Supplementary Information

Conduction band-edge valley splitting in two-dimensional ferroelectric $AgBiP_2S_6$ by magnetic doping: towards electron valley-polarized transport

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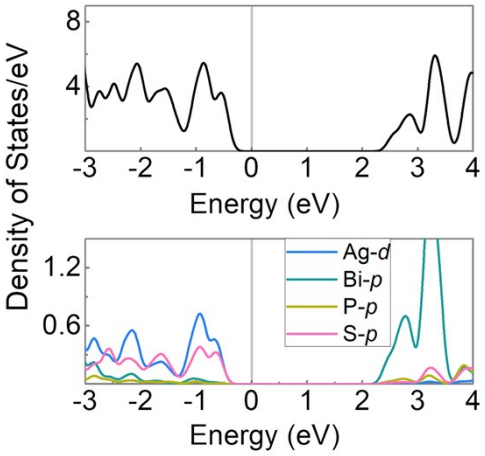

Fig. S1. The total DOS and orbital-resolved PDOS for each atom of $AgBiP_2S_6$ monolayer calculated by the HSE06 method. The Fermi level is set to zero.

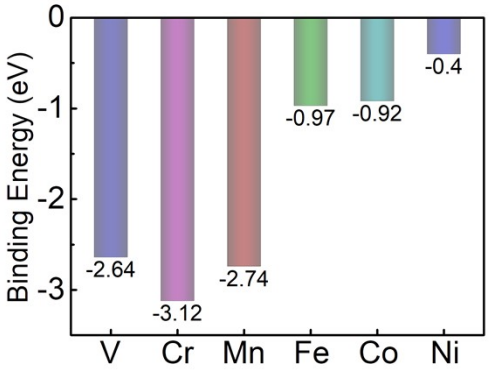

Fig. S2. Calculated binding energies of TM-doped $AgBiP_2S_6$ monolayers.

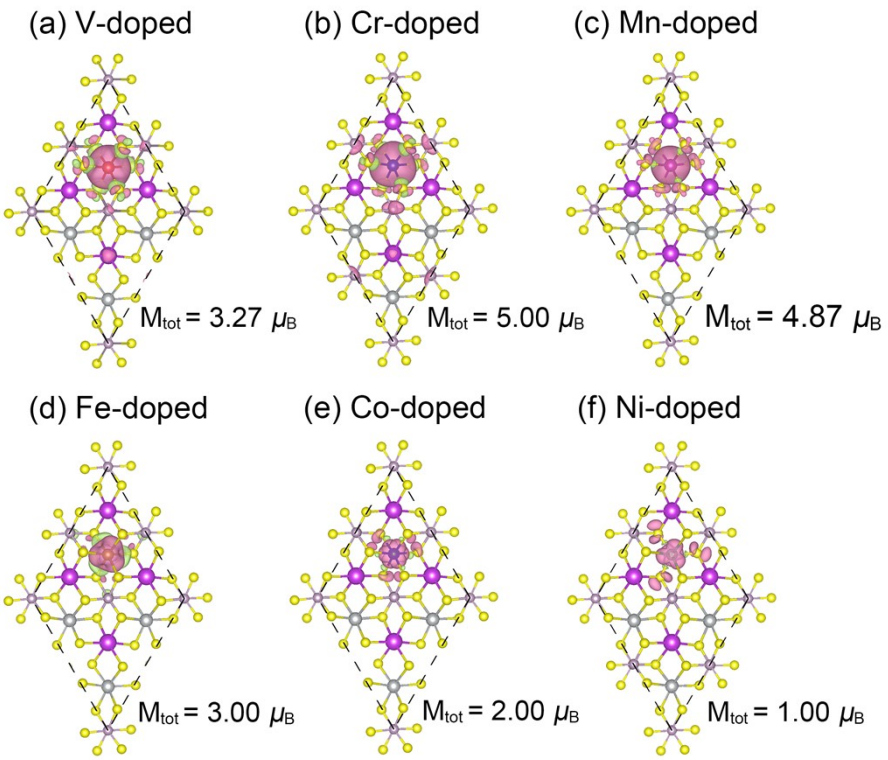

Fig. S3. (a)-(f) Spin charge density of TM-doped $AgBiP_2S_6$ monolayers. The pink and green isosurfaces correspond to the spin-up and spin-down states, respectively. The isosurface value is set to 0.001 spins per $bohr^3$.

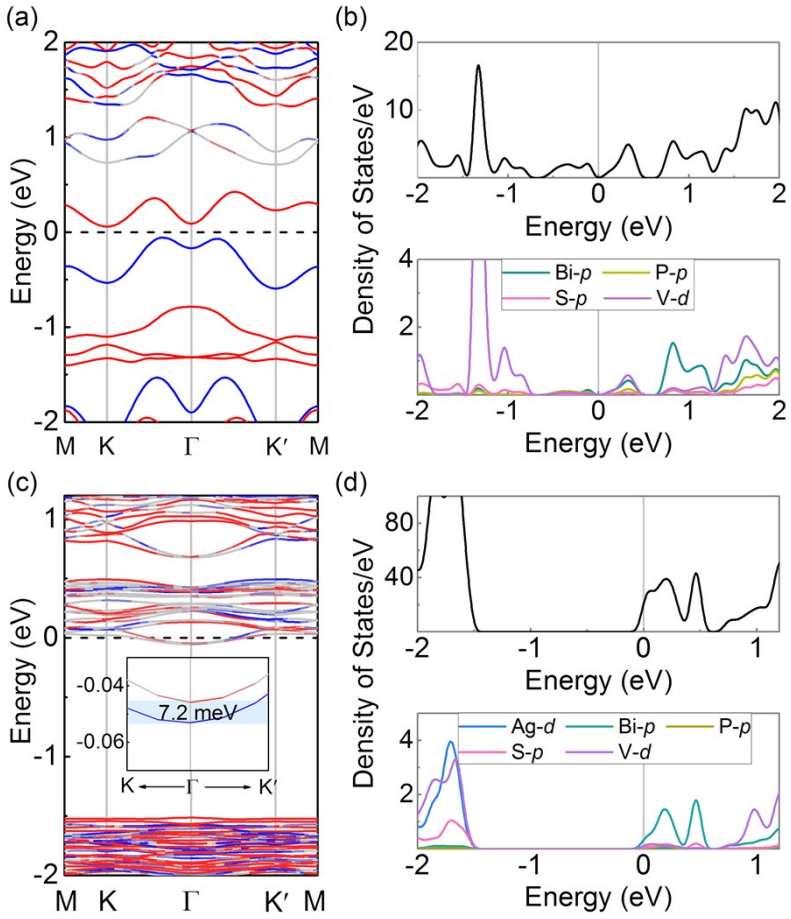

Fig. S4. Band structures and orbital-resolved PDOS with SOC for (a)-(b) $VBiP_2S_6$ with a doping concentration of 100% and (c)-(d) V-doped $AgBiP_2S_6$ with a doping concentration of 11% in a 3×3 supercell. The spin projections along *z* direction are represented by red and blue lines, which represent opposite spin states, respectively.

Table S1. The lattice vectors and fractional coordinates of each atom in V-doped $AgBiP_2S_6$.

a[Å]	12.8657064901794609	0.0000000494359845	0.0000000000000000
b[Å]	-6.4328532879025531	11.1420286334117531	0.0000000000000000
c[Å]	0.0000000000000000	0.0000000000000000	23.5874996185000008
S	0.6548579463045473	0.4890883335481567	0.5098919639639460
S	0.8342303872436092	0.3451420536954523	0.5098919639639460
S	0.5109116664518439	0.1657696127563913	0.5098919639639460
S	0.3436823654019980	0.4850030974970416	0.6501268895179962
S	0.1413207320950434	0.6563176345980026	0.6501268895179962
S	0.5149969025029590	0.8586792679049564	0.6501268895179962
S	0.3509391446914708	0.3462438974561883	0.5030093846765581
S	0.9953047527647176	0.6490608553085297	0.5030093846765581
S	0.6537561025438117	0.0046952472352823	0.5030093846765581
S	0.6457410784324674	0.6505358500755355	0.6529043810238895
S	0.0047947716430678	0.3542589215675322	0.6529043810238895
S	0.3494641499244646	0.9952052283569317	0.6529043810238895
S	0.5035458314862133	0.6470980912860445	0.5047630211356137
S	0.1435522597998370	0.4964541685137860	0.5047630211356137
S	0.3529019087139565	0.8564477402001627	0.5047630211356137
S	0.5118801504136585	0.3452378187526849	0.6480150927384950
S	0.8333576683390187	0.4881198495863416	0.6480150927384950
S	0.6547621812473159	0.1666423316609738	0.6480150927384950
S	0.1520587767200111	0.0011045934964447	0.5004077590839414
S	0.8490458167764340	0.8479412232799883	0.5004077590839414
S	0.9988954065035550	0.1509541832235663	0.5004077590839414
S	0.8412909907350090	0.9849479397359679	0.6473957900745945
S	0.1436569490009584	0.1587090092649906	0.6473957900745945
S	0.0150520602640324	0.8563430509990417	0.6473957900745945
P	0.5010814780799095	0.4963641483020060	0.6265499619854570
P	-0.0047173297779032	0.4989185219200908	0.6265499619854570
P	0.5036358516979937	0.0047173297779031	0.6265499619854570
P	0.5008946427396375	0.4947008668427069	0.5309127319758677
P	-0.0061937758969303	0.4991053572603626	0.5309127319758677
P	0.5052991331572937	0.0061937758969303	0.5309127319758677
P	0.0000000000000000	0.0000000000000000	0.6225475709000117
P	0.0000000000000000	0.0000000000000000	0.5255978598021375
Ag	0.1652537608570578	0.3338877729295850	0.5674708496970583
Ag	0.1686340120725274	0.8347462391429427	0.5674708496970583
Ag	0.6661122270704145	0.8313659879274724	0.5674708496970583
Bi	0.3263136704603770	0.1605544107509745	0.5795206841507511
Bi	0.8342407402905977	0.6736863295396228	0.5795206841507511
Bi	0.8394455892490258	0.1657592597094027	0.5795206841507511
Bi	0.3333333333333357	0.6666666666666643	0.5805803090938907
V	0.6666666666666643	0.3333333333333357	0.5788488941314359

Table S2. The lattice vectors and fractional coordinates of each atom in Cr-doped $AgBiP_2S_6$.

a[Å]	12.8765087487423333	0.0000000093358572	0.0000000000000000
b[Å]	-6.4382543824562539	11.1513836837954994	0.0000000000000000
c[Å]	0.0000000000000000	0.0000000000000000	23.5874996185000008
S	0.6518044905784184	0.4954822902703230	0.5076677195835120
S	0.8436777996919046	0.3481955094215816	0.5076677195835120
S	0.5045177097296766	0.1563222003080952	0.5076677195835120
S	0.3412565797144544	0.4872796018900415	0.6500050593964282
S	0.1460230221755870	0.6587434202855457	0.6500050593964282
S	0.5127203981099585	0.8539769778244131	0.6500050593964282
S	0.3503038282465109	0.3435671376664864	0.5048514918290654
S	0.9932633094199756	0.6496961717534893	0.5048514918290654
S	0.6564328623335133	0.0067366905800242	0.5048514918290654
S	0.6442447341818026	0.6595605603296201	0.6501113742832596
S	0.0153158261478177	0.3557552658181976	0.6501113742832596
S	0.3404394396703798	0.9846841738521821	0.6501113742832596
S	0.4944003319487371	0.6449738052166042	0.5029469244820770
S	0.1505734732678744	0.5055996680512628	0.5029469244820770
S	0.3550261947833954	0.8494265267321256	0.5029469244820770
S	0.5144400500028056	0.3562822539090889	0.6503868961097434
S	0.8418422039062771	0.4855599499971942	0.6503868961097434
S	0.6437177460909106	0.1581577960937167	0.6503868961097434
S	0.1554201113393837	0.0087074368354885	0.5036391164554682
S	0.8532873254961046	0.8445798886606167	0.5036391164554682
S	0.9912925631645116	0.1467126745038951	0.5036391164554682
S	0.8416835671983781	0.9863200329458471	0.6496847010803063
S	0.1446364657474685	0.1583164328016217	0.6496847010803063
S	0.0136799670541533	0.8553635342525315	0.6496847010803063
P	0.4996071519912832	0.5013293685852425	0.6265429521757551
P	0.0017222165939591	0.5003928480087166	0.6265429521757551
P	0.4986706314147575	-0.0017222165939590	0.6265429521757551
P	0.4997176694422530	0.4973979616083969	0.5306120249916005
P	-0.0023197078338561	0.5002823305577468	0.5306120249916005
P	0.5026020383916034	0.0023197078338561	0.5306120249916005
P	0.0000000000000000	0.0000000000000000	0.6260582207753019
P	0.0000000000000000	0.0000000000000000	0.5301325950657436
Ag	0.1648303277197019	0.3346759113259439	0.5593691725127840
Ag	0.1698455836062417	0.8351696722802979	0.5593691725127840
Ag	0.6653240886740565	0.8301544163937584	0.5593691725127840
Bi	0.3338054494605605	0.1664295387806212	0.5829379439346909
Bi	0.8326240893200607	0.6661945505394391	0.5829379439346909
Bi	0.8335704612193788	0.1673759106799393	0.5829379439346909
Bi	0.3333333333333357	0.6666666666666643	0.5814855125950904
Cr	0.6666666666666643	0.3333333333333357	0.5765377050597672

Table S3. The lattice vectors and fractional coordinates of each atom in Mn-doped $AgBiP_2S_6$.

a[Å]	12.8819772003869577	0.0000001144619014	0.0000000000000000
b[Å]	-6.4409886993204415	11.1561194492761206	0.0000000000000000
c[Å]	0.0000000000000000	0.0000000000000000	23.5874996185000008
S	0.6469008805739721	0.4855862928667921	0.5109674274186964
S	0.8386854122928209	0.3530991194260364	0.5109674274186964
S	0.5144137071332072	0.1613145877071717	0.5109674274186964
S	0.3430844230381752	0.4863674530247554	0.6538151217106818
S	0.1432830299865800	0.6569155769618251	0.6538151217106818
S	0.5136325469752434	0.8567169700134206	0.6538151217106818
S	0.3447777024432620	0.3464020911585713	0.5061126708509756
S	0.0016243887153017	0.6552222975567379	0.5061126708509756
S	0.6535979088414371	0.9983756112846998	0.5061126708509756
S	0.6463776422807602	0.6503693283819948	0.6543344151824433
S	0.0039916861012355	0.3536223577192560	0.6543344151824433
S	0.3496306716180052	0.9960083138987635	0.6543344151824433
S	0.4991240902461621	0.6465224393319368	0.5079290804321145
S	0.1473983490857827	0.5008759097538322	0.5079290804321145
S	0.3534775606680634	0.8526016509142155	0.5079290804321145
S	0.5071912259759351	0.3451597169682867	0.6509709772614266
S	0.8379684909923302	0.4928087740240663	0.6509709772614266
S	0.6548402830317145	0.1620315090076556	0.6509709772614266
S	0.1559555392427779	0.0093761871416233	0.4928815435442174
S	0.8534206478988532	0.8440444607572238	0.4928815435442174
S	0.9906238128583759	0.1465793521011547	0.4928815435442174
S	0.8407603888452931	0.9821614414942105	0.6407665771564813
S	0.1414010526489264	0.1592396111547141	0.6407665771564813
S	0.0178385585057812	0.8585989473510677	0.6407665771564813
P	0.4992469226416565	0.4965847595806134	0.6296279905034782
P	0.9973378369389583	0.5007530773583350	0.6296279905034782
P	0.5034152404193725	0.0026621630610434	0.6296279905034782
P	0.4957469874114995	0.4934356454837528	0.5338492398426491
P	0.9976886580722594	0.5042530125884999	0.5338492398426491
P	0.5065643545162503	0.0023113419277401	0.5338492398426491
P	0.0000000000000000	0.0000000000000000	0.6144864452078636
P	0.0000000000000000	0.0000000000000000	0.5170515653975373
Ag	0.1439276062965507	0.3225840821372049	0.5642433953137675
Ag	0.1786564758406470	0.8560723937034496	0.5642433953137675
Ag	0.6774159178628020	0.8213435241593448	0.5642433953137675
Bi	0.3271820304581467	0.1573486611825607	0.5777525214286943
Bi	0.8301666307244114	0.6728179695418458	0.5777525214286943
Bi	0.8426513388174459	0.1698333692755795	0.5777525214286943
Bi	0.3333333333333357	0.6666666666666643	0.5861009999271635
Mn	0.6666666666666643	0.3333333333333357	0.5861009999271635

Table S4. The lattice vectors and fractional coordinates of each atom in Fe-doped $AgBiP_2S_6$.

a[Å]	12.8403962079850960	0.0000000324739325	0.0000000000000000
b[Å]	-6.4201981321157966	11.1201092945354958	0.0000000000000000
c[Å]	0.0000000000000000	0.0000000000000000	23.5874996185000008
S	0.6579799124427795	0.4958187874722892	0.5100461583608371
S	0.8378388750295098	0.3420200875572207	0.5100461583608371
S	0.5041812125277110	0.1621611249704900	0.5100461583608371
S	0.3396411933338674	0.4844102236293238	0.6493647921170059
S	0.1447690302954567	0.6603588066661330	0.6493647921170059
S	0.5155897763706765	0.8552309697045435	0.6493647921170059
S	0.3526067386869859	0.3423967443857850	0.5042803553864217
S	0.9897900056987995	0.6473932613130142	0.5042803553864217
S	0.6576032556142155	0.0102099943012010	0.5042803553864217
S	0.6423255665289895	0.6549409644051003	0.6520680923527107
S	0.0126153978761110	0.3576744334710110	0.6520680923527107
S	0.3450590355948997	0.9873846021238892	0.6520680923527107
S	0.4972495946792806	0.6451433557988845	0.5041269540335553
S	0.1478937611196109	0.5027504053207191	0.5041269540335553
S	0.3548566442011155	0.8521062388803895	0.5041269540335553
S	0.5137224856669623	0.3514162641976066	0.6496130791804923
S	0.8376937785306362	0.4862775143330370	0.6496130791804923
S	0.6485837358023933	0.1623062214693563	0.6496130791804923
S	0.1546487937793268	0.0067277890304844	0.5030474739677105
S	0.8520789952511577	0.8453512062206733	0.5030474739677105
S	0.9932722109695159	0.1479210047488425	0.5030474739677105
S	0.8393633122063825	0.9813030018457031	0.6499803466892973
S	0.1419396896393204	0.1606366877936175	0.6499803466892973
S	0.0186969981542971	0.8580603103606794	0.6499803466892973
P	0.4989932027496640	0.4971868253128228	0.6268552792444542
P	-0.0018063774368409	0.5010067972503365	0.6268552792444542
P	0.5028131746871775	0.0018063774368409	0.6268552792444542
P	0.5009084593301675	0.4957678432515651	0.5313091284523211
P	-0.0051406160786019	0.4990915406698329	0.5313091284523211
P	0.5042321567484345	0.0051406160786021	0.5313091284523211
P	0.0000000000000000	0.0000000000000000	0.6260833416580608
P	0.0000000000000000	0.0000000000000000	0.5296336473266550
Ag	0.1662424565618629	0.3321203992439914	0.5603359092879607
Ag	0.1658779426821284	0.8337575434381365	0.5603359092879607
Ag	0.6678796007560087	0.8341220573178715	0.5603359092879607
Bi	0.3316480317326824	0.1646799828452171	0.5838721571136082
Bi	0.8330319511125351	0.6683519682673175	0.5838721571136082
Bi	0.8353200171547830	0.1669680488874653	0.5838721571136082
Bi	0.3333333333333357	0.6666666666666643	0.5817440499993179
Fe	0.6666666666666643	0.3333333333333357	0.5583199464568195

Table S5. The lattice vectors and fractional coordinates of each atom in Co-doped $AgBiP_2S_6$.

a[Å]	12.7880434369079019	-0.0000000675790626	0.0000000000000000
b[Å]	-6.3940216599287512	11.0747705148506732	0.0000000000000000
c[Å]	0.0000000000000000	0.0000000000000000	23.5874996185000008
S	0.6545307394057350	0.4884353790987767	0.5104101923430600
S	0.8339046396930391	0.3454692605942710	0.5104101923430600
S	0.5115646209012245	0.1660953603069522	0.5104101923430600
S	0.3413301487547981	0.4842631102584399	0.6502066917363674
S	0.1429329615036344	0.6586698512452008	0.6502066917363674
S	0.5157368897415598	0.8570670384963661	0.6502066917363674
S	0.3512376526736859	0.3445239436344114	0.5037532208875319
S	0.9932862909607185	0.6487623473263128	0.5037532208875319
S	0.6554760563655880	0.0067137090392749	0.5037532208875319
S	0.6449219257686022	0.6528942836044469	0.6527978599946804
S	0.0079723578358523	0.3550780742313989	0.6527978599946804
S	0.3471057163955533	0.9920276421641471	0.6527978599946804
S	0.5011422918463345	0.6472298391034103	0.5051780109374990
S	0.1460875472570837	0.4988577081536592	0.5051780109374990
S	0.3527701608965971	0.8539124527429214	0.5051780109374990
S	0.5145550640244473	0.3477946330789823	0.6484132719626460
S	0.8332395690545198	0.4854449359755442	0.6484132719626460
S	0.6522053669210178	0.1667604309454734	0.6484132719626460
S	0.1552079577930718	0.0068691664272308	0.4999055687588259
S	0.8516612086341574	0.8447920422069283	0.4999055687588259
S	0.9931308335727621	0.1483387913658413	0.4999055687588259
S	0.8388427183271688	0.9809248996750374	0.6474850273633138
S	0.1420821813478751	0.1611572816728380	0.6474850273633138
S	0.0190751003249629	0.8579178186521248	0.6474850273633138
P	0.5003760343986768	0.4961369531177888	0.6269390524000670
P	0.9957609187191263	0.4996239656013224	0.6269390524000670
P	0.5038630468822044	0.0042390812808813	0.6269390524000670
P	0.5021606028252803	0.4953544764715174	0.5314944906709872
P	0.9931938736462442	0.4978393971747200	0.5314944906709872
P	0.5046455235284888	0.0068061263537559	0.5314944906709872
P	0.0000000000000000	0.0000000000000000	0.6229525752666047
P	0.0000000000000000	0.0000000000000000	0.5262758174436668
Ag	0.1622883058455144	0.3275857195668966	0.5630168385959219
Ag	0.1652974137213824	0.8377116941544849	0.5630168385959219
Ag	0.6724142804331028	0.8347025862786189	0.5630168385959219
Bi	0.3333141748020887	0.1650322491778484	0.5811167944016155
Bi	0.8317180743757651	0.6666858251979101	0.5811167944016155
Bi	0.8349677508221595	0.1682819256242334	0.5811167944016155
Bi	0.3333333333333357	0.6666666666666643	0.5819487803889790
Co	0.6666666666666643	0.3333333333333357	0.5771519307431562

Table S6. The lattice vectors and fractional coordinates of each atom in Ni-doped $AgBiP_2S_6$.

a[Å]	12.8451228042110639	-0.0000002261694508	0.0000000000000000
b[Å]	-6.4225612062370354	11.1242027762623064	0.0000000000000000
c[Å]	0.0000000000000000	0.0000000000000000	23.5874996185000008
S	0.6564460813090357	0.4948107693602374	0.5070866601817167
S	0.8383646880512028	0.3435539186909645	0.5070866601817167
S	0.5051892306397621	0.1616353119487979	0.5070866601817167
S	0.3387085809695705	0.4906022508760313	0.6476208068759507
S	0.1518936699064607	0.6612914190304293	0.6476208068759507
S	0.5093977491239678	0.8481063300935394	0.6476208068759507
S	0.3504786566645607	0.3406336601772803	0.5051192065423394
S	0.9901550035127198	0.6495213433354389	0.5051192065423394
S	0.6593663398227193	0.0098449964872803	0.5051192065423394
S	0.6416759970833460	0.6571880672032888	0.6513246066981971
S	0.0155120701199436	0.3583240029166547	0.6513246066981971
S	0.3428119327967107	0.9844879298800561	0.6513246066981971
S	0.5004187339654455	0.6432840042960900	0.5015554191617695
S	0.1428652703306516	0.4995812660345542	0.5015554191617695
S	0.3567159957039101	0.8571347296693483	0.5015554191617695
S	0.5079985295646285	0.3549626459835969	0.6538804528726213
S	0.8469641164189611	0.4920014704353718	0.6538804528726213
S	0.6450373540164033	0.1530358835810316	0.6538804528726213
S	0.1541607666043134	0.0051815893511293	0.5065158526018575
S	0.8510208227468156	0.8458392333956862	0.5065158526018575
S	0.9948184106488707	0.1489791772531843	0.5065158526018575
S	0.8427682919595175	0.9889621304600609	0.6528604183879323
S	0.1461938385005428	0.1572317080404820	0.6528604183879323
S	0.0110378695399392	0.8538061614994572	0.6528604183879323
P	0.4973837008751829	0.4989804091635743	0.6268685627045026
P	0.0015967082883915	0.5026162991248170	0.6268685627045026
P	0.5010195908364256	-0.0015967082883915	0.6268685627045026
P	0.5000370685340066	0.4938997477024863	0.5308633614533850
P	-0.0061373208315210	0.4999629314659931	0.5308633614533850
P	0.5061002522975140	0.0061373208315211	0.5308633614533850
P	0.0000000000000000	0.0000000000000000	0.6283657443858565
P	0.0000000000000000	0.0000000000000000	0.5323668915432981
Ag	0.1668109415629730	0.3354290718226154	0.5634909141981940
Ag	0.1686181302596425	0.8331890584370270	0.5634909141981940
Ag	0.6645709281773848	0.8313818697403573	0.5634909141981940
Bi	0.3349775462683822	0.1677366260628877	0.5857535157489675
Bi	0.8327590797945057	0.6650224537316181	0.5857535157489675
Bi	0.8322633739371121	0.1672409202054942	0.5857535157489675
Bi	0.3333333333333357	0.6666666666666643	0.5775445360762760
Ni	0.6666666666666643	0.3333333333333357	0.5333836597122509