740497 0.5389751403260852 0.3297190491424994  
0.6230245851926101 0.0459030776569400 0.4499794804891888  
0.5719168829962923 0.5424801618542813 0.5875620186615051  
0.6572441782895767 0.0517159267399330 0.7033786684211493  
0.6610988219300313 0.5557881852943665 0.0048182081062594  
0.5683692518048041 0.0553347575966641 0.1203731229479766  
0.6257546643508572 0.5620104595280526 0.2553968689453487  
0.5877297389884742 0.0729524553049547 0.3758112818813690  
0.6486065555320749 0.5813373566884045 0.5141795861268140  
0.5725488230121347 0.0689886507061375 0.6302802913873867  
0.3121946041681324 0.4067120822676238 0.0210118746343208  
0.3209279050253475 0.8823616829800223 0.1613655269359128  
0.2994267644640416 0.4144714103052712 0.2833659442322177  
0.3190557601968906 0.9020934168399510 0.4134675830931416  
0.3155310731649348 0.4271623005347483 0.5355181366639329  
0.3227882835076376 0.9082095605605459 0.6736466884980201  
0.3251504052510557 0.6962280426887728 0.0333013762959244  
0.2993510129610313 0.1791901660533153 0.1689828803911843  
0.3211934763278523 0.7106568215071931 0.2902908724547566  
0.3022025684661201 0.1982333784394013 0.4209676535051652

0.3294655804392483 0.7217025478275823 0.5462531220204907  
0.3254285743822323 0.2072564616036142 0.6789528264850213  
0.0520926414010639 0.0774648806312799 0.0768205585092909  
0.1295169694329117 0.5609157971204092 0.1947252125632507  
0.0854366725236382 0.0748152439385981 0.3281289756392208  
0.1340130754140076 0.5739283565518074 0.4515817899135526  
0.1038757821212286 0.0927981911951604 0.5795866488927923  
0.1587325885195022 0.5747712989402664 0.7038289460657595  
0.1543951206490372 0.0434009343182572 0.0050203496185612  
0.0682608399599169 0.5390593659760307 0.1206138886054416  
0.1326071026595430 0.0398410058473493 0.2542703208789512  
0.0772888148673525 0.5422531822816230 0.3778060155580397  
0.1260933488172360 0.0512083753258887 0.5059443602434248  
0.0739633427038825 0.5474446105927737 0.6302391775695199  
0.8064383650858212 0.1925031022546568 0.0222840168039622  
0.8199608453177851 0.7109850146519502 0.1615208903140317  
0.8043569111529719 0.1915396151799200 0.2804066041843873  
0.8220257098747759 0.7172158046944225 0.4171829676087735  
0.8044354343186974 0.2034036930254969 0.5346550988015987  
0.8350748942642232 0.7177604504287950 0.6729299858242047  
0.8209466430423584 0.9018274872378346 0.0338854544900318  
0.7984544902635687 0.4141058249410481 0.1691401314984286  
0.8259289414254456 0.8971261742811657 0.2902196898359067  
0.8035152228287558 0.4224771097955003 0.4262530280048284  
0.8323966170385313 0.9103500608393810 0.5457212529185530  
0.8207913694985338 0.4262228259503844 0.6817464192912696  
0.4650441671499427 0.5461495962750194 0.0328775733781410  
0.4513590152804862 0.0377521363457566 0.1613972791106429

0.4533491245766261 0.5559781516621097 0.2895095521850109  
0.4540577065563521 0.0555503758893146 0.4154049659308620  
0.4638044414333991 0.5678599009119117 0.5459924021912894  
0.4682872232739942 0.0587292310474142 0.6728362057371354  
0.9598035534285482 0.0523242294317573 0.0334363206674919  
0.9504289199802785 0.5555553672816339 0.1616215243546618  
0.9595536028580929 0.0518834041325321 0.2881159066993955  
0.9561659346621252 0.5636067091418199 0.4183883734884127  
0.9638619877501539 0.0652040662906647 0.5420209190057089  
0.9770941768891418 0.5676946811229855 0.6726745104700138  
0.9697734128980628 0.6920035963340326 0.0632639755759560  
0.9532601259460890 0.1482227666486922 0.1855540257319603  
0.9558752142575792 0.6904935515714336 0.3251782422950653  
0.9552592216547131 0.1675749043412672 0.4431873577106316  
0.9544781276381827 0.7249654308953531 0.5855221271348224  
0.9762529450876510 0.2377769501077165 0.7109452529259895  
0.9674259332160717 0.4427402566309427 0.0117356327177661  
0.9474615916795524 0.9108957578431798 0.1246812339820458  
0.9569792619219620 0.4550486890097880 0.2636174632583562  
0.9535263388986179 0.9306742964340381 0.3828425116412219  
0.9678022379919434 0.4718726520474755 0.5247897964021698  
0.9795149889140902 0.9014853055297647 0.7042772886593808  
0.4623424451761344 0.1543099465607513 0.0122529843261261  
0.4480288657764828 0.6828390790036396 0.1245440799005692  
0.4598150847454441 0.1558104726119161 0.2612883658582797  
0.4602915357701786 0.6898196803366297 0.3821510702794081  
0.4591956851994961 0.1602962644370292 0.5170520893540456  
0.4718326134430776 0.7073859230969352 0.6397007630688563

0.4657328799355702	0.9049351742573758	0.0638872575846637
0.4522578009660624	0.4456541576661741	0.1856368558215561
0.4566862468243899	0.9245762110260132	0.3227450199631567
0.4594605620602848	0.4592597362065718	0.4444870389057404
0.4441142561449338	0.928210555592796	0.5804656020306679
0.4697746690242575	0.4581514493500634	0.6941008193907708
0.5784603728063490	0.2878474378068920	0.0976953517136236
0.6646683722269423	0.7988998343738070	0.2258111629163153
0.6055104994751961	0.3057035631251295	0.3524701558054611
0.6603361777731217	0.8152630040984084	0.4823121994436168
0.5976202383503131	0.3013969365038087	0.6067998532997475
0.0788224771153564	0.3080875051951895	0.0979070961431621
0.1630914960636085	0.7983474216712767	0.2255170354794695
0.1001128989562697	0.3083286195162185	0.3531431935221034
0.1613464039621262	0.8094679004168440	0.4808467712623958
0.0967211829335928	0.3153240328821340	0.6065775352696456

Surface connecting  $\text{OOH}_{\text{ad}}$  :

$\text{Ag}_3\text{PO}_4$

1.0000000000000000

6.099900999999840 -0.000004516858560 0.0000000000000000

0.0000000000000000 8.6265610671518971 0.0000000000000010

0.0000000000000000 -0.0000000000000040 34.1294861280913295

O P Ag H

50 12 34 1

Direct

0.0099664794968408 0.0865681422805523 0.7905311323695003

0.1261615099913893 0.0718636729637949 0.7524900034249745

0.5534501533751267 0.5189313373413758 0.0761420121407772

0.6309671423827112 0.0332829058072415 0.1946331154622831

0.5796271613437305 0.5385744379451933 0.3298379189480874

0.6236278873481950 0.0452399257290386 0.4500749076679591

0.5706107524203775 0.5453670207429439 0.5871627965414870

0.6682592091902165 0.0512317775584754 0.7031222354233996

0.6624849821559596 0.5554460874469479 0.0046021805214664

0.5684198118017965 0.0555973653361142 0.1205289486708394

0.6263018475486811 0.5619251607724909 0.2553626512052978

0.5877435265294625 0.0724596291384974 0.3758249478608121

0.6489182293948517 0.5820726551982163 0.5138368046565345

0.5756391954803768 0.0729394483970555 0.6302442656562265

0.3122756359113974 0.4068296569405400 0.0206757016930115

0.3209659166012488 0.8824356654577448 0.1613968741891042

0.2996855998588436 0.4144049256814178 0.2833139971931421

0.3194438774605509 0.9024077124900666 0.4134073810441342

0.3151673066407201 0.4281992438369558 0.5352924400807350

0.3270779108876145 0.9113457562405949 0.6746967320412404

0.3259349835765308 0.6962924869786178 0.0331315353240649

0.2992987315819268 0.1791394666832004 0.1691044364476094

0.3202290260371810 0.7109685708988529 0.2903679094526204

0.3015176790674192 0.1982689344576392 0.4209752000234107  
0.3297679233353942 0.7228906526457939 0.5460708664468202  
0.3344219037350303 0.2075396022270553 0.6811762076131790  
0.0526720746227418 0.0770502109172015 0.0767312512425646  
0.1300370687578986 0.5610033999544639 0.1946872609322454  
0.0857365119244459 0.0748607638922400 0.3280718611441083  
0.1333175191498396 0.5738332624850608 0.4516051445970050  
0.1047405928585236 0.0924993836013332 0.5796439805907564  
0.1473683084297598 0.5737595272000238 0.7038702850968568  
0.1537242622415763 0.0434475447670096 0.0048457994247667  
0.0682981879239997 0.5394980030408937 0.1205159728094699  
0.1328904236436279 0.0393250387189654 0.2542139164662336  
0.0772772227225368 0.5423415274086629 0.3776993661584511  
0.1261096236716873 0.0501637134639042 0.5059677075297182  
0.0693765914508954 0.5444245618946079 0.6300985608301570  
0.8063514202244585 0.1924543030270378 0.0223973614646805  
0.8213892526555728 0.7104619641025908 0.1614419719103030  
0.8045994482862706 0.1910538807528583 0.2803436542594873  
0.8222014718642366 0.7168471001852632 0.4171397543389602  
0.8046290163330552 0.2024269219472289 0.5344326751306792  
0.8269877212594609 0.7146074854372135 0.6721807682661953  
0.8213228613619228 0.9016507779583631 0.0339453496109998  
0.7973873590917797 0.4141685523462196 0.1690328111612246  
0.8261991506947576 0.8965921518862896 0.2902886584858136  
0.8032953131224083 0.4226637926984850 0.4261104933656479  
0.8321513794096962 0.9100550152751358 0.5458398594291739  
0.8143403257367322 0.4207878229124417 0.6807758167492206  
0.4648361733032634 0.5463441103191210 0.0326786949506981



0.4517549030300134 0.0370688581298636 0.1615777060977618  
0.4544219213805168 0.5562820632884590 0.2894041234519266  
0.4531502484177897 0.0563331689633100 0.4154580012709920  
0.4632680028873679 0.5695198877246960 0.5457897960419837  
0.4750927281975416 0.0587651660713516 0.6737964406548549  
0.9604951218992964 0.0521881934674260 0.0331639661312242  
0.9497658288604102 0.5549576959866949 0.1615705336091592  
0.9586175793063975 0.0516343601721073 0.2882183006578958  
0.9570953085256529 0.5632808788755476 0.4183920563548801  
0.9623072567444129 0.0642545708383089 0.5419720556655221  
0.9647408600689128 0.5645703912100036 0.6721571754321802  
0.9706807054185947 0.6923489280250871 0.0633780922516704  
0.9527059178120391 0.1483598232196984 0.1855945129110104  
0.9562558916522068 0.6904653529425347 0.3251794153492652  
0.9555324269370792 0.1677256081003066 0.4431924546737760  
0.9556498684028093 0.7244187808406464 0.5860239005418663  
0.9880292998751364 0.2361627887664546 0.7109928924240405  
0.9667421600376144 0.4427550774578626 0.0120340361028600  
0.9477128846979711 0.9113049691459484 0.1247357318751285  
0.9565525359692556 0.4549794213531395 0.2635771873158956  
0.9538132517812095 0.9309041213295808 0.3828142047644599  
0.9674786406258415 0.4717178561232352 0.5247996174716998  
0.9813819467042200 0.8954224507124778 0.7085129432299846  
0.4616841373017616 0.1540355155059067 0.0126489404112430  
0.4485764354918969 0.6824563192261096 0.1245970118288343  
0.4600960394083145 0.1558786029056680 0.2613093677673013  
0.4606136446850831 0.6897337203997651 0.3821294504241347  
0.4587004634768098 0.1604163808244614 0.5171530750062051

0.4678400158077729	0.7080776117386020	0.6402996440984889
0.4666238570393655	0.9043274469064522	0.0640797155950354
0.4533090897021777	0.4456068460500142	0.1856190482513827
0.4568947357393967	0.9246010624886002	0.3227326011231384
0.4594345963276339	0.4592779029027729	0.4444782999436229
0.4430748095964695	0.9273680714628727	0.5804527665879359
0.4641298037086423	0.4568842745984832	0.6930277921183429
0.5784266770225498	0.2876456026682642	0.0977419397882629
0.6648272312795590	0.7987237273346091	0.2258121979192619
0.6062764781393023	0.3061967440930811	0.3525590415808385
0.6607298536230481	0.8160033231750911	0.4823434014334858
0.5978691267355101	0.3083361223499131	0.6072697483611647
0.0792164063189808	0.3084157231018563	0.0979241893113792
0.1632696902720669	0.7981115376207302	0.2254777088406415
0.1005496703691931	0.3083789058384180	0.3530838360036476
0.1611598369267976	0.8085906970276004	0.4808365094456515
0.0957554049394346	0.3147730965999812	0.6062899179775387
0.1099203034434200	0.0267764045256509	0.8071550202676833

## 111-01-12

Bare Surface:

Ag<sub>3</sub>PO<sub>4</sub>

1.0000000000000000

7.4708232263539216	-4.3132767318909231	0.0000000000000000
0.0000000000000000	8.6265677671561374	0.0000000000000010
0.0000000000000000	-0.0000000000000010	29.8929711337085706

O P Ag

48 12 33

Direct

0.5297166461378057	0.8008472792146776	0.0759876523145415
0.1670513189840529	0.1294026963141456	0.1900932253937236
0.8385446967689908	0.4655855616482242	0.3083883782538511
0.5047830672528187	0.7971595089035968	0.4272063453212753
0.1727712219378350	0.1308922941835464	0.5486917651239501
0.8342337707924092	0.4552551191347982	0.6635650693815817
0.3968262068066699	0.5896306858688524	0.0099824118918384
0.1080250094590698	0.9312575138013806	0.1218437797682454
0.7678052859216590	0.2700680139169923	0.2390075034690336
0.4289981089116127	0.6020777230423013	0.3575227273404077
0.0981787613724601	0.9350970469213550	0.4789304212832524
0.7689823392574706	0.2716746998894130	0.5908541974673336
0.3916857131326033	0.8860634533631279	0.0127993217183954
0.0639182620730053	0.2045520379348922	0.1174744212893541
0.7256652359253046	0.5442587414618035	0.2376335439355662
0.3878265591659866	0.8768400226952096	0.3575969685355224
0.0506655931647352	0.2059973094743925	0.4792550372076128
0.7118505953770303	0.5332132989883533	0.5930324355660096
0.6819766550482723	0.8770621379183161	0.9982138808756614
0.3819648580618821	0.2524001702774648	0.1248753498792388
0.0421203104489078	0.5872140063385857	0.2402172466562970
0.7040742975132761	0.9182116637820171	0.3581940205049456

0.3694373533784606 0.2538763595945595 0.4791507625778468  
0.0308220441141501 0.5909390560914258 0.5930080844949608  
0.2182316321135442 0.1728703351178111 0.0188563477532531  
0.8460453729056503 0.4508007960181082 0.1293285965780456  
0.5108356854030118 0.8035163776804539 0.2483097976601195  
0.1748711148736227 0.1321863454857775 0.3676793948181503  
0.8396380609541140 0.4659587246855749 0.4854223701946757  
0.5064871823959727 0.7997415472846570 0.6065020705199602  
0.7291916706087876 0.2631719562495753 0.0575847886683552  
0.3846129419444471 0.5954196463839453 0.1810630996084068  
0.0507664067092942 0.9330634647742341 0.2986371973811093  
0.7183982746216230 0.2667793082460469 0.4163829184125112  
0.3825380177298232 0.6011101059965519 0.5371859811065208  
0.0171762667920485 0.9369640255366286 0.6702901123095378  
0.0517284016393971 0.5256827847921475 0.0623708146763189  
0.7064606913444881 0.8633509105155851 0.1796121945337405  
0.3680537573838520 0.2059851137090309 0.2973364100663423  
0.0359950386547160 0.5390049637126417 0.4161058268425841  
0.7002162213751422 0.8726024089462148 0.5362273845797071  
0.3579072611769241 0.1643003334358109 0.6702983919805080  
0.7963745851968439 0.5925562028471397 0.0599559901771470  
0.4367874874250174 0.9143918690706895 0.1766408832675685  
0.0964382577636218 0.2513202065225010 0.2982807275401994  
0.7634957907846247 0.5842819350592575 0.4154174060973201  
0.4282899247276626 0.9186568326005403 0.5367085685121368  
0.1298554129827877 0.2766882045985358 0.6657299797700685  
0.5005262857724898 0.7921204356081435 0.0227139605254555  
0.1822415481474699 0.1282812759851919 0.1365225765627583

0.8432747639266253 0.4671035883223014 0.2548780662979577  
0.5066043309744201 0.7988388872797580 0.3736633019318993  
0.1729134441274535 0.1315596035969940 0.4944371242390885  
0.8367204005980807 0.4630838192096183 0.6137404990858815  
0.8519025336726088 0.4571104116929166 0.0749859243428003  
0.5098201876467254 0.7935800977174003 0.1946930430211727  
0.1722250570488806 0.1303443271222670 0.3139310282944294  
0.8392722116950554 0.4642024155503817 0.4320056113870990  
0.5043365186260887 0.7983808145904345 0.5533159305238210  
0.1687697033629717 0.1263578256546855 0.6693500302085472  
0.5048132067321219 0.4872971104340687 0.0743537786375994  
0.1306222343311471 0.8610694986264794 0.2148246242565423  
0.7976663304203936 0.1961500315092106 0.3344744706459633  
0.4604194443744513 0.5296356060576928 0.4544599319420726  
0.1200449921025187 0.8622829826241423 0.5735574270464104  
0.1492260654332694 0.3579639239500258 0.0387145194167327  
0.8025849887644660 0.6862302408847681 0.1508531138068999  
0.4617804642785263 0.0230944742084540 0.2741608564951449  
0.1289319082462667 0.3539910704501058 0.3944920955886438  
0.7891596996320460 0.6828632630844299 0.5141883474950615  
0.5068299939960849 0.0649499261027328 0.6294689015619636  
0.7911205001243344 0.0067832775991951 0.0981796597868001  
0.4474706249190614 0.3617411628195403 0.2131888992885254  
0.1086161271823137 0.6909136777105860 0.3350946733595695  
0.7731132777882765 0.0209677545998050 0.4549709937654737  
0.4393291339218577 0.3502041473838436 0.5740746357390630  
0.9500756674299189 0.9942688431220803 0.0125256456271810  
0.6254469990956375 0.1894392215780823 0.1549684986134734

0.2847602102867904	0.5311032118662822	0.2753745542697145
0.9490893746775333	0.8646931012169472	0.3948594398674423
0.6168829384892864	0.1975823848946835	0.5139100877010284
0.2449693615144085	0.5297134320587631	0.6267662762788796
0.2803171322023075	0.8274174629631366	0.0954307952218442
0.9487998707409685	0.1765391194224693	0.2152448210419221
0.6112442824544202	0.5070242391721170	0.3338332753734940
0.2829400694874128	0.8431458041411013	0.4546954448644779
0.9512206455227346	0.1786884774350978	0.5732586578171280
0.4515301336059469	0.1640712855585845	0.0334680425045409
0.1128676377089560	0.5073905475663947	0.1568674906258430
0.7752929079642177	0.8406165133361455	0.2746816987851755
0.4413876079874525	0.1746217341482721	0.3940445880349339
0.1053952529222257	0.5127267639903021	0.5142404519194016
0.7709554491491954	0.8045565817411990	0.6285622235920678

Surface connecting  $\text{OH}_{\text{ad}}$  :

$\text{Ag}_3\text{PO}_4$

1.0000000000000000

7.4708232263539216    -4.3132767318909231    0.0000000000000000

0.0000000000000000 8.6265677671561374 0.0000000000000010

0.0000000000000000 -0.0000000000000010 29.8929711337085706

O P Ag H

49 12 33 1

Direct

0.5898521815490383 0.8729226504008317 0.6919942130696449

0.5355278054319913 0.8382333932054949 0.0735944414673527

0.1702997720063587 0.1255917748916487 0.1900030270464297

0.8397464272402579 0.4601712411254144 0.3090781488500199

0.5051237066558877 0.7922162276891754 0.4277552455835481

0.1159997461980116 0.0807684401756680 0.5473276520568843

0.8050811007434858 0.3693066304908725 0.6701410592394665

0.4086819196137304 0.5981964676504992 0.0137124969858328

0.1059609887308471 0.9376572989201571 0.1193794155226009

0.7652801456176787 0.2686627030554948 0.2386225247560703

0.4280981732198568 0.6017318171946882 0.3573675862979165

0.1049578526244260 0.9509851508859111 0.4701533374344037

0.7660161096636604 0.2890208777118841 0.5900891792488813

0.3893616056456324 0.8860338085349611 0.0054845347638168

0.0712796789737522 0.2167923633969770 0.1192514532148341

0.7174989101208931 0.5392944017899830 0.2406530855811423

0.3826905301819048 0.8740890527088159 0.3594511842040123

0.0455680023434511 0.2115552670540794 0.4789940573537987

0.7300367561081332 0.5519651118328978 0.6133347213289231

0.6837900246317067 0.8818050228935679 0.9958334226243977

0.3848514323081124 0.2535503231395804 0.1248696555058999

0.0365970160828345 0.5875111444041849 0.2398879654755059

0.7003794424115801 0.9204471361863853 0.3582582176238983

0.3620901499920055 0.2677694373268379 0.4913331639054181  
0.0410939863430244 0.5910535126908110 0.6137263189623567  
0.2177279120212588 0.1884637631952110 0.0097338986541453  
0.8540530504262986 0.4289042102677397 0.1276362443843131  
0.5062253364658791 0.8032696912048213 0.2481305900472414  
0.1780266865611250 0.1428249227449220 0.3679431487470792  
0.8364080772220597 0.4829867164504377 0.4881902983365070  
0.4808520461149742 0.8313671262346062 0.6054760958776672  
0.7234821121756637 0.2737058519685052 0.0526170993044593  
0.3859461309233629 0.5955541927576981 0.1804964368535892  
0.0476747576820202 0.9320320267734055 0.3015265811931030  
0.7044694911981202 0.2665357192965433 0.4226043127908881  
0.3673721818408017 0.6057076941970974 0.5418436003813484  
0.0245506652047372 0.9748635109455073 0.6572860797638089  
0.0461182616400694 0.5353590734180594 0.0575240581983468  
0.7065883948357232 0.8625101985328414 0.1811625651777109  
0.3659384479881158 0.2038404923309100 0.2972975085587544  
0.0254617065774562 0.5342398973396733 0.4184867921774017  
0.6900696831181340 0.8667597020556446 0.5405717269650666  
0.3501507115279155 0.1931221992827774 0.6311627366917114  
0.7885136613494103 0.5958596448092850 0.0676535163726763  
0.4351069902927358 0.9133031488339418 0.1758822879259824  
0.0938667985640003 0.2496633879257816 0.2971618361449804  
0.7553828391453031 0.5845136489446359 0.4159289223239856  
0.4280573919300303 0.9239679743954052 0.5290460045700150  
0.1613982188956045 0.3147146552672141 0.6698112677313278  
0.5042781134111781 0.8056233798646821 0.0210179142431822  
0.1833163678397723 0.1321191498173369 0.1363685792981692



0.8394735776946658 0.4641325937471869 0.2553530459347714  
0.5037762609660774 0.7970106082739453 0.3741892666254159  
0.1576457495062853 0.1262873553028590 0.4959797089820381  
0.8405813694210559 0.4575925393754124 0.6237578488259731  
0.8507556150955413 0.4569523433829789 0.0750254993922434  
0.5083925383356072 0.7938572175574555 0.1945996115430579  
0.1711699993659636 0.1319864865327683 0.3142818697905381  
0.8308068885165937 0.4675802901325265 0.4343616905681301  
0.4933903644283800 0.8086021221244001 0.5534761461223008  
0.1793226407151974 0.1600959736795189 0.6526679697479845  
0.4738435758400896 0.4645944038615442 0.0716244208781620  
0.1210613462280637 0.8573080196827244 0.2145271626028869  
0.7883492577754463 0.1921431006166217 0.3341285808173294  
0.4518555308387132 0.5217836636717955 0.4542890334941458  
0.1025963677021022 0.8370387758548892 0.5771473200693750  
0.1389235531918645 0.3679714141824154 0.0303371935020619  
0.7764799855930801 0.7346162754237121 0.1282292069634373  
0.4536703877484076 0.0186786510203567 0.2734645950113817  
0.1180052780078850 0.3522937462094555 0.3947600388745561  
0.7813217553217502 0.6909457112009481 0.5154174177235098  
0.6524140040178975 0.0849946360003330 0.6453062523450713  
0.8028802397169247 0.0558302301561614 0.0905796823267787  
0.4449182556916785 0.3603039843470048 0.2140550846160819  
0.1057245017964655 0.6899648996803706 0.3356086175903033  
0.7690714153168808 0.0244400915558253 0.4550637651328707  
0.4674256247023326 0.4073974810862703 0.5695757958573826  
0.9517888122660435 0.0114113339884477 0.0064143292563976  
0.6242855177563456 0.1884845128302501 0.1554115908690056

0.2801719528945394	0.5314946996710215	0.2753694182756852
0.9402934786023217	0.8687050998251994	0.3942707952022997
0.6111853571626970	0.2099895801936761	0.5149915989545204
0.3063843063009683	0.5844041081610848	0.6422808639999383
0.2808955813212251	0.8373579728809198	0.0945162943443807
0.9471907293164615	0.1725474719578438	0.2152452686294584
0.6094809919290384	0.5056435587267671	0.3331443318065238
0.2816741581418676	0.8449261794030932	0.4525280085423688
0.9306995640423595	0.1765599401167859	0.5675104288855050
0.4414201388544966	0.1610960000538504	0.0261478150181712
0.1186595641058957	0.5077794357380468	0.1553204050793243
0.7759119258178924	0.8353410163751337	0.2727837140994886
0.4378698512853059	0.1824172744794477	0.3951039488583544
0.0985632433496003	0.5267533076664439	0.5165523185904602
0.6818620025270353	0.7130967125182562	0.6599373819153506
0.6363981169920244	0.9090269733639306	0.7222240753390721

Surface connecting  $O_{ad}$ :

Ag<sub>3</sub>PO<sub>4</sub>

1.0000000000000000

7.4708232263539216    -4.3132767318909231    0.0000000000000000

0.0000000000000000 8.6265677671561374 0.0000000000000010

0.0000000000000000 -0.0000000000000010 29.8929711337085706

O P Ag

49 12 33

Direct

0.5529217169165367 0.8729986136902913 0.6807503886967627

0.5373614668098436 0.8435595839592085 0.0725356039471707

0.1716433409607330 0.1250714112967722 0.1895312591420411

0.8397761792976949 0.4572666170581884 0.3088100810869376

0.5010319111405716 0.7739232762507756 0.4248914572262180

0.1235406273535206 0.0613493800128506 0.5483194508029404

0.7930366959083865 0.3166742746909523 0.6694761962629688

0.4099488716725558 0.6021236243713513 0.0131847601163199

0.1053237274829780 0.9364950741808968 0.1189713108042863

0.7636877800781781 0.2670456091996610 0.2379448041402629

0.4293072497095435 0.6022629512392289 0.3513189295946948

0.1009428891183342 0.9404265254764730 0.4689607835783390

0.7544424851704136 0.2863718270304827 0.5887346209240588

0.3888022040292077 0.8884833272698299 0.0043572776631183

0.0710693411353711 0.2160850837948597 0.1189621508385925

0.7161801748611372 0.5377821390075553 0.2407052874042512

0.3825810641717883 0.8726051519573761 0.3590843328741221

0.0342505987301342 0.1938086375788920 0.4842701230157101

0.7409193808542401 0.5479097579741637 0.6249582914528452

0.6838097322330025 0.8869578553679333 0.9945077728245324

0.3845380046858903 0.2521089350354102 0.1238890591521970

0.0349464922710142 0.5852414899975390 0.2392897211515411

0.7005554230869330 0.9200568480372312 0.3571750155947191

0.3545244516656342 0.2567433401646731 0.4893756284257119  
0.0407326257829601 0.5634398248812948 0.6189289462009674  
0.2178179096476673 0.1912592700773905 0.0071925278194039  
0.8553474011188748 0.4323433374837458 0.1258985499258423  
0.5112368181117259 0.8044267185096838 0.2475915956208992  
0.1793674056384364 0.1438436107765901 0.3678902254550680  
0.8528331727575372 0.4918322976814433 0.4897275723039444  
0.4424534247635566 0.8683789067934204 0.5939616072211471  
0.7180472131339589 0.2702461888590676 0.0519725091155570  
0.3851692829556081 0.5960640196377875 0.1802071190337700  
0.0477517353639215 0.9303731027177088 0.3019651884190766  
0.7002838717521463 0.2636220260102607 0.4267707089423123  
0.3793272130881692 0.6215074710363416 0.5388863935429659  
0.0393224587917725 0.9795522715898460 0.6560198401819006  
0.0410355562907745 0.5336528451973852 0.0546325672068740  
0.7079622977820429 0.8604964381857841 0.1798930846697585  
0.3655644770495853 0.2013033841571464 0.2971683410193605  
0.0218926923566180 0.5258607226468357 0.4174383229057294  
0.7009989516552471 0.8463881896911786 0.5581748427104001  
0.3624671837773055 0.2097901953482024 0.6319288751977654  
0.7832086752085488 0.5929327194647904 0.0653762854399813  
0.4386846035676304 0.9150693474180147 0.1756759715706415  
0.0927696675633948 0.2469700975359364 0.2965264946347056  
0.7547640385530093 0.5814975518989244 0.4183405810570016  
0.5186694983838694 0.9501485367710109 0.5119592258701197  
0.1600474172503859 0.3192623711312854 0.6683458079067643  
0.5049961793354902 0.8098189636375616 0.0200841877776789  
0.1832786909099983 0.1315360881812175 0.1358658605688070

0.8379999821298670 0.4621041191025578 0.2550234327775582  
0.5025495301121894 0.7916987789214630 0.3719193986649636  
0.1530829309556829 0.1106123978927883 0.4972129636000994  
0.8387154074269364 0.4401066583615712 0.6277803306506126  
0.8473900627236642 0.4556281920478624 0.0731830297281347  
0.5109386728222463 0.7941861370049446 0.1940955090978681  
0.1711572412486883 0.1313980835639750 0.3142253574036108  
0.8316379214239988 0.4652265709913939 0.4365589110378993  
0.5126898472354978 0.8251064336879330 0.5495493107712854  
0.1867785232044467 0.1695102946755536 0.6523702176057190  
0.4683291691658300 0.4622461351756152 0.0706412761151526  
0.1210899216384437 0.8557771616459172 0.2140393805824823  
0.7853191649597605 0.1903382111876249 0.3340005421569529  
0.4464854123112627 0.5104962076719134 0.4529596473392448  
0.1113786122594980 0.8227217714058052 0.5829682731102780  
0.1379752190860108 0.3702707035799496 0.0274619572110183  
0.7742490122088695 0.7337939965659092 0.1259371562812975  
0.4516773344536156 0.0145542777416879 0.2734597738838914  
0.1069202385744123 0.3384503132205205 0.3960364828177002  
0.7895814321224371 0.6874224095525512 0.5206306104281501  
0.6246129221430075 0.0689301136045859 0.6358072954940528  
0.8052429315339911 0.0585301568153246 0.0893952431654909  
0.4433544544510791 0.3581257355008822 0.2144599314340341  
0.1026838322398725 0.6896476026362687 0.3366214802510708  
0.7606599533267913 0.0198413937933602 0.4549412027809905  
0.4666619317235473 0.4621772868971508 0.5850434365480791  
0.9517916557889794 0.0146855872692953 0.0043443004745807  
0.6274707120963323 0.1905611447246992 0.1547064259724827

0.2754501220160259	0.5319172346327912	0.2747957269195015
0.9340653161190735	0.8678270314640111	0.3954191647491496
0.5696929902916147	0.2502820655258478	0.5293577631510749
0.3169038667785989	0.6201771320946530	0.6614913975628363
0.2843778660285247	0.8418026970085355	0.0941298797358492
0.9468181435305790	0.1706847183421964	0.2148512761272298
0.6164474749456583	0.5044681707860313	0.3352652043941599
0.2845963010786811	0.8394950029534897	0.4521379120365185
0.9335468911597337	0.1729639862029966	0.5654566521634780
0.4394773779601762	0.1624780399571447	0.0243078543214108
0.1202113494354505	0.5102885195531868	0.1535076705915930
0.7775145784295515	0.8338520374180797	0.2728268628321668
0.4393406239681276	0.1830464196830194	0.3961599744527335
0.1087709749069086	0.5381387562346870	0.5171990492795460
0.6922825806495071	0.7450165343989577	0.6574847437408172

Surface connecting  $\text{OOH}_{\text{ad}}$  :

$\text{Ag}_3\text{PO}_4$

1.0000000000000000

7.4708232263539216    -4.3132767318909231    0.0000000000000000

0.0000000000000000 8.6265677671561374 0.0000000000000010

0.0000000000000000 -0.0000000000000010 29.8929711337085706

O P Ag H

50 12 33 1

Direct

0.5977478872829038 0.8797446538567866 0.7342891076605267

0.5755444742441674 0.8595092884370933 0.6867763851989341

0.5356179245332144 0.8457504384861700 0.0717697897182014

0.1703492246622741 0.1255865287570363 0.1900889572462794

0.8387060563960034 0.4567410747833872 0.3089039884661148

0.4997239431566042 0.7786191198147638 0.4261706076673732

0.1218430368344468 0.0706643850941345 0.5480874419046036

0.7927590268744313 0.3449717741155598 0.6656929941776951

0.4048001192315143 0.6007478985454613 0.0133030508554698

0.1050793092563246 0.9371995500170269 0.1195617819225798

0.7633648892452261 0.2678772641868788 0.2378202006181517

0.4265866319457590 0.6032465095055582 0.3529863349583006

0.1003428539616003 0.9391425215627204 0.4703462421206770

0.8002345565159721 0.3129260295503035 0.5818072637427503

0.3822958903133022 0.8863840180581931 0.0039977861441750

0.0706848242015526 0.2166146933141761 0.1193616300363568

0.7161676238950579 0.5386505237064670 0.2408671072136852

0.3837885605864233 0.8759612715824741 0.3594621532875703

0.0348510521507709 0.1952850673933574 0.4813220697935143

0.7316945811677538 0.5441316740036194 0.6111922951564996

0.6775992317106357 0.8849528251975636 0.9933202347876937

0.3841931948947291 0.2534266745318881 0.1246449965321815

0.0347857995074614 0.5865042845142755 0.2397038330353511

0.7004475356550545	0.9204033188517012	0.3581757191028508
0.3548864873503377	0.2575608266163247	0.4895390113638196
0.0459436777341121	0.5987385949263664	0.6202168980271636
0.2115773438728910	0.1891280680016464	0.0088517637951361
0.8518165466668547	0.4279317392944587	0.1274835148411342
0.5066053273601165	0.8025950047733773	0.2480451146638804
0.1789834890972838	0.1414846600739169	0.3684093459306703
0.8527213306051651	0.4987781715546492	0.4873914790565177
0.4389384591455696	0.8389433033914967	0.6013947201560947
0.7168055247343600	0.2738808138825729	0.0526355443026773
0.3846885239393625	0.5945032701631628	0.1804520085258204
0.0471534976324330	0.9290886394406976	0.3021818263456774
0.7012010468883709	0.2637359921417827	0.4262554061564386
0.3704280252175026	0.6107611221414502	0.5400916677850295
0.0190331219393930	0.9813678925582530	0.6682261988843248
0.0406410317760121	0.5351346937875622	0.0570094066330691
0.7057509288384765	0.8621358811764461	0.1809407072880088
0.3649226577316226	0.2011749071235828	0.2974049408996184
0.0207100701909136	0.5281459295680153	0.4151158445370686
0.6946669496523904	0.8404719490749565	0.5578616936505860
0.3351200523153520	0.1778712237904491	0.6334572626247111
0.7836126354548734	0.5955091019298882	0.0679126490441453
0.4335949453174404	0.9115897465923063	0.1758314519590422
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