

ZCuOH

CIF file

1.0000000000000000

9.4422998428000007 0.0000000000000000 0.0000000000000000

-0.7718446244000000 9.4314702197999996 0.0000000000000000

-0.7410140138000000 -0.8132947143000000 9.3735478129000001

Al P O Si Cu H

6 5 25 1 1 1

Direct

0.9034099444262126	0.9535155422550144	0.2777376557181237
0.3576956598874385	0.7236754992100856	0.0562078378960513
0.6998314990844859	0.5192142262457297	0.2994599857313218
0.9237342101755666	0.7422513110054744	0.8423020840254024
0.1533747961604436	0.2839130101585681	0.0784388270489020
0.1282438232345420	0.4945841986276127	0.5176102530191773
0.1369334134787369	0.9549571869295250	0.0488645390647184
0.9137971152961899	0.7330961386442010	0.5114046095055698
0.9165825452723420	0.2835262751863166	0.2997373759506075
0.1441184249938670	0.5095720027814756	0.8471714342553571
0.6885886488711105	0.7423402623001573	0.0673852428305795
0.2742445941401377	0.8815674163643389	0.0715809837131843
0.0524060502427216	0.6572468180537997	0.5099011332987172
0.9335185081906882	0.8681918619360729	0.4335485173710111
0.3525100763138784	0.6426227677822788	0.2135735022816065
0.2956005137344153	0.5055714447119060	0.4465887172853658
0.0555957137594324	0.9488201615186739	0.1840301217592350
0.7810811317733320	0.3612838636546788	0.2796357759895778
0.0040860886724892	0.5825346499757438	0.8482180412048385
0.7712091481943180	0.7310991954336660	0.9343157690410074
-0.0063061109364551	0.2867387109257018	0.1629338190033237
0.1281432211982335	0.3770779228396451	0.9281914239154508
0.6927078678126390	0.6015608292679125	0.1399656329864616
0.2971889752244079	0.3574777349409533	0.1910342892374435
0.0428016454389745	0.8833034987538032	0.9184031857939757
0.7878672460793569	0.6333661571911312	0.4385841942264762
0.7549698329310589	0.8677222506792991	0.1726639070600674
0.0135718041798030	0.3557800124169549	0.4285795098886389
0.2711010149009990	0.6130057706275895	0.9108384621902113
0.1701483441907286	0.4596700447041456	0.6931712656445123
0.5347972258087099	0.7684082418804775	0.0203975392458422
0.8725876647783128	0.1294445970536101	0.3288836059862427
0.8803476591276725	0.7745365664277570	0.6647762163788987
0.5281666821779863	0.4781491521155680	0.3539107529178002
0.1775755148337338	0.1089908841356881	0.0197439408376749

0.5422010246155899	0.4254760586081379	0.7248118287236474
0.3622931286109158	0.4974253104667005	0.2876991429069392
0.4750336876488092	0.4586107182101802	0.5510373812073913
0.5282115094761584	0.3258816679794246	0.7455313778586852

ZCuOH-1NH3

CIF file

1.0000000000000000

9.4422998428000007	0.0000000000000000	0.0000000000000000
-0.7718446244000000	9.4314702197999996	0.0000000000000000
-0.7410140138000000	-0.8132947143000000	9.3735478129000001

Al	P	O	Si	Cu	H	N	
6	5	25		1	1	4	1

Direct

0.9023202126381070	0.9604239258089249	0.2746860931840305
0.3559616745627176	0.7243184722135234	0.0561145201076803
0.7045338599482083	0.5260891340178848	0.2853581821181830
0.9277916166505757	0.7498357707972912	0.8428875002966051
0.1619678121229118	0.2880927666723331	0.0736254426126731
0.1359160211685865	0.5023293946942673	0.5097207107476147
0.1387793899708246	0.9601967489775418	0.0454623027533139
0.9232321751582359	0.7347940658302575	0.4995591046562827
0.9221814526458275	0.2895291744953246	0.2914984141157567
0.1367146835758667	0.5177473284501852	0.8505517550572091
0.6880943076458437	0.7524252902034045	0.0600418461289106
0.2708539887798712	0.8807809532056996	0.0738801618332635
0.0631806169453675	0.6655609855635478	0.4802481607068143
0.9310332134864611	0.8779394457105660	0.4335897983188471
0.3556979783204229	0.6433116769645475	0.2134741937240986
0.3053795130623790	0.5013752126377617	0.4480673710642038
0.0511787940851004	0.9559690945155433	0.1767514706762269
0.7866162186254341	0.3674300340139228	0.2677979604016549
-0.0016972988908384	0.5895953292793844	0.8809599573447532
0.7673307236555301	0.7515102469609034	0.9237850384497535
0.9997382062187862	0.2865816185019820	0.1553597040619287
0.1332900776280412	0.3782180088175643	0.9213187333818516
0.7002073054975143	0.6080185355937562	0.1253000455706602
0.3029469325976705	0.3602381260167666	0.1890395615848109
0.0465821110101298	0.8937611737614102	0.9107401393842494
0.7956587621483663	0.6365621026132350	0.4267633518785476
0.7528198128321145	0.8745845517467620	0.1699722684066350
0.0165554068971406	0.3637481530308184	0.4209990781339152
0.2681871651612660	0.6188543263213665	0.9071164726744079
0.1340269383489494	0.4827191237671339	0.6897560156672246

0.5322180378194523	0.7732508557363974	0.0180815640529321
0.8735956381981987	0.1374221489213211	0.3257327862888283
0.8968513291424659	0.7578408290450009	0.6581918502119349
0.5377218680140777	0.4796466182853522	0.3452874509169827
0.1875978204447195	0.1127099443068601	0.0186782464130266
0.4177191270908910	0.3839520819779387	0.7085676280109982
0.3693872170672244	0.4984066643637886	0.2890551634773981
0.4975458210294849	0.4315249131210497	0.5461644351805999
0.4818885367823545	0.3494222592281448	0.7813467870244651
0.7562511937882848	0.4759441966186818	0.6522464877217075
0.6926631519546016	0.3163473934684889	0.6896345883400764
0.7473023477968174	0.3390851923922297	0.5304221501844036
0.6953784603740051	0.3850561683511460	0.6112454041345360

ZCuOH-2NH3

CIF file

1.0000000000000000

9.4422998428000007	0.0000000000000000	0.0000000000000000
-0.7718446244000000	9.4314702197999996	0.0000000000000000
-0.7410140138000000	-0.8132947143000000	9.3735478129000001

Al	P	O	Si	Cu	H	N	
6	5	25		1	1	7	2

Direct

0.9110496631852345	0.9649608585316322	0.2684685032604315
0.3675474943813323	0.7310212825570670	0.0551875301698942
0.7081244162117690	0.5294979543465215	0.2845395233245818
0.9341848752029919	0.7574589239251073	0.8333024254714185
0.1774950750818504	0.2980940037611808	0.0747999630266794
0.1326637999610604	0.5025686092898979	0.5083187717345765
0.1459372976931805	0.9661753438581085	0.0399520152359414
0.9240543649156100	0.7442063531090485	0.5012170115828212
0.9268693065608112	0.2974697821033645	0.2942751409529766
0.1519332294740197	0.5203429051772146	0.8433403939575169
0.6965430580548279	0.7558483673686458	0.0565171301567119
0.2792704285329455	0.8865949141259504	0.0626605812563565
0.0640885523768472	0.6718865293862356	0.5056269530606785
0.9416625402502884	0.8825000291844929	0.4269299055607988
0.3726347049673178	0.6551401932992066	0.2141615841468896
0.2840247197638026	0.5025611804093734	0.4219154135936499
0.0616642085418653	0.9574223804047732	0.1731873573184432
0.7934130245702468	0.3733618330387643	0.2539185550028908
0.0158704043795528	0.5999334952934330	0.8504218553035349
0.7782352834945653	0.7501090999159651	0.9216444922325929
0.0287454197104936	0.3047820768885248	0.1769925982081671

0.1320712935851533	0.3877740096757862	0.9241274342307602
0.7036928457457355	0.6140485761237585	0.1255657568936495
0.3318236774523062	0.3711101640690551	0.1695711075816672
0.0518922406329635	0.9009029607052991	0.9059448913759452
0.8025696197934569	0.6434867318885872	0.4221263915120284
0.7611164609104398	0.8802233679212187	0.1641431277294256
-0.0020517189668370	0.3677634575733654	0.4390568324399041
0.2854998911813575	0.6181837742239918	0.9060224015497466
0.1738045830874609	0.4750179365409323	0.6877036680227845
0.5418404357067869	0.7796584952462836	0.0088001282148843
0.8772961053432998	0.1414802849659454	0.3148778308652304
0.8830210364349315	0.7809995639595356	0.6541753722806297
0.5445205525507149	0.4923866411756687	0.3539656338045553
0.1908825632214714	0.1203468500674642	0.0163901903028028
0.5292126547979086	0.3942830189478430	0.7558815224387960
0.3780445074622794	0.5049078889414657	0.2858814093683444
0.5579121355507241	0.4643990377218585	0.5779181534916642
0.4763064430627376	0.4554770506925724	0.8163668012074221
0.7800500314144888	0.3170341408004632	0.5614386998824134
0.6453119046520169	0.2456042518442133	0.6431304908057995
0.6463617848873685	0.2235703766407969	0.4645034121357426
0.4241132216662449	0.6590559185206990	0.6948187210259499
0.5924053587225269	0.7215707074471041	0.6929416548052032
0.4817358188759914	0.7145353804313270	0.5454873592071554
0.6717526144372320	0.2928186748381924	0.5533691052579732
0.5091923154806079	0.6628446230620882	0.6335540520119693

ZCuOH-3NH3

CIF file

1.0000000000000000

9.4422998428000007 0.0000000000000000 0.0000000000000000

-0.7718446244000000 9.4314702197999996 0.0000000000000000

-0.7410140138000000 -0.8132947143000000 9.3735478129000001

Al	P	O	Si	Cu	H	N	
6	5	25		1	1	10	3

Direct

0.9103096931113526 0.9869463737658246 0.2725696453257884

0.3637632151374275 0.7541122495097835 0.0644230069828107

0.7063870794971377 0.5527810222829641 0.2939880364128631

0.9296543029632731 0.7827086025845327 0.8370173410415456

0.1698391783398371 0.3228861491468386 0.0831566068377616

0.1346914165990389 0.5236571357183402 0.5173470294049541

0.1443068034403014 0.9913995261264240 0.0424541399676044

0.9251062258696413 0.7671118998006805 0.5069010173459458

0.9254437038226399	0.3185521662788890	0.3095674615021348
0.1472719627300695	0.5428254397374983	0.8500485703346905
0.6951960112051311	0.7760808131847342	0.0638052395237863
0.2784576635297829	0.9128049803539289	0.0655766205989440
0.0632520343283236	0.6912013237427210	0.5152409860702962
0.9477633996895812	0.9036292233513515	0.4296668971947191
0.3638165529028058	0.6782696200554867	0.2232388350185426
0.2801685539465736	0.5114669173540252	0.4240064469921032
0.0603384200319565	0.9852554454496567	0.1759257350824836
0.7940289260334884	0.3962333475788862	0.2692261412438539
0.0116053684353936	0.6233383076626293	0.8464870996782320
0.7771872301982085	0.7706419284278699	0.9294291873092785
0.0288978844059941	0.3263146369783591	0.1934467225570911
0.1190006109584810	0.4095075093135555	0.9301505473087973
0.7046035978306128	0.6333942127223802	0.1313979317798014
0.3300610135644784	0.3963990335046328	0.1658343023543290
0.0507199295817040	0.9249492399294491	0.9088776095553831
0.8024290609444846	0.6683705726990300	0.4289692433511650
0.7596923914626097	0.9003402005258008	0.1720161354721550
-0.0022699829865975	0.3854540112989286	0.4554851909995408
0.2782357279394788	0.6378700128001946	0.9197052662945490
0.1779534076066533	0.4923867881064473	0.6971402644627969
0.5395565400646529	0.7984677153669602	0.0191288510889540
0.8754444826969411	0.1617289061105768	0.3275627906771631
0.8848022764814818	0.8124748381256792	0.6584488130654846
0.5417875220723917	0.5090966139226799	0.3509217465032088
0.1885688985981910	0.1464439317854766	0.0173797420115505
0.7058275580811434	0.1684210749727337	0.9182026121582575
0.3773317996419714	0.5260104908282801	0.2907538616319110
0.6351052652360853	0.2510844520579883	0.7553344941380222
0.6410696414584389	0.1660974055551973	-0.0065459574171078
0.8818666383523553	0.2656205676064880	0.6190210398330549
0.8887356540050777	0.2116787048150239	0.7836834531368366
0.8252409923652370	0.1006054662471960	0.6465333721882955
0.4871736744015471	0.3398114691393520	0.9626878307525438
0.4777411588688843	0.4520913125993289	0.8392638860824015
0.3780552988023990	0.3007648840583230	0.8185090525705061
0.5524273730441052	0.3790025082156013	0.5149979223170017
0.5901989929748934	0.2155771933478977	0.4796298572095063
0.4387416339840787	0.2472399173557743	0.5432615683562847
0.8294314915173111	0.2047341642977074	0.6871288399138530
0.4782052393687060	0.3458321392120666	0.8541869141126838
0.5457265138642439	0.2793275683878377	0.5539000006656509

ZCuOH·1H₂O·1NH₃

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1.0000000000000000

9.4422998428000007 0.0000000000000000 0.0000000000000000

-0.7718446244000000 9.4314702197999996 0.0000000000000000

-0.7410140138000000 -0.8132947143000000 9.3735478129000001

Al P O Si Cu H N

6 5 26 1 1 6 1

Direct

0.9207701948423346 0.9564019767354699 0.2880888834937171

0.3782602982729927 0.7214589150187237 0.0790201868914197

0.7182621896920602 0.5198505238602318 0.3082073658248909

0.9434655488481244 0.7466669612209952 0.8533704869967259

0.1786609167227369 0.2856882998609811 0.0924907463439124

0.1471094551038447 0.4932469143347221 0.5294407872225656

0.1574119061402802 0.9572299167706861 0.0638908485185964

0.9298491614262948 0.7319930134449096 0.5225371088637661

0.9377408745322046 0.2842882879435921 0.3193219871035625

0.1611675546128071 0.5096288431297259 0.8637468314497978

0.7076303568682129 0.7457238404033483 0.0750325329602327

0.2908941651834676 0.8778960905949472 0.0872989151434924

0.0678229528596113 0.6562531837985223 0.5238433265682113

0.9467748840187278 0.8651368642174445 0.4406241454839018

0.3895890785243642 0.6458199312525258 0.2376692012212372

0.3008932057019255 0.4966541496740948 0.4468890847429742

0.0764581025318661 0.9568149946895380 0.1996394155922169

0.8070056990737473 0.3655733305733671 0.2848941533876493

0.0235467332651582 0.5869064998045654 0.8622451798801352

0.7838415486003848 0.7284705179614682 0.9365017339925167

0.0294554294567924 0.2835324930421019 0.1929596393795768

0.1364524750477795 0.3741437343836841 0.9394971976812323

0.7183031873556309 0.6091631000213994 0.1524292723570565

0.3295503335935989 0.3638596728798121 0.1883413486073832

0.0598023118026049 0.8864892627504951 0.9348704270530690

0.8025249388514978 0.6315490962120317 0.4534873911449386

0.7764586314769145 0.8756260489750358 0.1723660418624131

0.0207618975964508 0.3525479467686398 0.4582172550537759

0.2900704766032234 0.6070321677838947 0.9353085185976070

0.1951067517455526 0.4680718826962438 0.7097100257792236

0.5520743636810725 0.7675583760580333 0.0290990797881204

0.8832761737684083 0.1301661250745256 0.3442156860382271

0.8977359654807147 0.7783341338281679 0.6760789778086377

0.5527736779485057 0.4652002437415554 0.3637050526818689

0.2029399700086416 0.1096091524250242 0.0320036969101763

0.6176890593451519	0.2644202699883226	0.9073189914193213
0.5839925584909362	0.2640041380590704	0.5315079731466442
0.3876341802743934	0.4938041875020749	0.3058195740760224
0.5857659577850536	0.3271265083045197	0.7352034634910399
0.5343003300825974	0.2300958173166223	0.9540521345956197
0.6577144010037060	0.2056266954154778	0.4991911380975818
0.5688252415747799	0.3388333694019403	0.4594071820283299
0.4347148549418020	0.5330907136704479	0.7252816986054312
0.6022944731237573	0.5978726858398842	0.7726205622425887
0.5485755786175573	0.5462465327869488	0.6016504020118617
0.5391919475217429	0.5234428387841898	0.7054043128607028

ZCuOH·1H₂O·2NH₃

CIF file

1.0000000000000000

9.4422998428000007	0.0000000000000000	0.0000000000000000
-0.7718446244000000	9.4314702197999996	0.0000000000000000
-0.7410140138000000	-0.8132947143000000	9.3735478129000001

Al	P	O	Si	Cu	H	N	
6	5	26	1	1	9	2	

Direct

0.9010593094418778	0.9846381326226031	0.2851657694777943
0.3570323970492775	0.7522049781654090	0.0796659812790323
0.6990174793705128	0.5513483598926674	0.3059937277621952
0.9228646168366097	0.7782937695750227	0.8494250912216721
0.1632954695838982	0.3191425973704857	0.0913214820288459
0.1303933721896749	0.5240301573192204	0.5308242958271400
0.1380521501353654	0.9869137610282943	0.0572965007089459
0.9151939562803917	0.7653120370665498	0.5203968241515741
0.9210951779393499	0.3169144482460629	0.3202317072002577
0.1366201074057635	0.5395755220051930	0.8626808595304748
0.6874311481135096	0.7757726116973852	0.0763488369065762
0.2737488334350168	0.9124587791447000	0.0857698197990524
0.0526881949958579	0.6883416185834101	0.5282566216101705
0.9377247107007326	0.9012500578839009	0.4421073909107376
0.3656021245070511	0.6803959456118959	0.2406733253597230
0.2770821578239506	0.5159438568878875	0.4399976229189627
0.0503339363372629	0.9803268608053689	0.1884133796851410
0.7910819816706439	0.3972629629124254	0.2826714363407252
-0.0029461624702072	0.6144662134104519	0.8522720408008307
0.7709728742746664	0.7736721525023221	0.9428232910776788
0.0198146940511983	0.3205145007691002	0.2003445354809901
0.1061265187515735	0.4036149779153061	0.9383740983927698
0.7022839912458049	0.6342918891152901	0.1449495479170498

0.3163231631994368	0.3998465182766130	0.1791491492572022
0.0481402053944674	0.9153142173223333	0.9233961819597519
0.7912464765818836	0.6668107947686736	0.4443124189467573
0.7483747446752781	0.9019848876685853	0.1845940864459121
0.9971307072563758	0.3825366395297461	0.4653537532267268
0.2603814487032801	0.6375622087633470	0.9402482580625656
0.1762788058264359	0.4936808269589608	0.7110469821890297
0.5315457221091026	0.7934211971893755	0.0290778238849520
0.8680186324759096	0.1608910903846710	0.3412321786535090
0.8770287544034759	0.8129323048962671	0.6722390324526493
0.5350509799762768	0.4992962460176812	0.3597873634701467
0.1779938824310408	0.1416183137833502	0.0299043467897790
0.6735419281598544	0.2931980394898690	0.9049201220407338
0.4388848413192667	0.2897255511980173	0.7632609335239151
0.3711176794582097	0.5256458740489801	0.3041748800284622
0.6476552358861619	0.2647717094784893	0.7036250333155278
0.7393318916661180	0.3748086434152455	0.9425226954300251
0.9031403190434137	0.2608145211613964	0.6120828679524886
0.9056360808741120	0.2418516397538998	0.7860678454044221
0.8524670585149720	0.1046471341436657	0.6691478724301261
0.3859280185997988	0.3707775845000116	0.7400859145770707
0.4944934225969649	0.3126074787015803	0.8590530460803190
0.5533004857632053	0.3331369428796747	0.4565501915278581
0.6403561985812467	0.1897812061189911	0.4308760835856348
0.4795205893563492	0.1750505690593386	0.4885440050971551
0.8498567177861104	0.2126203054637558	0.6890455446413695
0.5744869056914758	0.2372014814965340	0.4981271206375965

Z2Cu

CIF file

1.0000000000000000

9.4422998428000007 0.0000000000000000 0.0000000000000000

-0.7718446244000000 9.4314702197999996 0.0000000000000000

-0.7410140138000000 -0.8132947143000000 9.3735478129000001

Al P Si O Cu

6 4 2 24 1

Direct

0.3005514834578334	0.7324504593460091	0.4721412809836213
0.7566894900706183	0.5030659757346880	0.2586823399702677
0.1047878079797094	0.3184683463879106	0.4853992991908022
0.3359695295804707	0.5216643044459455	0.0403035737201268
0.5717105098514685	0.0676092702517842	0.2660998713807661
0.5354053234582211	0.2827319140232479	0.7004319466686185
0.5445280502305774	0.7287789309304067	0.2533916375656464

0.3268673949101075	0.5131480654538909	0.6945461602555575
0.5400900210965390	0.2934246819057126	0.0484454338777812
0.7663288189267640	0.2786177297520897	0.4857208623271467
0.3323532990779230	0.0717980092673116	0.4867895892975258
0.0967596267714887	0.5293456707487172	0.2481142811183668
0.6879492165397555	0.6676882723090217	0.2846451775969053
0.4577115558780838	0.4370931233957617	0.6509865628675994
0.3331781885878656	0.6607344214217191	0.6387757317305952
0.7268437637853651	0.4099039148088764	0.4102170738673195
0.7033253269884164	0.2819250682066258	0.6310001437442319
0.4545310757560241	0.7090429839699908	0.3794701677987791
0.1968703878624344	0.1672165810595629	0.4484904572962189
0.3908656699303069	0.3448412195031990	0.0951216803078662
0.1747651421829081	0.5392150748078300	0.1037562044948953
0.4094603645016150	0.1074698056156210	0.3352865868245467
0.5594950557452338	0.1479414452352351	0.1040242008840934
0.1379672621647427	0.3734064160035789	0.3125092064230823
0.7116347711312045	0.1417232780089607	0.3894313161081008
0.4674776177215511	0.6543139383521025	0.1138534364073029
0.1873707069358793	0.4244402778607581	0.6326139712324874
0.1515007291930049	0.6467078980276068	0.3770197410273191
0.4318446926895831	0.1342811087774283	0.6254199426960313
0.6575785149749395	0.4051337123141622	0.1113590603255785
0.5377576452518705	0.2820310327558016	0.8868580068113068
0.9277031676920220	0.5169717589096232	0.2176334059148600
0.2789048454788286	0.9104978171484870	0.4924417082538617
0.3278683314894755	0.5255850940413803	0.8569995170184465
0.9284135749892183	0.2784735439212230	0.5132381414370658
0.5765506713789744	0.8869742759764575	0.2311852344739825
0.2856803347389805	0.2512245723212863	0.2751269711013133

Z2Cu-1NH3

CIF file

1.0000000000000000

9.4422998428000007	0.0000000000000000	0.0000000000000000
-0.7718446244000000	9.4314702197999996	0.0000000000000000
-0.7410140138000000	-0.8132947143000000	9.3735478129000001

Al	P	Si	O	Cu	N	H
6	4	2	24	1	1	3

Direct

0.4288792943896360	0.8134606600554599	0.5472737343084823
0.8853303416578284	0.5946444623355062	0.3299565562970597
0.2120935487570849	0.3956588360553723	0.5831450710616092
0.4545772318557351	0.6140952364651777	0.1094526347524445

0.6710182027032425	0.1546426089681666	0.3478888664523575
0.6545746108817305	0.3510851586313457	0.7878293229178255
0.6663797281396763	0.8286636253343530	0.3275274348984946
0.4354043438983565	0.5995425850739329	0.7823962289343760
0.6754483548684551	0.3777176885159279	0.1130894577932413
0.8804858698449278	0.3693845195248377	0.5629622846438583
0.4409839375248445	0.1390172172153139	0.5829396562322453
0.2192657710414824	0.5922991052840988	0.3249703393711497
0.8023853108169618	0.7527439319390558	0.3499305669260626
0.5537363688698773	0.4976616324110605	0.7815866157597464
0.4762650411701222	0.7244370124177145	0.6975543581820715
0.8729586641491662	0.5057526246018526	0.4862924898656341
0.8064506260663800	0.3875952925477710	0.7000581063454413
0.5904270124348897	0.8351481504763751	0.4650125426810626
0.3095328727899915	0.2447739403819852	0.5612552921467668
0.5331785353680567	0.4486505781151217	0.1002053849102599
0.2986393063688577	0.5682941015754051	0.1814591480072453
0.5027649090795746	0.1595304072142126	0.4212335298887949
0.6482345876001526	0.2452403446716275	0.1945609286240870
0.2248547096866165	0.4362429477630231	0.4032472946628350
0.8112513013303098	0.2389367295501105	0.4655184427660917
0.5690465058632815	0.7517467124133140	0.2011322789717337
0.2918276545710138	0.5185025757593025	0.7187147093750860
0.2992929172672120	0.7127387749641972	0.4387095508388864
0.5563247783615102	0.1995116471540124	0.7105826447093863
0.7929306490470552	0.4816847009578851	0.1899055196139789
0.7162134063489840	0.3295991994682211	0.9643549524958624
0.0564937124698019	0.6218285657006588	0.2890466769168240
0.3773421794325933	0.9803377282828613	0.5959759105637508
0.4173688473165106	0.6581795696681025	0.9352888257987833
0.0360154028913899	0.3437494623402332	0.6072055429309051
0.7084182921523129	0.9821541956158587	0.2918161156165914
0.3321171666678695	0.2674874025448007	0.3567038743593553
0.3043065097753028	0.2382751748874073	0.1488162219863536
0.2056388255988836	0.2645151604546841	0.1121022894346927
0.3793073857398748	0.3075285988090850	0.1096535712918723
0.3168454932024385	0.1366510818546087	0.1085649316667047

Z2Cu-2NH3

CIF file

1.0000000000000000

9.4422998428000007	0.0000000000000000	0.0000000000000000
-0.7718446244000000	9.4314702197999996	0.0000000000000000
-0.7410140138000000	-0.8132947143000000	9.3735478129000001

Al	P	Si	O	Cu	N	H	
6	4	2	24	1	2	6	
Direct							
0.4426108068769233			0.8132146005781865			0.5448240554953588	
0.8941011727300230			0.5860272794370128			0.3199895545121472	
0.2185499106461674			0.3905018021605968			0.5738897151199868	
0.4601517977627370			0.6100328237026624			0.1107364973384408	
0.6885386776168092			0.1537809539463899			0.3434595942541439	
0.6473264854794677			0.3512830897806921			0.7775766439759242	
0.6669962829785941			0.8240558445575323			0.3207378706592995	
0.4465776403403248			0.6010896571696391			0.7788758301371740	
0.6913562843535792			0.3730984101183788			0.1089253958061579	
0.8888657601863867			0.3640793929876008			0.5530998389677069	
0.4403033972724800			0.1459919386109085			0.5654094312741542	
0.2239103844716244			0.5923505218894548			0.3233031826386213	
0.7927131463090610			0.7320980946749454			0.3179796926212093	
0.5801726485853276			0.5192876024677946			0.7750291386734384	
0.4716915978481372			0.7392302341456987			0.7079060582893798	
0.8771681995647502			0.5040938148219308			0.4813422982357017	
0.7939614983813870			0.3596952061264449			0.6761975456033343	
0.6083546088373282			0.8250880226348107			0.4681051287096443	
0.2930814480292537			0.2294194828116102			0.5268749663557117	
0.5632742687486050			0.4634989557625318			0.1185432345310994	
0.2985808886765525			0.5605061011913501			0.1757287108406710	
0.5367634545931753			0.1667852761105568			0.4320899816269224	
0.6610565943137462			0.2372905941564386			0.1844562323442961	
0.2087763704740180			0.4343197022546423			0.3937315684011121	
0.8462977821877969			0.2350275844790838			0.4420225711164096	
0.5498340122818040			0.7658287811076183			0.2013522359963925	
0.3153610098490253			0.5072187959033508			0.7039797988942278	
0.3211377057540499			0.7026573775924668			0.4344255127397335	
0.5162266560434827			0.2179885732074541			0.7157328756671725	
0.8286504889976708			0.4578561255901304			0.1784208403836990	
0.7134254614709049			0.3290578673910790			0.9528494108799858	
0.0665142093168544			0.6433824203235299			0.2931776752695587	
0.3821287450360035			0.9808196297068684			0.5684082232422023	
0.4163167560681272			0.6408894550483005			0.9334105324512220	
0.0431710944526827			0.3553462911876409			0.6171956318517640	
0.7201643402736789			0.9765254333311505			0.2915927458521550	
0.2350566147246796			0.2328868794466761			0.3171359524413782	
0.1942558528007052			0.2739979955904628			0.1142879440208646	
0.2332542302418236			0.0200010696482997			0.2828253261493779	
0.0873632704782400			0.2637746759993198			0.0816985999038426	
0.2309373015868946			0.3815990137528092			0.1141231806346549	

0.2450283021045276	0.2156043078088621	0.0408469860415237
0.1398325964703310	-0.0326827265853057	0.2362301245935556
0.3137511694370256	-0.0082130946506760	0.2223318289341812
0.2544593313472305	0.9812340490231040	0.3812897275244727

Z2Cu-3NH3

CIF file

1.0000000000000000

9.4422998428000007	0.0000000000000000	0.0000000000000000
-0.7718446244000000	9.4314702197999996	0.0000000000000000
-0.7410140138000000	-0.8132947143000000	9.3735478129000001

Al	P	Si	O	Cu	N	H	
6	4	2	24	1	3	9	

Direct

0.4419131696315520	0.9106259657286345	0.5887282816982006
0.9015480149285781	0.6791558054839563	0.3657644679716183
0.2375426033138200	0.4802693144104539	0.6028356875551140
0.4728052568006108	0.7035266737634640	0.1464215290349695
0.6987747700226603	0.2439226000347810	0.3885046762724398
0.6703110302419131	0.4525212661557301	0.8239526846427597
0.6810388178340578	0.9120591650924207	0.3570510189546837
0.4641259621133813	0.6890262714996596	0.8174154314808426
0.6903878549742809	0.4648813994960366	0.1520334970200372
0.9079586621556469	0.4528097922251844	0.5981737090086009
0.4548257659314132	0.2414802988505454	0.6127355004626197
0.2289077843745030	0.7064633376690823	0.3725646372030515
0.8140492788069202	0.8348273805465206	0.3964711688142364
0.6070262136409478	0.6215928957905167	0.8276044488448721
0.4871201338389200	0.8235436458327590	0.7400583035680487
0.8960886410718583	0.5904536653184559	0.5228819184929009
0.8210700183246165	0.4565646971163312	0.7276249820543312
0.5856107863244944	0.9092526558238126	0.4799903343231036
0.2998546516508561	0.3095827799744886	0.5699308597050666
0.5501831647554311	0.5383909956877760	0.1517790122576715
0.3259271757597038	0.7027761955104458	0.2400125692229932
0.5435406254747325	0.2496512727164495	0.4712768465849619
0.6726982983568321	0.3296762383780445	0.2315497540317684
0.2254714428528156	0.5513147736605629	0.4389892371261035
0.8549765252455735	0.3212683695157473	0.4920979667799849
0.6032064583111283	0.8433568526643027	0.2161568564140803
0.3431974910593615	0.5856744411663021	0.7382740047033812
0.2859393292175464	0.8325462629920118	0.4965500061457071
0.5365770778328713	0.3297006255375636	0.7510192556328081
0.8148121584059262	0.5662284381544468	0.2247405104963127

0.7252240567398098	0.4201171957040028	-0.0001571192894187
0.0671393601766996	0.7412273661592246	0.3203312680555079
0.4095867575421054	0.0807890714903207	0.6444735235529828
0.4219165176753247	0.7299268588380470	0.9682705265849247
0.0633602220195091	0.4384740519050321	0.6524874302634689
0.7370095238474875	0.0674781276458920	0.3359746043716323
0.1809170921681316	0.1766928130707237	0.4081585920601582
0.0599963795125994	0.0454187186740907	0.2536916806717462
0.1010875418246797	0.0594801244247461	0.5536681553092074
0.2822937066060618	0.2988267799810152	0.2790206109469045
0.9539387510391099	0.0604748335711930	0.2619194283435389
0.0823283546375729	0.0606286573344808	0.1514076551821799
0.0709605738318685	0.9389627837609665	0.2699056395651965
-0.0067545148973842	0.0328866863509169	0.5402494118445448
0.1540224282914472	0.9672158889204404	0.5466603348333519
0.1281979836295907	0.1118850632870945	0.6521870879066661
0.2629886256589455	0.4026335466342502	0.3128100230899359
0.3892043467570018	0.2904999370810830	0.3057625290453286
0.2627829126864716	0.2831172483699698	0.1706094571588612

Z2Cu-4NH3

CIF file

1.0000000000000000

9.4422998428000007	0.0000000000000000	0.0000000000000000
-0.7718446244000000	9.4314702197999996	0.0000000000000000
-0.7410140138000000	-0.8132947143000000	9.3735478129000001

Al	P	Si	O	Cu	N	H
6	4	2	24	1	4	12

Direct

0.5833075187467323	0.0800338983600330	0.5456232591003416
0.0430528542652473	0.8495409625359492	0.3267854865035724
0.3712477787991051	0.6434293813004315	0.5661149001632860
0.6083591766650522	0.8731254531789147	0.1075090051089203
0.8349891338502704	0.4144208301923317	0.3546759167602196
0.8032604540817078	0.6146911739692000	0.7886229908427921
0.8182614308770162	0.0872889777332140	0.3194737647873545
0.5957927152696941	0.8549348261432249	0.7791107865766554
0.8321188497140416	0.6327443392064650	0.1157479144454921
0.0431763553167567	0.6270677357051710	0.5597273562169214
0.5873329152496825	0.4065510772412489	0.5826734708266190
0.3690653702807487	0.8662551839598137	0.3274587529970439
0.9479707868565095	0.0008864493930420	0.3366437127664848
0.7360761614996885	0.7835307934428922	0.7972695876242702
0.6209704810011109	-0.0168097789589708	0.6936615278504693

0.0360033088208164	0.7691070346402861	0.4897098848618360
0.9480644194665900	0.6255560147010523	0.6839167109261495
0.7421207670542669	0.0889608615480167	0.4566069941839898
0.4413375983755635	0.4803070070124945	0.5341133732369686
0.6991505727057540	0.7174567026577833	0.1090467968275053
0.4511251653365990	0.8407879490200711	0.1832131465375195
0.6890834557839506	0.4131672747946032	0.4508692998249032
0.7946220890247071	0.5009429713120448	0.1970244595876438
0.3571426527002543	0.7201801454066509	0.4063341593115588
-0.0066384642818114	0.5006021452359797	0.4469457777090930
0.7179876214857109	0.0235431438143573	0.1882464477764786
0.4713432462439813	0.7511413031506052	0.7088020617244859
0.4456499151582920	0.0000040301458677	0.4299714508653588
0.6671980081438239	0.4871827825692493	0.7298735637284391
0.9618056089047913	0.7232860792617941	0.1916040196748054
0.8669965209609624	0.5831984645134635	0.9643655072019032
0.2085278226715014	0.9108309062309308	0.2773183735800725
0.5402656644553064	0.2440258409755161	0.6142835559442993
0.5571770655297137	0.9100719626298712	0.9298925889439871
0.1960818764124843	0.6105211231928847	0.6213132001491017
0.8744438209028710	0.2407451162102749	0.2931788542622444
0.3603282101772348	0.2847433028033330	0.1092922846958167
0.3022715485938443	0.0824883615124452	0.0216797024238610
0.2603343644991945	0.2439678697331147	0.2893632559285628
0.4217133873002329	0.3418441297904873	-0.0873803926179854
0.4491699566360383	0.4726272902566740	0.2055439032571304
0.2279924181996680	0.0806015389075051	0.9361519917115656
0.3881436296895825	0.0342220122604773	0.9844427605169923
0.2598908413430027	0.0163088107522579	0.0929376669611965
0.1564042578816094	0.2695637675590017	0.2805932293814554
0.2567978153218066	0.1374770229072314	0.3077868123862335
0.3100280824425432	0.3013203578975153	0.3796767533056471
0.3441656278995524	0.3979265914890284	0.8665653546815807
0.5145455307749062	0.4078426257585984	-0.0829972844860603
0.4376017733838650	0.2619667126793394	0.8359407645235901
0.4050596994280049	0.5619559123597615	0.1733796749147114
0.4444847813717226	0.4787513944409122	0.3151887719610316
0.5560874097277093	0.4866720074655552	0.1903961390258972

Z2Cu-1H2O-1NH3

CIF file

1.0000000000000000

9.4422998428000007	0.0000000000000000	0.0000000000000000
-0.7718446244000000	9.4314702197999996	0.0000000000000000

-0.7410140138000000				-0.8132947143000000			9.3735478129000001
Al	P	Si	O	Cu	N	H	
6	4	2	25	1	1	5	

Direct

0.5194889119611378	0.9610274831367979	0.6361867789823361
0.9696075292799200	0.7344535279002511	0.4098332014435641
0.2906230458244476	0.5382820472190128	0.6729961789681478
0.5350545277473432	0.7548467958367185	0.2048300232372011
0.7616828863424884	0.3019566779288241	0.4342721843628863
0.7200089293866926	0.4997893450122234	0.8690362422421085
0.7415435843552182	0.9704947848836383	0.4138042489994739
0.5181106972261453	0.7499290239329877	0.8735659966322836
0.7687137379198036	0.5207326608896671	0.1997880823496327
0.9614869260974399	0.5123512775417075	0.6436476089244455
0.5155828053266209	0.2946889913613592	0.6568555716730343
0.2989351176239319	0.7395155214945243	0.4173079476779134
0.8691043184707213	0.8811309644854203	0.4060495777160795
0.6502617682601145	0.6664007771083931	0.8665687885119624
0.5418681828634470	0.8867639227041382	0.8000910524878073
0.9531976123433085	0.6521203601874259	0.5707278294706601
0.8635294750227116	0.5103433243280160	0.7640602994712614
0.6874424534031179	0.9697848982043825	0.5632489188054406
0.3669678947635062	0.3786090473622603	0.6230790674538305
0.6412223442741163	0.6115100736132953	0.2121314903434787
0.3727951454396915	0.6976151238792072	0.2691341312609370
0.6106501585986537	0.3211073063606726	0.5232355989558735
0.7395526976639634	0.3843244062750789	0.2742766183350135
0.2826214717042194	0.5849578823997074	0.4934041817163871
0.9200404241328790	0.3828216872950987	0.5328598427865613
0.6216493737441049	0.9103544713648866	0.2979284263616279
0.3842898005846835	0.6570661621532107	0.8026727250016716
0.4002603854341152	0.8518476090196828	0.5214973471555241
0.5913709020596251	0.3638849518461706	0.8081109669156987
0.9066947551464124	0.6054400596587445	0.2683959091163980
0.7898537109155523	0.4785529659432147	0.0432187132707232
0.1427916920861850	0.7916699931416530	0.3849183479209899
0.4589731684303033	0.1286797829092809	0.6546302888905496
0.4921070591328437	0.7910595367983129	0.0290578329780351
0.1142336273211621	0.5019594001100068	0.7114124896594487
0.7906962231945136	0.1237660821857644	0.3840033087412876
0.2752635130539384	0.4350382888519288	0.2135107863549841
0.3070390657638240	0.3876895519597051	0.4160645894600905
0.3015602569514880	0.1785934113073027	0.3700587435975614
0.1754587551624554	0.4287898340137439	0.1755414133750144

0.3114327684483616	0.5417340300824479	0.2197871209566715
0.2045031016284724	0.1303096109262164	0.3280176764943309
0.3750619284292702	0.1562528629473916	0.2989711999506663
0.3300873104810677	0.1321734584395154	0.4627505949904135

Z2Cu-1H2O-2NH3

CIF file

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-0.7718446244000000	9.4314702197999996	0.0000000000000000
-0.7410140138000000	-0.8132947143000000	9.3735478129000001

Al	P	Si	O	Cu	N	H	
6	4	2	25	1	2	8	

Direct

0.5627051814863572	0.0303198389966250	0.5491083053170863
0.0206084694423668	0.8036584523353525	0.3246684031699613
0.3569302150645597	0.6044987301476586	0.5632536625950832
0.5932051194119187	0.8289343434449370	0.1069569709824333
0.8128370084725386	0.3691943359021115	0.3478661700940912
0.7904992542619876	0.5756250870715759	0.7846845220602405
0.8014250763289416	0.0364204752867578	0.3165853297861002
0.5831199212796210	0.8135063478305405	0.7789997759202322
0.8097809434354243	0.5898195751304536	0.1118456328523004
0.0244626063202941	0.5794583539388108	0.5588314756056211
0.5735045236094748	0.3635498057875641	0.5708390218409510
0.3500031357603238	0.8266421695283938	0.3337942136494572
0.9367008542464303	0.9618555005504784	0.3543570921340599
0.7240699844226902	0.7431709801140859	0.7900706051448807
0.6099602391264540	0.9490370599077960	0.7038349101001073
0.0110225088123480	0.7162026228334891	0.4823839350577548
0.9439209548089569	0.5861202848235159	0.6924720011451725
0.7056070133724153	0.0278237033830757	0.4391895477019816
0.4162533606911972	0.4314665008540126	0.5388430057378009
0.6705835696132405	0.6644296327389616	0.1126104375664875
0.4484845749295719	0.8315969445598520	0.2031951641203488
0.6519533151755802	0.3756528600994765	0.4226193927660447
0.7928414697851277	0.4547903460761690	0.1912224059390444
0.3494468364823632	0.6665147952592108	0.3932693480431090
0.9660265419583047	0.4470911645825291	0.4564217408611376
0.7249969261465877	0.9688520795254442	0.1745818226967803
0.4624275998966766	0.7122221034893728	0.6962711399652866
0.4053882411387075	0.9467112519258793	0.4641683883328970
0.6627186524380946	0.4495498959254920	0.7057582113170158
0.9348044780534304	0.6912133034942742	0.1831413821156027

0.8438976715707177	0.5430895755786710	0.9600908695684507
0.1885391160926731	0.8617924244871150	0.2834062152404535
0.5298026880090625	0.2017402584263090	0.5988587836259326
0.5387693458176236	0.8534948928230762	0.9291075271041527
0.1812693485000712	0.5646652596488655	0.6074021461367028
0.8545084675914515	0.1933326053825550	0.2998104808750169
0.3954068973123934	0.4249070120478993	0.2463090894826857
0.2995748012747921	0.3019154354353911	0.3830978867909952
0.1887580507002238	0.1797643818644341	0.2208765075056562
0.2180051180595736	0.1787704302738702	0.5232711001670962
0.0818397530559004	0.1942059016274273	0.2209248774116514
0.2228723457266284	0.2067189537308441	0.1254595587226140
0.1979020914614136	0.0720909506427481	0.2295453856367849
0.1100539407094598	0.1535254606332463	0.5074347696286260
0.2697406112099881	0.0859491182868488	0.5141266132808096
0.2437705522738023	0.2279621133274893	0.6234622551547203
0.3792986532934064	0.5253222801055557	0.2852242184519784
0.4977519343688215	0.4175144651337511	0.2747776715965883

Z2Cu-1H2O-3NH3

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-0.7410140138000000	-0.8132947143000000	9.3735478129000001

Al	P	Si	O	Cu	N	H	
6	4	2	25	1	3	11	

Direct

0.5851214144304832	0.0845398413832909	0.7438895760502334
0.0487276211452986	0.8551867099489842	0.5256022764042462
0.3739963619170885	0.6466393262806026	0.7739757355357639
0.6121011085711694	0.8732955226159568	0.3103473118484574
0.8385466384483486	0.4187411142322576	0.5521443152189592
0.8058222372547104	0.6230200965545593	0.9858788245727472
0.8217002937692871	0.0889291177925645	0.5254690032967454
0.5911389941352512	0.8557552590186369	0.9822151637518279
0.8394145925352687	0.6375760426051663	0.3119578884959434
0.0454867585287014	0.6308952525407600	0.7559824404488799
0.5919488341965951	0.4131971199976384	0.7831764492943276
0.3747550281158308	0.8726885141541838	0.5272235749198225
0.9556227535684626	0.0080074186308640	0.5389129208342363
0.7358537168512289	0.7910335312737218	0.9905122393836396
0.5981344433168641	0.9792646502080624	0.8880888155848887
0.0421004519772132	0.7737762803162443	0.6873674270185148

0.9466207788217120	0.6311244439392104	0.8770329686063586
0.7502822769168418	0.0884689737676431	0.6660390856179341
0.4467869182557556	0.4863186700790533	0.7325092749510362
0.7037250472483513	0.7182211373109835	0.3039299405560727
0.4561276600519553	0.8326883667143016	0.3853761611242093
0.6942187643537031	0.4212326475101803	0.6518923325962056
0.8044034943413781	0.5035450854180231	0.3914038543601514
0.3715267267666295	0.7410016633263218	0.6255822009555574
-0.0034916273478534	0.5054842943748484	0.6421266226351758
0.7193998996719956	0.0204185404015627	0.3980994966478941
0.4675749490873100	0.7440193913460408	0.9270917641332963
0.4519397592899936	0.0198385727183233	0.6124553307556256
0.6695124755404749	0.4919880026593975	0.9331845874801024
0.9655777819949397	0.7307223604627936	0.3898948191468843
0.8753964703660889	0.5922656918195907	0.1599241048924344
0.2139463104715616	0.9099597114201526	0.4734130773415074
0.5468261906200466	0.2496260224097137	0.8161633411647113
0.5634030613580442	0.9168869598371828	0.1344331709429135
0.1965261068493948	0.6112451534225527	0.8192056221692834
0.8697739710896432	0.2425942842001102	0.4947468736123236
0.4887589785105376	0.3196768078290733	0.1158730027561950
0.3959129361950691	0.2866439026453431	0.3085148674451631
0.3109724527633402	0.0940429896845738	0.2220448742769686
0.3157586382796059	0.2506113639449706	0.4977407446648036
0.4767762576114979	0.4795981912895124	0.3883822035021939
0.2297880250745505	0.1030658397893678	0.1454210269778494
0.3862690455341875	0.0379962277468453	0.1738225831059205
0.2699263205496866	0.0301437915190436	0.2960545668860595
0.2074528391805812	0.2257256338731845	0.4865259593254946
0.3619172422485680	0.1635810943572219	0.5387666776960807
0.3379391767465456	0.3354206631380295	0.5745941792475645
0.5562863290910190	0.3997293688101343	0.0967672840889919
0.4835437265342983	0.2589136132399836	0.0250232428678856
0.4264077399089090	0.5632702878395374	0.3506240815893009
0.4775964635873025	0.4926421900713599	0.4982008307989599
0.5821455626745485	0.4958222465303286	0.3676153824216467

Figure 5 - A1

CIF file

1.0000000000000000

9.4422998428000007 0.0000000000000000 0.0000000000000000

-0.7718446244000000 9.4314702197999996 0.0000000000000000

-0.7410140138000000 -0.8132947143000000 9.3735478129000001

Al P O Si Cu N H

6	5	26	1	1	2	6
Direct						
0.9521332078380467			0.8710774421270963			0.0445479962579097
0.4053456417101752			0.6371908401678478			0.8344659920722405
0.7517361978804820			0.4369384383722630			0.0621131517482821
0.9718320627692149			0.6615673209366423			0.6081511871558204
0.2127795276335607			0.2035971264581622			0.8516255093231607
0.1814133658899705			0.4108247885765482			0.2864530072920141
0.1872638440443359			0.8728029254328730			0.8143545417176520
0.9687356110495117			0.6508305189394820			0.2764832174366182
0.9709509380498214			0.2013190436539238			0.0785421086583380
0.1880644371037628			0.4263810468712942			0.6207345133079745
0.7385962188689508			0.6603503898597121			0.8337760903575993
0.3233270786574833			0.7985293275612025			0.8410118010908830
0.1072774872340172			0.5757576096051891			0.2793651223246260
0.9926446675109860			0.7893095033844337			0.2020249283118776
0.4021612540905965			0.5589862116578231			0.9915666603980539
0.3328624666775541			0.4006083334851813			0.2028251908122908
0.1026170916428683			0.8701459533277739			0.9473700248178889
0.8395145475836819			0.2807283109164671			0.0437131878698134
0.0475832016694010			0.4996718887916053			0.6206980926358581
0.8171547754590931			0.6589656175958224			0.6969955005033309
0.0649295186400744			0.2047004143011799			0.9538025247263454
0.1678193691065067			0.2909806102684043			0.6985935855461157
0.7552005793930179			0.5184680117761721			0.9005897801245271
0.3665876027021533			0.2751796140128836			0.9450826440812871
0.0952133717770119			0.8012298825852540			0.6817341525102868
0.8446192801477570			0.5541866585949544			0.1985690212078609
0.8028829606322665			0.7856677838051971			0.9410907395302415
0.0518879131063017			0.2684273247550693			0.2198609482171664
0.3144990826199267			0.5277549942735241			0.6885075063639745
0.2162882599729868			0.3787956982490966			0.4665221114255390
0.5820057647325081			0.6798150981633453			0.7921916958050109
0.9207983904661143			0.0458220490602874			0.1008402024737287
0.9321579461256096			0.6923860136012655			0.4295766704868917
0.5859918555570591			0.3927206643267656			0.1154033805120726
0.2272747922192884			0.0269170541113168			0.7812573809864221
0.4990283388057567			0.9072393342323004			0.3532174619871964
0.4217953865854651			0.7973387957134271			0.3752177055551975
0.4194950479508538			0.4090895051819842			0.0615411342285986
0.4170929602160056			0.1130553428897050			0.3791595722801059
0.5935905663198110			0.2167033445967151			0.3455931637390352
0.2294066384170169			0.0463216503492805			0.4267137079990225
0.6719274421122937			0.1510133230378851			0.3246864670057185

0.5832073606952406	0.2800974740889045	0.2596443894963293
0.6321920367544067	0.2846332568458271	0.4325800246020867
0.1578327538488905	0.1203544330103734	0.4088124330620487
0.1886852104699462	0.9524945770804175	0.3705531231018093
0.2304861082622409	0.0301445253671073	0.5334406358531414

Figure 5 - A2

CIF file

1.0000000000000000		
9.4422998428000007	0.0000000000000000	0.0000000000000000
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-0.7410140138000000	-0.8132947143000000	9.3735478129000001
Al	P	O
6	5	26
Si	Cu	N
26	1	1
H		
	2	6

Direct

0.9443368814719429	0.8701214286014486	0.0466084880616933
0.3967045405641584	0.6352284527511295	0.8338040400653074
0.7445027635710934	0.4362889255485263	0.0589890220522972
0.9632590122298762	0.6631441801230024	0.6086085989982042
0.2046830333939967	0.2017886011605646	0.8557748512441504
0.1724187667997585	0.4108419251081170	0.2881001191238931
0.1780916559731969	0.8714564889561039	0.8130172684959222
0.9615868191445325	0.6496857919744532	0.2771246395780937
0.9604825904965030	0.1999802969272260	0.0772483116471972
0.1786709689130475	0.4261387352825666	0.6235267505463372
0.7303367730444335	0.6614353220508830	0.8354484957843670
0.3123758553911195	0.7948170182250519	0.8393705201063316
0.1018951867640904	0.5776166195590194	0.2843828416222574
0.9849502121223777	0.7888365450603996	0.2041903137989222
0.3908793497915220	0.5571620141936021	0.9909363101737566
0.3287697198757840	0.4066575558739953	0.2113775614843888
0.0902049227628618	0.8668544085613349	0.9432848377357086
0.8263663670128520	0.2762519105504913	0.0425153643336859
0.0398892787573965	0.5020145364369241	0.6261975826411521
0.8101788643926471	0.6655678981532227	0.6998008275053494
0.0514274567387761	0.2005549311006741	0.9502613127750456
0.1606098234881872	0.2925412583126596	0.7042544789851474
0.7474850481699196	0.5172721354744871	0.8977676720479408
0.3551273938606856	0.2738814417075650	0.9547564902052468
0.0879814317189475	0.8041222236439856	0.6769669135701731
0.8415913938504288	0.5509475486270694	0.1947148551888746
0.7927273161685916	0.7838907047405822	0.9469737984594464
0.0427636733563852	0.2721995265124615	0.2152324829516183
0.3081285763331295	0.5267861121937973	0.6850319186128976

0.1992740762569877	0.3720905362195255	0.4681541678270943
0.5735328991184985	0.6802001023875260	0.7941940658571515
0.9123431684765672	0.0449473625624356	0.1038516979125732
0.9193256811875329	0.6876159459358357	0.4290143441602582
0.5786864336189284	0.3963693425908854	0.1163413622807996
0.2219015233757778	0.0262406973459325	0.7839898195250122
0.3758059193663518	0.0474997644737268	0.2196427343230283
0.5008649136007894	0.2051518115577726	0.5545839497818514
0.4100730261069505	0.4106351605003653	0.0662390878830610
0.4364752721997673	0.1297371792810499	0.3863937873054648
0.6096072335226465	0.2023749362681245	0.3133234644117112
0.2585121549288190	0.0652303963126021	0.4600751865121177
0.6565816394541828	0.1210619926063229	0.2621895897251768
0.5882282305988049	0.2790932044784688	0.2393203594167418
0.6750605556498295	0.2488894073530869	0.3994046641013665
0.2018772944871075	0.1540832912032582	0.4668988316977348
0.2041538050410361	0.9865646637192929	0.3905244005258236
0.2742906248511845	0.0322397667924209	0.5613017889576261

Figure 5 - A3

CIF file

1.0000000000000000

9.4422998428000007	0.0000000000000000	0.0000000000000000
-0.7718446244000000	9.4314702197999996	0.0000000000000000
-0.7410140138000000	-0.8132947143000000	9.3735478129000001

Al	P	O	Si	Cu	N	H	
6	5	27		1	1	3	6

Direct

0.0496547745752859	0.1715912891061960	0.0527145507711041
0.5018256536147890	0.9356626525983092	0.8400813182820338
0.8478441205014368	0.7366151435301711	0.0699837188141652
0.0685241025860924	0.9633567826459377	0.6161248085550721
0.3092534196720740	0.5035805061622208	0.8610196022635291
0.2756295337882501	0.7139714745410203	0.2930952900175466
0.2838940020323722	0.1732145767546431	0.8213339597783821
0.0668686793042181	0.9530338690226645	0.2846483817435274
0.0649510502095939	0.5018707928490742	0.0820069713456378
0.2864017678809077	0.7266539704287887	0.6279113474105484
0.8360642434017398	0.9596145302046198	0.8425751833241032
0.4180946122026939	0.0956570695678971	0.8456867428624796
0.2078032064552172	0.8815617119916800	0.2909389201791399
0.0907977398489104	0.0932480455255881	0.2127968821883801
0.4919006800997102	0.8579256322497546	0.9970815782471941
0.4339158196136146	0.7084433791735198	0.2185525916677357

0.1994692401628095	0.1690940560799439	0.9545043739325171
0.9312284039886040	0.5779391817539630	0.0485164789785464
0.1486089760727798	0.8036372747956665	0.6317122418078209
0.9146266230515611	0.9591273718406016	0.7058864787367791
0.1555477190280851	0.5034062113377034	0.9545078400200633
0.2686350377226830	0.5927958829960669	0.7079207605540953
0.8519330502440505	0.8167765098787465	0.9072324699776921
0.4589616550453412	0.5741626720767340	0.9623837828051039
0.1906997618334328	0.1052121374404704	0.6875609317076068
0.9476612714622940	0.8546464179262333	0.2017532620748629
0.9007179657298719	0.0841913516181045	0.9507945917850735
0.1487870683600867	0.5740132954360749	0.2196358387808401
0.4175874264061341	0.8256383451875144	0.6899258381880922
0.3080616709682066	0.6751695692324808	0.4723934084595063
0.6793837309258244	0.9799346683088643	0.8022305246415045
0.0192107945024191	0.3465604979899598	0.1087367412323271
0.0261020476845420	0.9905933382018158	0.4369405875492667
0.6826774690397706	0.7002899871197017	0.1246721766269804
0.3270539550062619	0.3274046744121366	0.7915601059048317
0.6151124628800140	0.2122605960543234	0.5049408695702555
0.7131186872411719	0.1355401277815759	0.4699017572045293
0.7053818731419252	0.1842772906250528	0.2356104698412848
0.5165581465405683	0.7117991550583147	0.0725190534294292
0.5268293123262706	0.3520723472883636	0.3697508499586737
0.6069262632158493	0.5558542020218274	0.4149203845994976
0.3254902769253297	0.3368479176166113	0.4295104177659317
0.6131968834866193	0.2598617942055980	0.2313345010765082
0.7128757506237596	0.5711868920033142	0.3991698924884361
0.5543929009017849	0.6208679335159041	0.3479508506183187
0.5954228623819442	0.5934192878103917	0.5177782776639095
0.2821555505024882	0.4330166117396338	0.4316832160096943
0.2574635119337371	0.2651806255383298	0.3640264738014863
0.3229880968768828	0.3049004457558872	0.5308826947579633

Figure 5 - A4

CIF file

1.0000000000000000

9.4422998428000007 0.0000000000000000 0.0000000000000000

-0.7718446244000000 9.4314702197999996 0.0000000000000000

-0.7410140138000000 -0.8132947143000000 9.3735478129000001

Al P O Si Cu N H

6 5 27 1 1 3 6

Direct

0.0509693033644231 0.1749009896725355 0.0524650078291219

0.5037799043808808	0.9370731348450786	0.8396107919537519
0.8497652940866781	0.7390591091473833	0.0694324050997357
0.0701322712707846	0.9628969303938383	0.6161938942325514
0.3129677222163758	0.5047553709382228	0.8598764997183272
0.2764689349262434	0.7165429226477662	0.2896859070878995
0.2848401107948323	0.1743871098005944	0.8225234330445590
0.0700659892665018	0.9548026648285480	0.2825027465171099
0.0666710063423963	0.5051226621810093	0.0794126994901481
0.2894026466924481	0.7286846730802659	0.6272038490862901
0.8372653224908947	0.9623687154908965	0.8404759891895972
0.4188911599367549	0.0963098368625485	0.8454961925583288
0.2118607149677375	0.8847381416662690	0.2835270968983056
0.0897889435196707	0.0958947556682134	0.2119290220132694
0.4936732236441366	0.8561995349627325	0.9948081231959707
0.4342506401123888	0.7041399242699899	0.2154153976190120
0.2035692143766502	0.1740678501237820	0.9576020423568656
0.9340127869939499	0.5816134552555872	0.0427932847386839
0.1512950816624694	0.8041676858238772	0.6358387326941325
0.9134179788284755	0.9583487206380659	0.7019947141495925
0.1600800873915746	0.5073908067723868	0.9538342081974567
0.2748329554319074	0.5928423245229146	0.7050567834685114
0.8512241456256762	0.8204231828691003	0.9070684521261644
0.4645607286988275	0.5728380739285692	0.9595754659464604
0.1891263949720745	0.1058798960940253	0.6909790905641530
0.9505112037567826	0.8552283447908743	0.2014764623288734
0.9047674945584434	0.0875514813325216	0.9460604651892510
0.1482565538224592	0.5769379357069797	0.2183919914271585
0.4211345665847485	0.8274846996489195	0.6879833657842291
0.3076940826296091	0.6796047467267634	0.4701287336393117
0.6806479251571494	0.9850521736713950	0.8012472782402795
0.0201986172312351	0.3500329351073723	0.1050659165881031
0.0340016985296743	0.9898982646438894	0.4366945795478805
0.6851329435236958	0.7007904053619669	0.1250875025585474
0.3282048761776115	0.3279686677660846	0.7890001836579073
0.5263547528317930	0.1394574815356883	0.4035207330438124
0.7209249399782227	0.0372064319001923	0.3515518524107490
0.7166064972040834	0.2719070487496896	0.3687334760968911
0.5194740097835034	0.7106002657337380	0.0708635242318189
0.5315271706135208	0.3533402149246644	0.4129326382145136
0.6018477206513655	0.5562933890793786	0.4131338536744942
0.3277953266432958	0.3543226644836217	0.4534422908535840
0.6588146674293186	0.1426070764999292	0.3731586036833094
0.7034241040590424	0.5648668157843222	0.3816089956323173
0.5413081376323764	0.6114960211011312	0.3421124610275992

0.6041857507357606	0.6111829106039466	0.5114105001681205
0.2890420783287779	0.4522108390668028	0.4484503648322821
0.2647645011727238	0.2818666355792714	0.3842359776787505
0.3167778579700558	0.3255740937166687	0.5551865677141991

Figure 5 - A5

CIF file

1.0000000000000000

9.4422998428000007	0.0000000000000000	0.0000000000000000
-0.7718446244000000	9.4314702197999996	0.0000000000000000
-0.7410140138000000	-0.8132947143000000	9.3735478129000001

Al	P	O	Si	Cu	N	H	
6	5	28		1	1	4	6

Direct

0.0500593403310239	0.4495601326981952	0.0572664572056317
0.4996350077015574	0.2133340135714930	0.8454974001388348
0.8480959799883280	0.0143720332812705	0.0773936269826528
0.0676263357339901	0.2408707605164398	0.6219230659134857
0.3064288861777992	0.7808033933489705	0.8683878220821322
0.2746192750953250	0.9908700074666252	0.2979202280070221
0.2833918953420653	0.4520511618374726	0.8298347916233285
0.0653831523581107	0.2275783173502537	0.2914736942157449
0.0620203317142230	0.7791265777666119	0.0841346028002620
0.2882027170730646	0.0061290903187063	0.6331325185416038
0.8387722528248257	0.2367619053397990	0.8453279782840206
0.4186708429258637	0.3743605596356034	0.8464920503027219
0.2078403299480940	0.1587540257840506	0.3000135190832819
0.0837641732640339	0.3613367859245918	0.2106687709292381
0.4776823379382996	0.1289030225857452	0.9961851666178400
0.4365488334765241	0.9914944584989651	0.2292780225339568
0.2070780982763074	0.4507570955192681	0.9677669258308341
0.9263334542488623	0.8531690417877406	0.0535112451523462
0.1506239628705319	0.0827860879263604	0.6389728352394058
0.9065264541714821	0.2262264861170467	0.7015358676248343
0.1477384528388359	0.7814855815304271	0.9525844228065176
0.2752927825176280	0.8740241404684366	0.7160851089367184
0.8615314749589540	0.0999316371252760	0.9183622114785276
0.4535143620519796	0.8454969452299783	0.9770314894173556
0.1828888612789499	0.3835748292887931	0.7016663835851957
0.9462241662660874	0.1215293609967161	0.2185410092768471
0.9086106254341059	0.3682666209460687	0.9394406974046905
0.1495816416767425	0.8538232719360903	0.2183053562186905
0.4205394970610913	0.1066761526610785	0.6895528209707139
0.3058012666425198	0.9509448061328156	0.4775828578631968

0.6795609085178952	0.2534617105096423	0.8112565883891850
0.0208254303047764	0.6241320772518728	0.1128025727835789
0.0279368027678111	0.2726438362439093	0.4437748718640114
0.6795760883069167	0.9847598351947092	0.1246063707934652
0.3268542001107864	0.6055701579240379	0.7960640245820118
0.5620781893111656	0.4772677344396939	0.3022485814306547
0.7490640844702426	0.4034091774754099	0.1993879218122613
0.7530417517955793	0.6221550350589573	0.3036124566379214
0.6633121338796309	0.2202648988886974	0.4584463498483376
0.5117744818373370	0.9890593204354703	0.0783924488905220
0.5739436119773851	0.6800854796770679	0.3983323720929471
0.3856948161180465	0.6504718898118459	0.4798430846984418
0.6371224840858959	0.8859147940803502	0.4349147496535876
0.6918843679616077	0.4965473707759614	0.2642318586243242
0.6193385914597164	0.3190885733724128	0.5133667908159917
0.7402158290251395	0.9064260749845011	0.4107581154199061
0.5735989170032167	0.9387416206201344	0.3645476886336970
0.6292533885599811	0.9303899540863696	0.5361443272480027
0.3337273463138941	0.7421064955519497	0.4828547752732520
0.3913330661387568	0.6199549362838741	0.5824683747913124
0.3217666938670261	0.5727907987422300	0.4178468296489601

Figure 5 - A6

CIF file

1.0000000000000000

9.4422998428000007	0.0000000000000000	0.0000000000000000
-0.7718446244000000	9.4314702197999996	0.0000000000000000
-0.7410140138000000	-0.8132947143000000	9.3735478129000001

Al	P	O	Si	Cu	N	H	
6	5	28	1	1	4	6	

Direct

0.0381145716441284	0.4346030238720139	0.0484177356164498
0.4936151395311846	0.1986736438502703	0.8265587101864156
0.8339216119264633	0.9991152775017808	0.0662470486475279
0.0585284336538751	0.2227724844457320	0.6114190685513410
0.2994456871407975	0.7652717342875037	0.8563724582100315
0.2622900862955151	0.9756343667434673	0.2848704037643138
0.2727153860914381	0.4344880156948575	0.8185168215970168
0.0524518400625815	0.2156139109997086	0.2803833402203463
0.0524572254475532	0.7654533168774651	0.0708464078624326
0.2791820272141393	0.9903673829195023	0.6196669271350214
0.8244030424196487	0.2217759743598166	0.8352151190928129
0.4076824635732977	0.3573487957727906	0.8418210688607065
0.1926723715799641	0.1430879274650041	0.2872949451469831

0.0775295002017510	0.3538380419831569	0.2066249022181036
0.4891069787734497	0.1109635532321112	0.9775448245784856
0.4183527269215371	0.9867794249499695	0.2075384533348884
0.1916433534244006	0.4328817392585416	0.9536876088361125
0.9189781405689307	0.8427609006053103	0.0395858244358189
0.1398018318089013	0.0641599563531548	0.6293460275669570
0.9030281735655318	0.2122994576502933	0.6985280285428332
0.1411398983349866	0.7693014911554011	0.9415883074412388
0.2712037935726652	0.8593681424051618	0.7045178694927186
0.8305118101282887	0.0800201076150662	0.9038884088683486
0.4478000017193440	0.8272683286609841	0.9649773311720737
0.1780141447514055	0.3647409660621975	0.6867759804397772
0.9320313570070684	0.1167542933713891	0.1991995113905494
0.8938574579601941	0.3455618057137159	0.9405803321291348
0.1381696769351936	0.8358935930545333	0.2080096554899341
0.4099951816210071	0.0946604573344773	0.6728056337926966
0.2932373455599185	0.9368764534291791	0.4637739025993478
0.6701623428806310	0.2495374579061676	0.7906274251115669
0.0069801893339122	0.6103286888414519	0.0957703659232657
0.0128400991093788	0.2533112143190919	0.4334427613139230
0.6700363607546301	0.9610055550410044	0.1264967030389952
0.3146936427976662	0.5884355254602089	0.7851860958745707
0.6235139373023803	0.5295483784476076	0.4097293423557504
0.7611490980742898	0.4375214025057210	0.2559508575592125
0.8437063414788781	0.6263009847529337	0.3989071377915632
0.4869710057283014	0.3266528452356694	0.1965892559680408
0.5047533505910926	0.9708654107243934	0.0659820578537427
0.5078575941875763	0.7296570621688117	0.4395798698435927
0.3312230934202717	0.6154453105180664	0.4569366605424618
0.6596794813714313	0.8742877001364388	0.4269197963648995
0.7469885418551442	0.5335909428718378	0.3565697924170610
0.5719029240398503	0.3208959228577548	0.2878675141146936
0.7565616784646386	0.8363970998828582	0.4518181086928980
0.6600737744498266	0.9075970735344908	0.3245833447670309
0.6513131047297244	0.9626681155833197	0.4947953125678336
0.2458294927111740	0.6709524470154726	0.4292371523886994
0.3229036328220337	0.5936344347864129	0.5614428507608613
0.3166991254620096	0.5199619247857241	0.3960848605289266

Figure 5 - A7

CIF file

1.0000000000000000

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-0.7718446244000000	9.4314702197999996	0.0000000000000000

-0.7410140138000000				-0.8132947143000000		9.3735478129000001	
Al	P	O	Si	Cu	N	H	
6	5	28		1	1	4	6

Direct

0.0370110068522130	0.4332914207678525	0.0483496303285625
0.4892603428071534	0.1983037313487207	0.8332022505374643
0.8335762201514911	0.9989232912238425	0.0671913618117958
0.0574635598563690	0.2269699673641617	0.6136139018240110
0.2909165453599484	0.7668324314910522	0.8580056438456353
0.2635728019664800	0.9770857897375137	0.2867905593876961
0.2714449929348029	0.4367524129431874	0.8187611067955965
0.0489231845907053	0.2142489209075139	0.2809797688421294
0.0515675892049433	0.7631668442145535	0.0731153829139400
0.2756084737719025	0.9902557483179758	0.6230058280985029
0.8247946726974311	0.2213513786243065	0.8374175198368410
0.4062058618140963	0.3582681272308587	0.8364646509739636
0.1878920849847186	0.1402848144029259	0.2832529778212142
0.0715971844247554	0.3522905758888724	0.2067888657314412
0.4757864090455788	0.1206015120141408	0.9890931480922669
0.4274298123494850	0.9891329039365179	0.2225338055336961
0.1899610169867575	0.4285097323757883	0.9535139068349580
0.9172272718681371	0.8409533815909102	0.0516950515418314
0.1403276545442319	0.0696301657506307	0.6358165644273631
0.9003208568897889	0.2182390564690466	0.6986009317868018
0.1282209358378589	0.7637679121522183	0.9356881228694698
0.2619576899599532	0.8549973309757285	0.7017969522469212
0.8426689408993649	0.0803180052677293	0.9049489451852123
0.4321504190963874	0.8374987548863476	0.9707066721938490
0.1756270319650320	0.3716649887010847	0.6853725748141430
0.9255183266460425	0.1163339332755938	0.2040170822050606
0.8893351569504682	0.3483996386675174	0.9417289235488632
0.1484684691754494	0.8336213786041695	0.2029433009073573
0.4104256173354261	0.0874669319078446	0.6804675224918770
0.2896948237777535	0.9400760973301676	0.4664823553985321
0.6674769237229228	0.2398249477607940	0.7964241188655412
0.0085728225482829	0.6085673766622278	0.1025808325259316
0.0134096677474854	0.2532725410116864	0.4349779175752295
0.6662986918400572	0.9626439154846949	0.1153854636268041
0.3153611582754960	0.5914854217081371	0.7926183667177890
0.6400866248009277	0.5730988130056343	0.3807290658096147
0.6846419202200096	0.3339739539510779	0.2181293986471070
0.8428896137702651	0.7050544910811061	0.4120028978235992
0.4811345185680992	0.3291310636672906	0.3237156191075988
0.4998874183447578	0.9779038213827613	0.0709649718149342

0.5133617997077281	0.7319964122979240	0.4438707071447467
0.3349651994022433	0.6124178490338195	0.4544851806248251
0.6281599501609491	0.9104009144500769	0.4535167642604487
0.7833841996445752	0.5902252750830955	0.3661558467681995
0.5957952244568006	0.3730367566220645	0.2914762822035683
0.7345258965696747	0.8966956981543295	0.4528177254236194
0.5945908603622920	0.9582202993778006	0.3632660086496216
0.6122578563279681	0.9769965468070290	0.5408565699175939
0.2765184038488780	0.6628413621026671	0.5273489351086205
0.3470494746543204	0.5129206606213423	0.4865378189294469
0.2724068652815397	0.5990447353656929	0.3596042576281678

Figure 6 - A8

CIF file

1.0000000000000000

9.4422998428000007	0.0000000000000000	0.0000000000000000
-0.7718446244000000	9.4314702197999996	0.0000000000000000
-0.7410140138000000	-0.8132947143000000	9.3735478129000001

Al	P	O	Si	Cu	N	H	
6	5	26	1	2	4	12	

Direct

0.3122037642473102	0.1271878866862688	0.8366978347049834
0.6584947641585164	0.9346165381120550	0.0782362843830624
0.8834620070189202	0.1548384971813659	0.6234289118810350
0.1151578040974985	0.6971443787335292	0.8659019074831549
0.0898186060997654	0.9030593601014532	0.2941813951291355
0.8650230010456622	0.3640486404475490	0.0574673354692741
0.0987465348615909	0.3664906524327844	0.8319024072598336
0.8681674603159460	0.1443086883108429	0.2891448132061715
0.8801187511864993	0.6942013874388594	0.0792464512053671
0.1022018126076436	0.9228339467176035	0.6288753591404447
0.6529742644514309	0.1526527907363254	0.8464193083187482
0.4730521664039563	0.4676933623460999	0.5244997303285279
0.4253210039740749	0.6017761423856725	0.5673913437468405
0.2371838514995478	0.2928457868997221	0.8496490030074778
-0.0039472816308525	0.0556859154317552	0.2799557714724537
0.8977018993433679	0.2824688811625929	0.2157169862713436
0.2863105448825493	0.0374870593696905	0.9828482356770079
0.2534586960853685	0.9336157179937298	0.2311649476281325
0.0217086037229485	0.3590489167741238	0.9696079555597492
0.7516543311929046	0.7820283720948330	0.0730754168246092
0.9623768829536317	-0.0040883615012999	0.6440514188620916
0.7227901558983437	0.1465968197299555	0.7043149787897284
0.9456059031811277	0.6960519666955085	0.9347198636213440

0.0974052831948083	0.7942866805805032	0.7168873115979416
0.6778826358025326	0.0136236795098969	0.9156443187147315
0.2490960927547351	0.7552229845462491	0.9943160883603251
0.0010800034563080	0.2967674696818155	0.7021265246049598
0.7313067515389357	0.0605256142603219	0.2189348266015136
0.7183029290822978	0.2822399498132804	0.9468954171320564
-0.0118447157330708	0.7520355561050812	0.2046026986788075
0.2333747093972234	0.0289499370959599	0.6774631262881199
0.1104825696051292	0.8681582897031541	0.4734931982192721
0.4941602666182925	0.1686411849426840	0.8125930576015415
0.8270152639551117	0.5395873529163326	0.1020095301221199
0.8445909852698185	0.1867441869229567	0.4457850169198017
0.4873088567447477	0.8903915851113773	0.1077772744742983
0.1367689411662969	0.5208228839175680	0.8013986493011852
0.3190344215220008	0.9057388081399685	0.0779204431816310
0.3152975339844227	0.3186593986484607	0.4531259770291451
0.5137902621754400	0.6218283199743400	0.7586457699898904
0.4799513350188761	0.5599111924811940	0.9463228989278117
0.6918374904766296	0.7367296512390691	0.6952366635027140
0.4192638808395062	0.1504896918700201	0.4328305947670016
0.1698713829664150	0.4539557748144672	0.4524437124254661
0.4111214598049538	0.6263601547162146	-0.0084212364210180
0.5677874792269926	0.5607834074490373	0.0174213166704169
0.4295858436019736	0.4590778360318313	0.9355445475941446
0.6785718330716181	0.7174140691799735	0.5864386811000222
0.7905581397674850	0.7097306197887926	0.7305715281286821
0.6930750817134543	0.8442039167007895	0.7196705493835747
0.4319580801777113	0.1071807492233694	0.5285902822952766
0.3704608419419762	0.0703853793089161	0.3595442916655811
0.5200015124272023	0.1756622277614690	0.4036283380294294
0.1020503633083099	0.4544414620811122	0.3623786018093181
0.1078183196449449	0.4483681877092343	0.5364805954837825
0.2338686148791808	0.5493586014935335	0.4711317008499595

Figure 6 - A9

CIF file

1.0000000000000000

9.4422998428000007 0.0000000000000000 0.0000000000000000

-0.7718446244000000 9.4314702197999996 0.0000000000000000

-0.7410140138000000 -0.8132947143000000 9.3735478129000001

Al P O Si Cu N H

6 5 26 1 2 4 12

Direct

0.2706336203231395 0.0717628581564883 0.8381038355937306

0.6221945273403288	0.8726174341813708	0.0752857486267365
0.8402252282343597	0.1014774813314415	0.6174030353090014
0.0822853786146992	0.6442395226534775	0.8578369642301714
0.0459649796782311	0.8470972206467046	0.2923051931010981
0.8222259471472116	0.3092837707245797	0.0493055709327052
0.0553524093511110	0.3105253495509860	0.8231792634128147
0.8348690950700582	0.0831402749917140	0.2857720972780940
0.8372440637908002	0.6428224554584415	0.0834948169843310
0.0555117798835401	0.8626189380389224	0.6273978568249613
0.6109588383766443	0.1017748153104092	0.8423610534226826
0.5114905495880019	0.3977725334033983	0.4840778599097300
0.3694938344407851	0.4668593939984436	0.4976621462394176
0.1903522457342349	0.2327023589202691	0.8381226898104222
0.9801529858044759	0.0194554287965938	0.2832217319994736
0.8375610994028651	0.2142720087612348	0.1995319593779822
0.2581050157240027	0.0029781271124009	0.0004914510755349
0.1928142777466416	0.8358834619697992	0.2021873613846279
0.9784314217216493	0.2985750561191939	0.9619396910033299
0.7022015284221331	0.7139699954432841	0.0387188263198964
0.9209243203385294	0.9441341824052902	0.6369438105309138
0.6818742699028614	0.0910921502923585	0.7015274592559708
0.9371333437476032	0.6534582540589521	0.9631576803759886
0.0309190070503020	0.7273061157443993	0.7043027211092523
0.6434821289890496	0.9712194588030389	0.9233960492447141
0.2398513613327224	0.7203454721118422	0.9418615951250444
0.9539168100707452	0.2469917101107134	0.6943630706073071
0.7142747790673601	0.9726787127743208	0.2241117696099166
0.6721554709804318	0.2402887829334627	0.9340406805368187
0.9087505491773284	0.7141263167177947	0.2254594378860048
0.1889010459824032	0.9563514490997140	0.6938347519666995
0.0784451567726509	0.8191971293187825	0.4721971640788192
0.4514509999783621	0.1087574940618656	0.8078500601547172
0.7947099679993093	0.4849118851584565	0.1014367857003175
0.8058998397376401	0.1327505021166659	0.4387914511287996
0.4514296313618209	0.8457938439367860	0.1144978115530355
0.0962815000670052	0.4658648557390140	0.8021982091184886
0.2844287525909771	0.8501926542795994	0.0664737248719870
0.3666098869774394	0.3276567374065130	0.3306157872363493
0.5262280256742813	0.5579001896893344	0.6374921748336715
0.4511827531549675	0.7339722881861627	0.7164488304716659
0.7163742437462617	0.5043828342222845	0.7191225879696136
0.4625093626152870	0.1959298468806264	0.2004756773774863
0.1609065110133686	0.3166781162717303	0.2560255269141410
0.5296621024973192	0.8104375969761343	0.7574747528685091

0.3852946572035190	0.7166272039165614	0.7968455303428631
0.3916928444395733	0.7772361224822392	0.6382153971957637
0.7676240070819351	0.4605774419449788	0.6369842811176992
0.6966463171660071	0.4264272837038771	0.7860610718478536
0.7845295120721149	0.5828288296953126	0.7742658620855787
0.5240195457182575	0.1344252340876347	0.2598858910507569
0.3931302018012288	0.1278254860615124	0.1316077268783097
0.5285556564483020	0.2518242041710994	0.1399395184310024
0.1126765927603918	0.2158165652166988	0.2580455682124333
0.1086740295234765	0.3839382034060789	0.3198231941152034
0.1432460355642312	0.3424562634490066	0.1532473103595684

Figure 6 - A10

CIF file

1.0000000000000000

9.4422998428000007	0.0000000000000000	0.0000000000000000
-0.7718446244000000	9.4314702197999996	0.0000000000000000
-0.7410140138000000	-0.8132947143000000	9.3735478129000001

Al	P	O	Si	Cu	N	H	
6	5	26	1	2	4	12	

Direct

0.2742688715317858	0.0741554509702794	0.8421727665019311
0.6238706746685651	0.8745304214395079	0.0748988129246396
0.8423215430882548	0.1058483010279986	0.6194431311504719
0.0833044503605161	0.6478157951863854	0.8572449207694631
0.0490320500208083	0.8475546887690162	0.2932201827933945
0.8277922504558005	0.3102834676084447	0.0517493591723073
0.0584237790207228	0.3142207630592525	0.8261982044171142
0.8404528989843315	0.0859560804200598	0.2858457499593324
0.8394181017010695	0.6436941624828898	0.0838674848632181
0.0586329932145048	0.8657540638981719	0.6300476857148997
0.6130234375730558	0.1010331906347189	0.8423648184603250
0.5469387061516330	0.3741664341430768	0.4790817057855894
0.3347739109369957	0.4939547393574698	0.4926462803162169
0.1917756007490123	0.2334224406168404	0.8350683373695192
0.9842157113673959	0.0197528533430761	0.2820400376251904
0.8485721840860099	0.2208142841147749	0.2050218133235805
0.2657177260178182	0.0108010776476439	0.0080547993442781
0.1953642070120833	0.8359970882362633	0.2023415355142921
0.9866966765403479	0.3032847735122532	0.9681306031078711
0.7043495894263737	0.7154752138635050	0.0399698501788169
0.9264874773227495	0.9506901282689544	0.6412041607384004
0.6823939097967389	0.0915599680704958	0.7007138460293787
0.9384989495215972	0.6542079561507116	0.9629437093543622

0.0286150482173077	0.7284008504959657	0.7028828943625189
0.6406530046614259	0.9660685045338436	0.9181192304234804
0.2406856567798687	0.7286665090259941	0.9387488643368500
0.9512210445657687	0.2534497220984893	0.7003252783370558
0.7178241860564522	0.9804192868140346	0.2187800118272202
0.6790059154707166	0.2357711363388836	0.9376326430898740
0.9115645400780229	0.7143364165065702	0.2261703627525218
0.1935478419777394	0.9543382697464987	0.7005256357276084
0.0827392488608571	0.8257243320643338	0.4745100260223110
0.4541543343318414	0.1142319807464518	0.8101111197001752
0.7954610637835079	0.4857527583648795	0.1003831019971765
0.8105386538098172	0.1307625010026769	0.4394391722078167
0.4541070951776801	0.8453422133711422	0.1165909526880984
0.1017120635826586	0.4691762707962032	0.8052618250082546
0.2878281063248522	0.8541075279689588	0.0677443407602718
0.3777660961587562	0.3484555937994430	0.3644128971768402
0.5072920855069409	0.5256335658771538	0.6046227697660689
0.4479742461993429	0.7037441484656962	0.7026755983366995
0.6981864394540335	0.5097333840192270	0.7076798553330451
0.4588905085065818	0.2090506944837134	0.2317730879533335
0.1782449223898763	0.3341410665129280	0.2791369937448475
0.5304877744870161	0.7789257773770512	0.7360224864780822
0.3885742102400006	0.6910247212635378	0.7887633724584189
0.3835796493629682	0.7452747842980275	0.6269294994114708
0.7551245437569241	0.4627068283929973	0.6316436539196444
0.6854371167299473	0.4401864859976984	0.7844216510568841
0.7557393659785141	0.6002239539697959	0.7539585628889208
0.5229356163506746	0.1520288187363662	0.2937575248609108
0.3898028799491543	0.1392382230863443	0.1642510852628451
0.5239275414372890	0.2646008185653678	0.1699423920100298
0.1256654852948692	0.2351722350664611	0.2805612047163755
0.1336660415569433	0.4053155738688670	0.3462292859474487
0.1632820504134726	0.3624115475225912	0.1769927820223323

Figure 6 - A11

CIF file

1.0000000000000000

9.4422998428000007 0.0000000000000000 0.0000000000000000

-0.7718446244000000 9.4314702197999996 0.0000000000000000

-0.7410140138000000 -0.8132947143000000 9.3735478129000001

Al P O Si Cu N H

6 5 27 1 2 5 12

Direct

0.9872537701154940 0.2837431805245190 0.1122684219864954

0.4369974957438674	0.0481963087765859	0.8944015009178913
0.7898786954332979	0.8554323752672791	0.1338692359381842
0.0085608911276186	0.0733842152460744	0.6795096189700245
0.2510444845749478	0.6231256145777009	0.9190426117331506
0.2153024054679612	0.8316514025055213	0.3496929531557992
0.2193956330975686	0.2791205686378879	0.8905072723213636
0.0057074938362145	0.0673621793529382	0.3475936617705411
0.0086373636444306	0.6288087144587293	0.1326949126013519
0.2245863017482307	0.8413139779121447	0.6835272672226032
0.7766590055251371	0.0793409386675543	0.9027783985529887
0.3639513463230226	0.2156022670869930	0.9047581076084280
0.1495840507249843	0.0016274201269202	0.3462931555413616
0.0156135717418878	0.2060367724375038	0.2723724549588760
0.4160071592329618	0.9634778087137166	0.0451122485082362
0.3673634360224284	0.8187214115404335	0.2690634283292228
0.1392106689900480	0.2470602743639648	0.0228562979132453
0.8646739157457441	0.6906946135028275	0.1028526152056204
0.0831382101301442	0.9118226505399281	0.6978093399298245
0.8505410581125419	0.0772558472095555	0.7633303385258546
0.0985175881844655	0.6598830716826136	0.0083969890366273
0.2157707065468251	0.7053226361177263	0.7618176323896486
0.8078452216047185	0.9454303218907564	0.9772795060751434
0.4065748889691894	0.6781212361690393	0.0214070969364454
0.1296515350500102	0.2156272028103327	0.7533329154338648
0.8867269448719809	0.9612510620082380	0.2750912895146458
0.8343507939209566	0.2157264707389576	0.0005388654443823
0.0828443108867432	0.6940716847664530	0.2765609377271950
0.3525611874358524	0.9459483314687895	0.7415801667164550
0.2388701887187974	0.7936173664758758	0.5275135899084272
0.6175504859832452	0.0890772645501428	0.8656147966575242
0.9825214255056715	0.4671855970890975	0.1388740193634051
0.9726685135933538	0.1079663413636540	0.5019292704630686
0.6203579111186109	0.8232640181675240	0.1739621056102880
0.2429517893205359	0.4389589858395374	0.8821532861270163
0.7664199000165214	0.4400877455943977	0.3605249954407609
0.5870733574709390	0.4067550326227745	0.5453777190076475
0.3832683626419994	0.4662522629821516	0.6096525809069542
0.4528501995781646	0.8245938148566496	0.1279719819298228
0.5755939046223232	0.4274187055114934	0.3152754119934832
0.8073754175660504	0.4581221872973942	0.5543496794687163
0.0142210783630472	0.4765153534958861	0.5248408800074129
0.8099603256599435	0.4957055984219050	0.7683122681782935
0.6013879152140321	0.4626075909056735	0.1124003478694502
0.3631651634099238	0.4126247740255977	0.3028126983946413

0.5112754425715581	0.4599951751001822	0.6458004305522204
0.0549987467542170	0.3800125561227677	0.5308359060546444
0.7092054233792979	0.5231045517889478	0.7863962439209823
0.8825997773254912	0.5748199061588786	0.8162830728095780
0.8239219628452796	0.4059866712097372	0.8201732206861354
0.7056025836055069	0.5029314506660053	0.1144070581088266
0.5847275513763021	0.3717170397109961	0.0448392159203829
0.5361206103605675	0.5370043958806875	0.0755017643843363
0.3245571616447115	0.4958171443521358	0.2533588502402727
0.3154012849929933	0.3195080337467656	0.2512300601866301
0.3373777083104018	0.4203920547256420	0.4074147477017440
0.0799801727162552	0.5506326351557840	0.5893483576819051
0.0145852565250036	0.5027050650800426	0.4215262514599625

Figure 6 - A12

CIF file

1.0000000000000000

9.4422998428000007 0.0000000000000000 0.0000000000000000

-0.7718446244000000 9.4314702197999996 0.0000000000000000

-0.7410140138000000 -0.8132947143000000 9.3735478129000001

Al	P	O	Si	Cu	N	H
6	5	27	1	2	5	12

Direct

0.9863862757560199	0.2824726714983790	0.1083566054026323
0.4345330572525536	0.0425096478230065	0.8872449946844639
0.7899340564840661	0.8530354389929323	0.1287414794960872
0.0058162803831264	0.0666171240872681	0.6750194992273194
0.2524011668967556	0.6150301605971661	0.9148367200857920
0.2175825331303395	0.8312107424277353	0.3472594953987746
0.2208064027623124	0.2773555668022868	0.8818937920415114
0.0033322689034632	0.0641858423670153	0.3440877929106321
0.0075022734502310	0.6222203647032712	0.1284168285117397
0.2247560643350807	0.8391559327581086	0.6792243644773001
0.7766179132839646	0.0760350928590034	0.8990116889734987
0.3622517351252373	0.2099350332304163	0.9039905772919623
0.1468337558541987	-0.0015437841177802	0.3440852002233240
0.0140030156341601	0.2019426751964322	0.2670377264069276
0.4058849494378901	0.9476198892394356	0.0299644349046239
0.3752286634721168	0.8307622395912753	0.2744373618099662
0.1398840733266246	0.2606496414452363	0.0174062475237140
0.8668072218328809	0.6899141036310347	0.1009057979096134
0.0806671367485336	0.9050968412736137	0.6950200558337036
0.8472755475346766	0.0743495722931443	0.7576940008323385
0.0907654934731779	0.6347884970572220	0.9959374459661415

0.2263201792016737	0.7082377777769286	0.7643312075616884
0.8124443441394975	0.9431961918459498	0.9730488827757197
0.3947570497434985	0.6646998725059363	0.0372682375518583
0.1285679615984011	0.2064340884197452	0.7499743102972602
0.8834127691244665	0.9587032025317341	0.2723877863483177
0.8353249108909747	0.2128073735109889	0.9958617331579495
0.0921912987903291	0.6932931500026280	0.2639539860299808
0.3505512070553292	0.9502580957104674	0.7280252965797157
0.2329297402112728	0.7850409829987959	0.5234493913686362
0.6167778671433831	0.0839633945669914	0.8661089410470374
0.9717068146696901	0.4636497593630584	0.1499325209872434
0.9706373983584997	0.1059683723230745	0.4983739656293617
0.6185962855080253	0.8206745091245311	0.1610863718681379
0.2494033207279015	0.4340787237567142	0.8582533580910334
0.7354289938020279	0.4460022470891442	0.3861981429425172
0.4788458886859887	0.4455568843153603	0.5302181961359717
0.5505059267219167	0.5118713879311134	0.7500728154894672
0.4493932036545033	0.8198231543832033	0.1260469872009878
0.5504864135598737	0.4339622425720896	0.3167797045778684
0.7923715282019967	0.4700139554264749	0.5759089609060980
-0.0066199421171446	0.4644484596317627	0.5147966008220936
0.8428213557245132	0.4960592848916904	0.7872410834207779
0.6043369819831105	0.4550109138003945	0.1170136148775499
0.3388695966084818	0.4296521318143271	0.2666125855694413
0.5792817927662243	0.4782853066924401	0.6257408017256416
0.0323448561159781	0.3682898053818063	0.5289426870115423
0.7498418374308033	0.5236768525492395	0.8286164570358795
0.9236060926465510	0.5724677778583500	0.8227764290055433
0.8675860485242166	0.4032776925130838	0.8281764944141945
0.7088925271823073	0.4950937894617633	0.1315153686977694
0.5962786984538179	0.3636039549187256	0.0502964965644389
0.5448457730533666	0.5281599150488377	0.0699413451623928
0.3218482326372140	0.5207737347116623	0.2178505132430731
0.2945859677334524	0.3446888983270469	0.1989549207234330
0.2866769159274143	0.4315436303549732	0.3577551533889191
0.0690899750836563	0.5439429089973731	0.5554927418836508
-0.0297498976206008	0.4711361731353979	0.4075038029947395

Figure 6 - A13

CIF file

1.0000000000000000

9.4422998428000007	0.0000000000000000	0.0000000000000000
-0.7718446244000000	9.4314702197999996	0.0000000000000000
-0.7410140138000000	-0.8132947143000000	9.3735478129000001

Al	P	O	Si	Cu	N	H	
6	5	27		1	2	5	12
Direct							
0.9869348828237434				0.2836824729171784		0.0916906577419136	
0.4362456452689760				0.0428890516771946		0.8741696424001790	
0.7924057945366484				0.8543599934806723		0.1184568380737000	
0.0064757280828475				0.0683414764623909		0.6599132735197302	
0.2569379782164533				0.6135253535529379		0.8996850491925176	
0.2197832136192359				0.8314453321479880		0.3358784086146608	
0.2220486245851860				0.2770858720828786		0.8689312198417966	
0.0030228343872184				0.0621398728805293		0.3316952882437533	
0.0107040078332252				0.6203811192672244		0.1194609561321057	
0.2251832874742155				0.8397243323003382		0.6655508209465013	
0.7784790167031654				0.0789928458819871		0.8848808904876929	
0.3636455385463672				0.2099039398526468		0.8913721023367592	
0.1484438834044302				-0.0006399423108387		0.3325843023675069	
0.0045965689571550				0.1944502322991327		0.2462683404328309	
0.4106436178249173				0.9503262251527765		0.0186457171214128	
0.3736655228869067				0.8278157112292180		0.2573246898046248	
0.1408881516301713				0.2608616254992945		0.0044428056093920	
0.8728683340908320				0.6925290760594836		0.0836886164014476	
0.0805678033389591				0.9061298042955381		0.6708251745767836	
0.8476525183067666				0.0676793568075891		0.7429663788595451	
0.0985899646799892				0.6234050756405137		0.9911281358429590	
0.2202607887781362				0.7133052708161316		0.7560643741085903	
0.8174209248452381				0.9529065605905990		0.9689264988775925	
0.4021685884566431				0.6671183952326093		0.0170959541560775	
0.1291887476246649				0.2047780228740545		0.7386053822266994	
0.8848204523373293				0.9497093174564959		0.2688823980586150	
0.8366212411449762				0.2211832728806696		0.9736311808916387	
0.0904389555776805				0.6929860438613963		0.2571101864569838	
0.3501186095085346				0.9512462009201168		0.7160276417267266	
0.2404179604497534				0.7820158633950601		0.5114295740249717	
0.6183550681506288				0.0843763243193443		0.8520315484455951	
0.9655831527762581				0.4632968966130439		0.1464488310232333	
0.9731429804810736				0.1131033335804900		0.4846096930971714	
0.6211920311236833				0.8198849514860733		0.1503069539601228	
0.2514075599866045				0.4328687311058806		0.8455222464414900	
0.5790466814204288				0.4829585727909289		0.5073958021954843	
0.3526491699919144				0.4338749632064695		0.5538714145204355	
0.5049889831446497				0.5599638363859148		0.7115612966512621	
0.4519570073213403				0.8193610180309743		0.1112270387808561	
0.5499442772291453				0.4508543490576305		0.3014590226458332	
0.9071060479490439				0.4970082699606293		0.6349147620778752	

0.0350268007159270	0.4683557577982802	0.4940673760255624
0.7924045867953013	0.5197519543954729	0.7877191020231492
0.6099199273029030	0.4652738459955336	0.1097482679503938
0.3261910980271533	0.4078951631374119	0.2582845015833928
0.4753409845511922	0.4918589399556882	0.5907307383579992
0.0726280898047288	0.3702937113623346	0.5014466908460282
0.6891428471108866	0.5428212938644765	0.7550357880171968
0.8347455150557318	0.5995108152297709	0.8628500859277014
0.7835800338478949	0.4279883063600921	0.8387982643756746
0.7139053829998184	0.5016999356562514	0.1034921164606722
0.5897748671226936	0.3710741566014731	0.0471133029352565
0.5464538105171080	0.5375945729905858	0.0653258720520854
0.2843211121874187	0.4989885842829576	0.2302539912074943
0.2891445687341599	0.3268137942133124	0.1834581448728936
0.2954098947287644	0.3862688703319567	0.3565183386466744
0.1221097290931511	0.5421167216101190	0.5099722986921205
0.9916287029100530	0.4714044324730979	0.3913843041106598

Figure 5 - B1

CIF file

1.0000000000000000

9.4422998428000007	0.0000000000000000	0.0000000000000000
-0.7718446244000000	9.4314702197999996	0.0000000000000000
-0.7410140138000000	-0.8132947143000000	9.3735478129000001

Al	P	O	Si	Cu	N	H	
6	5	27	1	1	1	5	

Direct

0.0479745378797967	0.1649410183208780	0.0345080021824356
0.4964638055422830	0.9294604050946399	0.8222381060295438
0.8440020164268859	0.7290814598526264	0.0540726259980247
0.0616068832577950	0.9556354890809431	0.5961876843931673
0.3028796441050726	0.4967315799530845	0.8448667164462492
0.2718371742215327	0.7027380374271841	0.2766493645746317
0.2791646341850961	0.1671481187283850	0.8051485204982424
0.0615265593544565	0.9421264964334627	0.2681186360970781
0.0590567393441056	0.4925378495941621	0.0662002766646553
0.2815952558546912	0.7201731154081012	0.6095377800024703
0.8334857573259664	0.9519654266972954	0.8225460273877173
0.4151842867425688	0.0914626546507251	0.8239475255402422
0.2015456602522411	0.8693732552707962	0.2791924907948291
0.0825794570266721	0.0744273662904043	0.1856725463617872
0.4810886754434696	0.8479896498358933	0.9759339490643936
0.4278359537863954	0.6987343374332936	0.1986073379268096
0.2040760304165518	0.1730304398291873	0.9436370251898359

0.9264844001770393	0.5699692442039290	0.0304465847396109
0.1433339523207885	0.7963569246425422	0.6069210727817109
0.9033753846902892	0.9420359950360763	0.6801596260108895
0.1506075950829217	0.4931546620685975	0.9388399364249889
0.2606380741679273	0.5892485922620629	0.6940925554586727
0.8528508299340717	0.8132134371970883	0.8938868991875445
0.4554343077709169	0.5639132514457069	0.9427393269807856
0.1786781843555654	0.0956343934321926	0.6791683748767227
0.9404373266537089	0.8384679421915072	0.1942334324647342
0.9045118908829283	0.0808596440178275	0.9207218283894435
0.1425102325362182	0.5645482284317571	0.2037191329160870
0.4115813997584806	0.8208350313112703	0.6708725347457848
0.3059700574093889	0.6623635532197829	0.4562136393830935
0.6754260757599877	0.9714820627721698	0.7878359377397443
0.0116875498319905	0.3376119253344300	0.0920882668112344
0.0218623539412277	0.9895700817236267	0.4189624083793010
0.6762623666902925	0.6955609917401797	0.1040746190190312
0.3199966986449204	0.3210154521064100	0.7654422774018970
0.3426718174269600	0.3504381935219238	0.4796932796972956
0.6279209143199553	0.2685484081958386	0.3790795755976291
0.5702348030209041	0.1451313151481946	0.3890094538719693
0.5091680299290864	0.7032365590175762	0.0525799988434685
0.5204838013623604	0.4465990314655368	0.4365389148984479
0.6617211369348907	0.5956649794689621	0.4042731551378820
0.7551008044065102	0.5598558356883349	0.3736088670188695
0.6215443089287302	0.6508697255463904	0.3216260076224042
0.6868235979309080	0.6674673600924300	0.4916477112261411
0.2704391921119565	0.4181122022051182	0.4667676877830202
0.3398897548534948	0.3283084236114915	0.5812222214394844

Figure 5 - B2

CIF file

1.0000000000000000						
9.4422998428000007		0.0000000000000000		0.0000000000000000		
-0.7718446244000000		9.4314702197999996		0.0000000000000000		
-0.7410140138000000		-0.8132947143000000		9.3735478129000001		
Al	P	O	Si	Cu	N	H
6	5	27	1	1	1	5

Direct

0.0465196003364096	0.1593795363393596	0.0366952001358475
0.4990197491780932	0.9248433603800230	0.8230563697041885
0.8422839428494988	0.7236797510776862	0.0551238832745675
0.0637290927854348	0.9503293962859115	0.5990824238201058
0.3017935755053391	0.4915272548114118	0.8476426869414484

0.2706693418358173	0.6974226114016387	0.2803502975943588
0.2794386031862467	0.1620546075997037	0.8062827395625434
0.0583318331718744	0.9365736213324310	0.2708164669631282
0.0580522265633421	0.4870562968028668	0.0688849618452938
0.2818891879213973	0.7128727724869753	0.6122084444570258
0.8315448494677418	0.9484599804244360	0.8244579969979280
0.4135344197374911	0.0842675919913538	0.8279561980794191
0.1978435469022736	0.8633073579281640	0.2812190094725345
0.0793160805890837	0.0695108257706339	0.1889620234915127
0.4968251197847500	0.8474583652588429	0.9807336960956979
0.4256017345140148	0.7013874560886870	0.2002429136772014
0.1999387608920027	0.1660845317786074	0.9423077910066346
0.9244945842418385	0.5641246115536080	0.0342615911900078
0.1440113130393322	0.7902459254832909	0.6091077203138465
0.9082762400217911	0.9381835020104391	0.6867431479790993
0.1484781638956831	0.4873312566678888	0.9410563033697229
0.2591779858389262	0.5812391826881345	0.6953401540296791
0.8445275240751330	0.8089475444060110	0.8967518998002277
0.4518098315830163	0.5645333506735823	0.9454803959617001
0.1813402197137985	0.0924694614552276	0.6774776668577905
0.9366287155588097	0.8335254349793478	0.1960836028314012
0.9008343665077745	0.0757296174507395	0.9261225444268385
0.1412693985657131	0.5596628641395135	0.2060973934957537
0.4103000870714539	0.8134559205161003	0.6765691330819896
0.3074800196344816	0.6564500014269482	0.4588254528480129
0.6755302389798906	0.9713326801874201	0.7830881337482267
0.0099445340289862	0.3322544381380335	0.0957399226341056
0.0190338460784113	0.9832287663701893	0.4219625409899936
0.6759626543911281	0.6817773041186727	0.1118515238355158
0.3239623520587698	0.3164757552546575	0.7705831660074390
0.3756644112271725	0.3432800795816369	0.4883264493010605
0.4669277735767693	0.3893233572594996	0.2435349280649805
0.6198796123866331	0.4952777367473618	0.5839310006649773
0.5091931899628184	0.7003912424151139	0.0565778669153282
0.5416293420451818	0.4425032582892164	0.4148026611266063
0.7038849695745339	0.5279442799288340	0.3390156490475801
0.7625680756702994	0.4476525542619584	0.3035631441631675
0.6784861795370091	0.5902321191933799	0.2514564878282234
0.7599226206646517	0.5885451072004591	0.4235283627338023
0.2946628381712487	0.3970696343434088	0.4613689837389613
0.3777370766779837	0.3403176385005918	0.5944490328945048

Figure 5 - B3
CIF file

1.000000000000000

9.4422998428000007	0.0000000000000000	0.0000000000000000
-0.7718446244000000	9.4314702197999996	0.0000000000000000
-0.7410140138000000	-0.8132947143000000	9.3735478129000001

Al	P	O	Si	Cu	N	H
6	5	28	1	1	2	5

Direct

0.0476907018399834	0.1716293668410303	0.0376625324581888
0.4938855007745029	0.9359510996879030	0.8257386120948397
0.8429018651932778	0.7354041436448908	0.0564826393351692
0.0601126033235125	0.9630339426566085	0.5989171502704321
0.2995879968074379	0.5022671401518658	0.8489445407927012
0.2685961142950971	0.7087694704694900	0.2809014104228181
0.2787013141132819	0.1746439178360589	0.8073560396717250
0.0600516459753530	0.9474384459763283	0.2719202817664242
0.0550825344118954	0.4985753032845913	0.0682016386492998
0.2798400686232331	0.7278988721370145	0.6132979605619070
0.8333539284824349	0.9596307863543596	0.8269627677304469
0.4150691603988233	0.0994062762012385	0.8279435928646554
0.2009901017062313	0.8763741637568339	0.2866552321552940
0.0809586757382940	0.0779789554082081	0.1869449371491509
0.4724915815676349	0.8510610854254618	0.9769228276811900
0.4265809877517808	0.7038782245729391	0.2046755189969816
0.2027491186589158	0.1804516089767277	0.9457332642090739
0.9202476050510779	0.5729821201512454	0.0327442302080512
0.1409488751044816	0.8026619675638414	0.6069350440481364
0.9024080243213588	0.9520609883391731	0.6840981019714176
0.1447154696511936	0.4977307212966692	0.9394043848922695
0.2612927516735236	0.5995239036866397	0.7009449581211893
0.8571776573118556	0.8216494663430512	0.8981577109554413
0.4507096168481806	0.5671566486256054	0.9508387411558855
0.1791723027299144	0.1011948412598233	0.6817237266390291
0.9408903553175493	0.8412200950483383	0.1985198090303036
0.9022045639066255	0.0900080057640965	0.9247047053527664
0.1387944129970914	0.5744762616772148	0.2035434559568532
0.4094706955413737	0.8307544009439921	0.6713173715802464
0.3052339012831751	0.6656248111520969	0.4605839446754713
0.6742270778420146	0.9756854429362966	0.7941167127781591
0.0107589422800557	0.3437377932411667	0.0975235124183682
0.0187002246226048	0.9970555156899588	0.4216539871103144
0.6739347168647446	0.7049535250947938	0.1037672191902868
0.3191043910311406	0.3282738442071842	0.7681752157437752
0.3896804315642202	0.3885818053154294	0.4907849620588740
0.5052464190284998	0.1632014592015171	0.3583456090233216

0.5714187555684371	0.0822123059332396	0.2775993729928776
0.7842150173074662	0.2189212455403020	0.3081088043475947
0.5058763663100333	0.7091623383614919	0.0562258443538185
0.5804738561074760	0.3666438024427519	0.4111172581160504
0.6273961036883327	0.5723451547886371	0.3879686584957613
0.7610750717212923	0.3015638553811281	0.4008932992647954
0.7201886037168317	0.5947308795647414	0.3415148198076660
0.5499453771916081	0.6173567943642309	0.3247417405164089
0.6372456742631506	0.6290745517987700	0.4859637861566048
0.3510484706080470	0.4821348469132810	0.4847725935933114
0.3656241778849481	0.3542877149917287	0.5829494356346057

Figure 5 - B4

CIF file

1.0000000000000000

9.4422998428000007	0.0000000000000000	0.0000000000000000
-0.7718446244000000	9.4314702197999996	0.0000000000000000
-0.7410140138000000	-0.8132947143000000	9.3735478129000001

Al	P	O	Si	Cu	N	H	
6	5	28	1	1	2	5	

Direct

0.0471231333363383	0.1709080652552118	0.0375930561582655
0.4941632023150848	0.9355146769303900	0.8260487232226704
0.8436381810700652	0.7342780949770091	0.0568716868788058
0.0596546877019543	0.9628412596851706	0.5987513072114652
0.3001240593819769	0.5017325168971867	0.8493366607493159
0.2694306189771805	0.7088046374141119	0.2805903024041999
0.2783082503213384	0.1744055254945701	0.8067752269023785
0.0615038914609009	0.9463948042989379	0.2713143580961241
0.0559384988802573	0.4978548226560872	0.0676810487551990
0.2800830825573797	0.7279380903446530	0.6141621089406936
0.8330801411846963	0.9589853097045756	0.8266776900743025
0.4141307369495039	0.0982244883181990	0.8277084815939418
0.2036684317018327	0.8769524275367185	0.2862213471697789
0.0817700220759991	0.0764371870997312	0.1857828211064001
0.4738788398518459	0.8507480060633494	0.9778239565401328
0.4292319599442281	0.7050734355961585	0.2072217672267435
0.2023834910542107	0.1801993977226331	0.9450077043504802
0.9212397850780140	0.5722647638809151	0.0324683190737195
0.1415915608027882	0.8029802393143377	0.6092244430514967
0.9017535266204444	0.9501001966287007	0.6835015153351328
0.1447267693182896	0.4977432858313454	0.9382391054081376
0.2626151502851262	0.5990856133462389	0.7011891769651803
0.8561263814806157	0.8212842418627947	0.8986100214449494

0.4502447258873216	0.5667252436908322	0.9527441301032215
0.1784678380492613	0.1016510066745246	0.6809567591733040
0.9439923355779953	0.8382141342090992	0.1983738903482146
0.9025642151402119	0.0896242217044984	0.9232602496223058
0.1410963274659374	0.5740043246961236	0.2022053285822743
0.4104363791484145	0.8300088293505585	0.6713708670157772
0.3041605655120838	0.6651125144947960	0.4609548431795116
0.6740757741876447	0.9757899607335880	0.7938080464001502
0.0126708413006840	0.3434000209801470	0.0971879085160498
0.0202822893419199	0.9957071861950227	0.4211893125078081
0.6748562974687015	0.7031589993491268	0.1044373888035111
0.3200878331828871	0.3279610287856533	0.7671893497860007
0.3817402330664226	0.3919948910097796	0.4857439881472546
0.5508353844778506	0.1669121863114422	0.3773235448270807
0.7186520514826594	0.0635797489515794	0.2656083121749565
0.7286580457587463	0.2980676728001875	0.3111648328126660
0.5071509176846644	0.7087553724100455	0.0576029174054584
0.5663879659287725	0.3802600286559134	0.4043264336167449
0.6274619867252731	0.5836217585215693	0.3993739080626496
0.6691545796192470	0.1687866819287643	0.3150567026021892
0.7226743925500712	0.5962194932379510	0.3546012287837964
0.5556449770396383	0.6344476669808219	0.3346577728348830
0.6395609011163028	0.6386850003754587	0.4981371288437926
0.3433877440147053	0.4866866491324041	0.4838491387899663
0.3649610709224944	0.3562242689611042	0.5795052364009070

Figure 5 - B5

CIF file

1.0000000000000000

9.4422998428000007	0.0000000000000000	0.0000000000000000
-0.7718446244000000	9.4314702197999996	0.0000000000000000
-0.7410140138000000	-0.8132947143000000	9.3735478129000001

Al	P	O	Si	Cu	N	H	
6	5	29		1	1	3	5

Direct

0.0528685302764956	0.4464400292225717	0.0546398223845431
0.4999981254608927	0.2118819680418613	0.8431267679376342
0.8481413940142679	0.0098069703468044	0.0762664444083677
0.0664998766529722	0.2394814826214094	0.6172417761680903
0.3060805357671642	0.7783352201826347	0.8675232816713537
0.2732703194428907	0.9856910483661057	0.2976895854094541
0.2841043899422782	0.4511271407701979	0.8248327682334894
0.0645248754301856	0.2224981569439006	0.2903233934816106
0.0612666244705123	0.7747077977756391	0.0838044433560680

0.2882797085978257	0.0046936150784842	0.6313729545465421
0.8402021058519339	0.2337542256279188	0.8440360143336972
0.4199447333926967	0.3739516625178284	0.8419744299713495
0.2069573930653827	0.1538713104808492	0.3058536675849981
0.0834490438211910	0.3512649732724362	0.2032356644075844
0.4766126540808101	0.1258514308298366	-0.0072583874784673
0.4337087899762558	0.9877196252971299	0.2255229787685454
0.2096565947073593	0.4535695098309815	0.9639274722308743
0.9253677780362093	0.8480491824725022	0.0506266763907659
0.1509353635946916	0.0814160995070755	0.6292018588011767
0.9071090814895487	0.2213218094366634	0.6997520465004439
0.1488648274538636	0.7776416228263028	0.9534507436154430
0.2724698474956025	0.8765108469807170	0.7191257633613268
0.8628528331062173	0.0977194918671249	0.9184454694097660
0.4547944919759641	0.8421772916396369	0.9741634838546004
0.1825243475524511	0.3803989150061409	0.6990663772275610
0.9468443224726292	0.1130858976666594	0.2196748925182588
0.9104794395241148	0.3661273045533711	0.9363669931752120
0.1464012732800818	0.8509354423040650	0.2184773918537403
0.4205813101852592	0.1060666023615315	0.6859829663312501
0.3090151140129642	0.9421828581756055	0.4776204025864983
0.6806572171443414	0.2502908582918075	0.8101428148528078
0.0210346690538673	0.6196118638673869	0.1125362388221508
0.0236770634225775	0.2728447857108753	0.4401622006650592
0.6788688430403338	0.9832806883299802	0.1234274031370455
0.3263255538135550	0.6047059442258672	0.7872664585561542
0.3953568403975475	0.6703981628279416	0.4940755350405260
0.5665192419039544	0.4801667691644023	0.3263093319814144
0.7394046161530741	0.3955102811822337	0.2076631981319652
0.7488064975218380	0.6231146076071934	0.2883140768912570
0.6602949864210996	0.2222663265079215	0.4611414948491567
0.5111107883435417	0.9862207766126077	0.0757240119030106
0.5806657116298946	0.6867537371140769	0.4008699174207572
0.6386866402628490	0.8916443348929776	0.4323227915413235
0.6889274648963108	0.4949327327814286	0.2697992129712745
0.6191936481703991	0.3205116759587408	0.5193564869172150
0.7409715089401359	0.9149432969256155	0.4068025408899470
0.5727258514712998	0.9414822684779161	0.3613520078570632
0.6300648292755546	0.9360919917842030	0.5333660195987072
0.3499809400781970	0.7612998789485748	0.4970340207205777
0.3841314189289303	0.6314693717842552	0.5867760022108279

Figure 5 - B6
CIF file

1.000000000000000

9.4422998428000007	0.0000000000000000	0.0000000000000000
-0.7718446244000000	9.4314702197999996	0.0000000000000000
-0.7410140138000000	-0.8132947143000000	9.3735478129000001

Al	P	O	Si	Cu	N	H
6	5	29	1	1	3	5

Direct

0.0432457305007066	0.4289153516178263	0.0449083563972854
0.4930231722719503	0.1897795392660521	0.8244359665185061
0.8390261045546203	-0.0078976721751135	0.0654343929589773
0.0592566868677837	0.2182856242567226	0.6089371576804263
0.2967349817544682	0.7588238037111681	0.8564410499310887
0.2671008370035439	0.9693885914681483	0.2837003406331293
0.2753888509288785	0.4296170876466576	0.8171032448698211
0.0546095681209723	0.2057102146608384	0.2795895321391537
0.0535174417702965	0.7567101921237575	0.0673762260376321
0.2815096271012195	-0.0161383762585805	0.6173461510824712
0.8312237793694920	0.2153030591903363	0.8325877945090044
0.4098347848654769	0.3506254535595478	0.8325414396392234
0.1968847435461783	0.1363891952014156	0.2881246714823509
0.0729369575912692	0.3378931886612803	0.1966883464820915
0.4721887271484357	0.1032007708108669	0.9745191000350649
0.4297709884717039	0.9851418475395118	0.2169010937905403
0.2025237754831643	0.4333772268533279	0.9572484790390581
0.9179897612337147	0.8318321960229408	0.0406614917952671
0.1449138442867735	0.0618032750973067	0.6261768501378556
0.8992317397382936	0.2012638784677831	0.6893588043338205
0.1331773683278218	0.7552175180719988	0.9313937067347547
0.2718304091413414	0.8556674413573594	0.7061008996418519
0.8513238682943679	0.0788800281442021	0.9071864431249214
0.4386531414603903	0.8202998886563871	0.9729727763469080
0.1723450312758750	0.3614708523648327	0.6915709017582418
0.9346650812389160	0.0994579121512501	0.2080330020980428
0.9027007222415638	0.3463191576960125	0.9267701625405598
0.1469069312936302	0.8325460736928059	0.1968903844935613
0.4154288799765090	0.0857547433302434	0.6666051398002882
0.2911751120177252	0.9229941915200637	0.4620463320022313
0.6730855843251794	0.2348408425512165	0.7978661950901536
0.0121288186979502	0.6028140854916363	0.0993041227764382
0.0181280447549595	0.2515913048268156	0.4317535057470161
0.6700074009528718	0.9606349405592435	0.1108460513294465
0.3191766214382943	0.5834186788919413	0.7800490912824084
0.3537456401818396	0.6218162656416664	0.4945401778346498
0.6031152214887509	0.5454548784181804	0.3813424834661148

0.7364664866125592	0.4403534340485744	0.2316625841230422
0.8227845688664879	0.6380933433865436	0.3590930715045328
0.4476519759832898	0.3422290568750442	0.1876125187421615
0.5024035595702915	0.9672474864926840	0.0655726792037090
0.5334766046339289	0.7337760975928876	0.4634302132262964
0.6552248257717004	0.9023132161055898	0.4439434998379500
0.7263517343892213	0.5436776970633606	0.3238283279086947
0.5347282351695566	0.3355669109312414	0.2763414550535357
0.7543078520633003	0.8773605981935048	0.4186973865300261
0.6099056978439246	0.9519085431436334	0.3599755588796060
0.6676679922897601	0.9739436788446304	0.5322321884306751
0.2786371183588852	0.6854420974994421	0.4771722313765576
0.3456674247301715	0.5975046197352143	0.5943664386228731

Figure 5 - B7

CIF file

1.0000000000000000

9.4422998428000007 0.0000000000000000 0.0000000000000000

-0.7718446244000000 9.4314702197999996 0.0000000000000000

-0.7410140138000000 -0.8132947143000000 9.3735478129000001

Al	P	O	Si	Cu	N	H	
6	5	29		1	1	3	5

Direct

0.0370199152928822	0.4295202250328342	0.0477869564780424
0.4908785751622616	0.1936739667769017	0.8332077900071124
0.8340184523155021	-0.0057197336743468	0.0658793280502174
0.0599041511732559	0.2214597417766099	0.6139288138919154
0.2927780902419133	0.7626574675164991	0.8562592910005266
0.2621548267104024	0.9742001732086411	0.2834967880584704
0.2721633890522672	0.4300708222243874	0.8185279414827530
0.0497030857693756	0.2088874881870396	0.2800772963704843
0.0503713298268822	0.7615542945128584	0.0682443768808438
0.2767681854482121	-0.0147600376615156	0.6217317138135631
0.8257335968417835	0.2192241770918755	0.8370143005461746
0.4078268569807806	0.3532763965737913	0.8363597025421328
0.1918456927460330	0.1404887110448722	0.2801084917708966
0.0647178409097550	0.3472543432495387	0.2059433091191126
0.4763795821124594	0.1174751914958027	0.9896803267642288
0.4264821206642018	0.9817751303876951	0.2202121487554995
0.1882424731049152	0.4176666422499154	0.9509436146816465
0.9128479364811249	0.8338904781800099	0.0426736120253076
0.1418360354047004	0.0635247646021092	0.6413071475634403
0.9030137096307786	0.2159972918087742	0.6992496604321334
0.1301237743789106	0.7653432314415402	0.9326206886901639

0.2654741995861123	0.8442163598860321	0.6937814988632955
0.8443948419301741	0.0791401296901593	0.9058556140853534
0.4352894446550286	0.8350626406069463	0.9657741220923819
0.1797562118279583	0.3666505646416218	0.6820564243577454
0.9285942002223982	0.1061328467667486	0.2053111114928984
0.8873851212657958	0.3477267732447133	0.9406406669406226
0.1417044151544005	0.8364388652544910	0.1991282335631905
0.4121120336041318	0.0800997249911389	0.6818644189335794
0.2889842557696806	0.9408354381717253	0.4641275498975915
0.6682053846497376	0.2350845981938138	0.7937698886434202
0.0111424108952247	0.6061597971260543	0.0968889608568523
0.0150778823706254	0.2449434496876525	0.4350332175174624
0.6671944074818587	0.9598605449369333	0.1152194242997361
0.3150753291706179	0.5857446502707737	0.7956583373424758
0.3457409529718967	0.6336666876729745	0.4789121493390808
0.6443234679822682	0.5703152885002629	0.3631601230276163
0.6602697233120591	0.3287942769668651	0.2155945907294949
0.8522566308211114	0.6980597487549537	0.3883026554588083
0.4681535794120030	0.3564935879779257	0.3341907495137146
0.5011262115132198	0.9738051977238388	0.0697019351431347
0.5416921401600646	0.7186556046068235	0.4415807624573787
0.6214304352837486	0.9154169688967236	0.4569241169342658
0.7991403386770031	0.5830979163913198	0.3448609747083428
0.5823268670166514	0.3842867657419525	0.2917019960852479
0.7298109933556245	0.9249756233293043	0.4544477138329065
0.5763755031766934	0.9578227551468900	0.3674944009922667
0.5959010734965070	0.9755677740095231	0.5450284702127748
0.2990248517667018	0.6979289827891568	0.5443382847292858
0.3349575612223037	0.5401856869968524	0.5154283300244287

Figure 6 - B8

CIF file

1.0000000000000000

9.4422998428000007 0.0000000000000000 0.0000000000000000

-0.7718446244000000 9.4314702197999996 0.0000000000000000

-0.7410140138000000 -0.8132947143000000 9.3735478129000001

Al P O Si Cu N H

6 5 27 1 2 3 11

Direct

0.3116733651778019	0.1272591188209390	0.8394750196592999
0.6597439355760244	0.9349395886494015	0.0818654183250003
0.8835811773540726	0.1528437343953809	0.6252684385665331
0.1174122535176227	0.6956201187703023	0.8681068383270493
0.0897457296078919	0.9015241662005129	0.2972008252179993

0.8624111871836205	0.3649661003453599	0.0604713714464843
0.0989928904826170	0.3652150411094417	0.8351158198594564
0.8693203400982860	0.1451925145975708	0.2920263018855110
0.8813655672811846	0.6941821440871280	0.0842302312166900
0.1024009411099686	0.9231894927131518	0.6307243447227353
0.6521600714776463	0.1522103421912488	0.8486069269208518
0.4751887057299055	0.4701727535498577	0.5074214307126927
0.4177766268775614	0.5913583488976220	0.5669521537663604
0.2397730793942207	0.2952401548481275	0.8593327661481293
0.9963354318828617	0.0549393690792412	0.2842330188172162
0.8994865025243433	0.2826148638587252	0.2177750792309938
0.2852692803793108	0.0299873742177930	0.9802535868378067
0.2507746141675063	0.9299137061938226	0.2293325613036169
0.0181540927000314	0.3600123918777056	0.9701288205478585
0.7562775940320857	0.7857758795871325	0.0749677764142389
0.9586383798208281	0.9906982600279858	0.6414806199962934
0.7235720557145301	0.1469124564431513	0.7070932558177958
0.9513079627590223	0.6969311853282074	0.9414934928399105
0.1027105857738120	0.7970225039132698	0.7220971530580289
0.6771443812088188	0.0127222092994231	0.9174260246882375
0.2563047180795207	0.7484747344860012	0.9950887428614892
0.0064006138124786	0.2899422882069104	0.7049490718900840
0.7325697058763000	0.0620525914021389	0.2208896968110972
0.7165703581401766	0.2811192944896845	0.9499607895367373
0.9878749078842517	0.7495420034366417	0.2119273352193402
0.2283246334079958	0.0356368205259450	0.6790485568796246
0.1147130719474297	0.8667336745352646	0.4765171053670725
0.4931660625234214	0.1668217613806854	0.8124937103180701
0.8273298749855269	0.5401588317453462	0.1053586006833942
0.8452412310728676	0.1885964536247406	0.4484715244334293
0.4888561049911809	0.8923477909010611	0.1126937704047848
0.1356358059314525	0.5191270504531382	0.8014986326858085
0.4603188240334664	0.5689461691209989	0.9407899370642362
0.3210147527844694	0.9024130238916720	0.0790954740835382
0.3176115849836357	0.3188054705968371	0.4357096113807077
0.5170627892894200	0.6304375104506946	0.7535617802775874
0.6970479832149374	0.7366332250017298	0.7017981076077234
0.4233745292803270	0.1520561287171955	0.4256489127003166
0.1686690527251593	0.4503864693849031	0.4429493970047914
0.3916725956518243	0.6364464237728167	0.9757456048661776
0.4047837458134534	0.4764230064007740	0.9233775746869389
0.6931738397743868	0.7172279826833809	0.5931474440252182
0.7912457180227074	0.7063125534881777	0.7456771700848639
0.7008751739649139	0.8443574537057243	0.7258929442957084

0.4310446828743513	0.1129744385553627	0.5239239580645756
0.3773982139810218	0.0698387107764053	0.3535755095127326
0.5255386663739154	0.1773467130891778	0.4008176717031869
0.1017253348151199	0.4548206050206240	0.3532342697924588
0.1059983408173415	0.4371845000792993	0.5255372864614998
0.2318801851153880	0.5455024910741598	0.4681107039700370

Figure 6 - B9

CIF file

1.0000000000000000

9.4422998428000007 0.0000000000000000 0.0000000000000000

-0.7718446244000000 9.4314702197999996 0.0000000000000000

-0.7410140138000000 -0.8132947143000000 9.3735478129000001

Al	P	O	Si	Cu	N	H
6	5	27		1	2	3 11

Direct

0.2755801312809150	0.0661261077122840	0.8335281337243401
0.6254274247784618	0.8664804801225574	0.0707220621810083
0.8414385259106846	0.0973863053203842	0.6124676771065508
0.0833644356094010	0.6386809909717701	0.8533996479598429
0.0493912981156156	0.8399915638883095	0.2899094025377083
0.8265698025848117	0.3021801811766984	0.0440578108317562
0.0581269487439125	0.3063312260829308	0.8198342834705962
0.8362960305517980	0.0745247723665453	0.2823641306996771
0.8412525695087046	0.6349596625201106	0.0839553311765429
0.0607975108072527	0.8570043290602025	0.6228475443889065
0.6166294543929747	0.0959311820235250	0.8380274943154938
0.5102128074845856	0.4136415394023047	0.4638848782545950
0.3729706102429339	0.4876381160472748	0.4943839395332810
0.1911786372932407	0.2248709536868587	0.8269586788670652
0.9826074385770942	0.0118819617819584	0.2843554185147070
0.8396970183167527	0.2019575220677795	0.1906947885555831
0.2603847320390481	-0.0004590014972966	-0.0029787237643567
0.1937877746747499	0.8289170978713052	0.1958212290674523
0.9881926190821406	0.2986898536436473	0.9632372583802312
0.7078223726186857	0.7076699682882281	0.0366293012857008
0.9303646179432279	0.9443450900808785	0.6278745760309703
0.6827067016272934	0.0781313083625026	0.6947499369688727
0.9438791825212310	0.6443087566780634	0.9654522617343306
0.0286983295514105	0.7239318113639113	0.7019966901248618
0.6534147683442701	0.9734404051464327	0.9276236620074882
0.2427110682747746	0.7176366089941124	0.9340267281398336
0.9492049458685400	0.2448367307123659	0.6960434873291914
0.7166699597065731	0.9616943644803044	0.2245169330026690

0.6811572216303943	0.2390397927873126	0.9210093251417393
0.9118474249168883	0.7060025963675867	0.2264457001863843
0.1969606273963068	0.9458870044932697	0.6906358068470008
0.0859372605272756	0.8096787602057166	0.4690398987423571
0.4566769171139800	0.1051404508177961	0.8072101153665481
0.7974739317417168	0.4769557163176513	0.1012207618720233
0.8077028019751407	0.1308136139719691	0.4339196069906872
0.4539462800311359	0.8399921052538227	0.1090800913430236
0.1009740382123141	0.4610573432933144	0.7960565591524982
0.4383436174894805	0.7372463700664540	0.7384787531137669
0.2872565189972312	0.8464867759279018	0.0619557386792619
0.3595521194163398	0.3365930382009422	0.3265141446692302
0.5182483732001740	0.5545637442318716	0.6392576546942050
0.7058528133187847	0.5256824208297687	0.7288613531898669
0.4573876314733988	0.1993424124195856	0.1999363710777239
0.1535550534058032	0.3270738753796376	0.2662020770450509
0.3694449636208560	0.7200407050075903	0.8120639189729831
0.3841481819641204	0.7807918333964926	0.6638481847289022
0.7675488391956954	0.4946188770627533	0.6494831113572589
0.6942795616948133	0.4428967129862210	0.7920181083914510
0.7599521004030640	0.6105692364418880	0.7891185159037338
0.5195404893336847	0.1401926311251948	0.2616603114489622
0.3896678774704881	0.1291457342334207	0.1314059409267738
0.5237020699397900	0.2549799955169358	0.1393083685065672
0.1052691865199451	0.2274111594527762	0.2743593354997638
0.1067854086397949	0.3977153566662301	0.3315704987415990
0.1302108119202764	0.3491818761899209	0.1629451389857469

Figure 6 - B10

CIF file

1.0000000000000000

9.4422998428000007 0.0000000000000000 0.0000000000000000

-0.7718446244000000 9.4314702197999996 0.0000000000000000

-0.7410140138000000 -0.8132947143000000 9.3735478129000001

Al P O Si Cu N H

6 5 27 1 2 3 11

Direct

0.2795572809065032 0.0656171104020498 0.8352580896242512

0.6273269980925293 0.8658301300964615 0.0705254987225974

0.8452946353605003 0.0991401295637671 0.6134235313469714

0.0859168369335701 0.6394646854024328 0.8506328781897091

0.0519755037585025 0.8395878098094207 0.2878990475868432

0.8296738902162253 0.3028902286127312 0.0445453400031038

0.0609472631734401 0.3066038169796172 0.8213670257252200

0.8410293569990925	0.0761365197200520	0.2814061674318498
0.8437516772537925	0.6353738236098925	0.0803343372935482
0.0641950729803865	0.8574931284167121	0.6232146742064036
0.6174735546021198	0.0953479800075572	0.8368653871788403
0.5398102136991176	0.3845574152790140	0.4652432169907875
0.3211176422596860	0.4943915968878023	0.4891025961628945
0.1920942376244211	0.2222460144347641	0.8272625517768922
0.9864213216403221	0.0119586629945875	0.2809167881615660
0.8466027856362813	0.2068486967190948	0.1941074690653703
0.2730160617705353	0.0034917870320613	0.0019415237806974
0.1946393320398909	0.8260215435090906	0.1910491378491581
0.9918419422103422	0.2984787184786641	0.9652672973560479
0.7104104307748715	0.7082418718014396	0.0328233107138361
0.9359576342216315	0.9474456484991057	0.6315503579580869
0.6865776481067513	0.0782020957270090	0.6953488926549839
0.9462179712010649	0.6435821335332310	0.9621062435980599
0.0290967955862968	0.7219821286497772	0.6979448787872842
0.6469542077184498	0.9685883898501670	0.9232743929488606
0.2460738663518645	0.7218581056444933	0.9277402100923204
0.9506041383120449	0.2479370227840682	0.6974742593657995
0.7198050808676555	0.9663922411424205	0.2198110951475211
0.6832140195372863	0.2357171998960428	0.9241408003983533
0.9135927553732893	0.7068629841222848	0.2231762713692452
0.2013147137339698	0.9420304449628465	0.6949424550329329
0.0895656607691017	0.8148135952086527	0.4683138723490928
0.4585349319382773	0.1085527711864661	0.8029504093590683
0.7989703760679416	0.4778365492659585	0.0984067998969778
0.8123139449545432	0.1277846767071233	0.4339658680142722
0.4570516394865101	0.8329329153390213	0.1114859602062213
0.1073064863994969	0.4610209318166262	0.7998733337858647
0.4316486572502763	0.7029646163433557	0.7169858715074994
0.2921827180806277	0.8458848553195645	0.0604062027926519
0.3695441917721651	0.3567815002477758	0.3600625634953222
0.4932308576147901	0.5255292027064719	0.6041637165885894
0.6827802403505876	0.5216472595322593	0.7095517842907881
0.4492402023578624	0.2178044612001494	0.2286359031629477
0.1702002301940665	0.3380372075851117	0.2793375978354720
0.3709264325296148	0.6970130681261090	0.7990409093895352
0.3737097079345905	0.7462030352449369	0.6447052327853592
0.7487305362334284	0.4911890853632168	0.6337126227134317
0.6784026098705899	0.4445959664281674	0.7798733469839161
0.7259908096686881	0.6149493509821987	0.7641391555184028
0.5146318001434677	0.1641409444466729	0.2931224153818761
0.3813378613258279	0.1455971262017178	0.1620974924358129

0.5137168517939502	0.2740067738374535	0.1665701582230604
0.1188539133017598	0.2395296709519178	0.2872981561114643
0.1293636492133284	0.4121406173992991	0.3467474625759449
0.1510106208060577	0.3615235589911389	0.1758574210763880

Figure 6 - B11

CIF file

1.0000000000000000

9.4422998428000007	0.0000000000000000	0.0000000000000000
-0.7718446244000000	9.4314702197999996	0.0000000000000000
-0.7410140138000000	-0.8132947143000000	9.3735478129000001

Al	P	O	Si	Cu	N	H	
6	5	28		1	2	4	11

Direct

0.8237851256995870	0.2939241225076304	0.1355132472221924
0.2788739728114608	0.0579816605047675	0.9173440716147566
0.6221559003470138	0.8614896265966521	0.1540176110537629
0.8462757791973510	0.0858842083314554	0.6971075540591695
0.0818834964186818	0.6276773025782491	0.9346914745751145
0.0481653113752596	0.8283481209907900	0.3726547827966372
0.0598811330358420	0.2950410445341131	0.9090448883998262
0.8386431311746708	0.0742501724565330	0.3665715476667234
0.8392809296761218	0.6254080781641074	0.1624059535846504
0.0608966295864679	0.8451617007311440	0.7060546454626448
0.6118790656080042	0.0832526033386287	0.9224628190020826
0.1948625189297449	0.2176359025247542	0.9355255719292840
0.9744945120394115	0.9949936073586046	0.3664550734567709
0.8639858949598580	0.2118141339224513	0.2913005859267560
0.2822543251078794	0.9907385528907887	0.0828030720779544
0.1954601412374399	0.8253512516368635	0.2800758974326096
0.9783542206686789	0.2904717644337586	0.0448627939363429
0.7098667809366022	0.7064004204835855	0.1208886353244257
0.9259538488145169	0.9266191984486002	0.7084849737207016
0.6922793135585573	0.0814627415760762	0.7877318156973495
0.9391421077052126	0.6304435069708622	0.0422180607824598
0.0317291600778903	0.7081880825720394	0.7796161263316221
0.6252363214402565	0.9407698371377703	0.9894950261661933
0.2396294440864653	0.7080549423638761	0.0184302495555518
0.9651781483455135	0.2262801631438629	0.7783679179380595
0.7116592017824958	0.9808095780001462	0.2885460836939767
0.6743489874468461	0.2086424182265713	0.0311397079880428
0.9153241793003611	0.6906502657741382	0.3052589733139345
0.1909584160450708	0.9369607740542001	0.7822631554618341
0.0933609280993941	0.8043373920191967	0.5523769574780333

0.4559642884039009	0.1044198223267920	0.8796213007888132
0.7837449531133485	0.4692001981552985	0.1759462493474462
0.8043117951362896	0.1167660504473825	0.5196398012492930
0.4546595755498715	0.8110391733613573	0.1981816908585069
0.1059571544475262	0.4490620379142687	0.8841913316585592
0.5251436606112238	0.5439921339098586	0.4195125977844625
0.3486926542962797	0.4146236802712719	0.5665467555185459
0.5411445697907405	0.7940479223103405	0.5308468004500129
0.2770957632244877	0.2033010848018898	0.6167461834128485
0.2907674956398838	0.8346469502564235	0.1458354163932067
0.3873889567354651	0.4009280499159633	0.3459733586051801
0.4838320413388893	0.5927725047406958	0.6041664144009331
0.4900411664064800	0.6345802567532496	0.8139761122165091
0.4265009936839201	0.4521757286235480	0.1453497633391089
0.2459189331687537	0.2323691762965535	0.2985535508190598
0.3336249123991586	0.3208183747385425	0.6639097766738887
0.4976727619645370	0.5413192900934966	0.8611068131060530
0.5419503843024527	0.7254454612245647	0.4421882983266412
0.4591974161762064	0.8484198749563884	0.5108176034574333
0.5330631615214395	0.4425014546277904	0.1377242174426577
0.3678955226346014	0.3946940439990844	0.0609142738484880
0.4114232748582483	0.5582088084137010	0.1425884478742097
0.1498639795755935	0.2597128339584661	0.2554521846498825
0.2730756195498031	0.1503056363797062	0.2294528499463607
0.2272959076184835	0.1913376093494720	0.3937222198966092
0.4025775534969038	0.6777101663497209	0.8530350300099235
0.5774165068428575	0.7021785675519598	0.8527715692758910

Figure 6 - B12

CIF file

1.0000000000000000

9.4422998428000007 0.0000000000000000 0.0000000000000000

-0.7718446244000000 9.4314702197999996 0.0000000000000000

-0.7410140138000000 -0.8132947143000000 9.3735478129000001

Al	P	O	Si	Cu	N	H	
6	5	28	1	2	4	11	

Direct

0.2775259974892821	0.0593436531961891	0.8346944114315858
0.6298598978165852	0.8606889747746755	0.0743242126709197
0.8471296608969802	0.0841190944038171	0.6138974707151044
0.0876163511931735	0.6286608433007418	0.8542729631592696
0.0563414934471004	0.8298102061545207	0.2922162183836967
0.8300193690685893	0.2943829774278852	0.0499097893266107
0.0654640248578028	0.2959521234184005	0.8258990293402723

0.8453315553096457	0.0699471836646279	0.2864327665113511
0.8475535371914062	0.6282018794650109	0.0851301959345069
0.0609561301921105	0.8495510840978174	0.6211542423490791
0.6179056751991981	0.0862956680572183	0.8406555441074351
0.6047602799087110	0.4020957013458876	0.3421184241394802
0.3729016924893730	0.5226547029913802	0.4656145096132375
0.2060578531488333	0.2268997945477790	0.8470921088841340
0.9876567791260571	0.0005211506510844	0.2914399870872074
0.8600712661383206	0.1996040143768741	0.1984238708371650
0.2637684986526656	-0.0174487209221344	-0.0071243474423932
0.1962889014496024	0.8148042610397881	0.1919347286112699
0.9892719085772085	0.2917187935429399	0.9654020807647423
0.7135932933259217	0.7024993351728271	0.0394713739840247
0.9187620074120700	0.9198584267804687	0.6147524917881692
0.6897885695737511	0.0793941377965973	0.7002727171068672
0.9493807464503977	0.6388035330001687	0.9667082283315962
0.0401474967534336	0.7186356308139953	0.7051833011007996
0.6486285275038403	0.9556192173835967	0.9206825337617932
0.2513325194343347	0.6996375976218540	0.9334602444501477
0.9685087919258296	0.2179280087155526	0.7010580997856958
0.7218542238886321	0.9646050594332980	0.2205198542089631
0.6792977663897575	0.2241499595302522	0.9355612284074313
0.9165045620515105	0.6977237857686339	0.2284717023413757
0.1829941879513902	0.9567089384109595	0.6898397225489499
0.0976551339299369	0.8002136116931817	0.4709760883820653
0.4587195627832418	0.0974708685962562	0.8047598905997672
0.8012155481913489	0.4706711599595110	0.0990884460830069
0.8121250549528426	0.1235465117365457	0.4373555869273303
0.4588956595776017	0.8286626393090186	0.1121751378097744
0.0973118582850617	0.4501931943028579	0.7924453153210006
0.3996751155698063	0.6932612922277473	0.6855959741346631
0.7864338018815229	0.4837942930673761	0.4889602853320561
0.2926482084670715	0.8310315167467073	0.0597009134098067
0.3731844112248556	0.3791549744740438	0.3262818548934019
0.5221072876818595	0.5418996219056396	0.6021112716759117
0.6650506561851022	0.5222847726556346	0.7615087181231025
0.4139403245963216	0.2121389174715363	0.1954865538802961
0.1605825179621190	0.3766477218199061	0.2980448308924144
0.6555048110332489	0.4670942603300344	0.4594893535241052
0.3535313926896659	0.6839220447689772	0.7761444135962986
0.3298714290942696	0.6580982755599246	0.6025074983874229
0.7604753628169805	0.5222186045831273	0.7160112302265953
0.6481554614802907	0.4283815607867371	0.8075330855184545
0.6728398813555221	0.6027365318462251	0.8420935679652438

0.4791922388667887	0.1525412410608757	0.2536350012583140
0.3350855762210789	0.1412613203846310	0.1417555545252857
0.4743909527856575	0.2510266457728133	0.1191923719135904
0.1073345648527896	0.2809605298785260	0.3119409528461505
0.1373493817254259	0.4511806520508909	0.3756066594432952
0.1248502839760735	0.4053002670485694	0.2003296940901435

Figure 6 - B13

CIF file

1.0000000000000000

9.4422998428000007 0.0000000000000000 0.0000000000000000

-0.7718446244000000 9.4314702197999996 0.0000000000000000

-0.7410140138000000 -0.8132947143000000 9.3735478129000001

Al	P	O	Si	Cu	N	H	
6	5	28		1	2	4	11

Direct

0.2872050037064139	0.0821745154148108	0.8302289412884992
0.6353833277094573	0.8809898501853484	0.0626662225672922
0.8551761807269616	0.1082230592268995	0.6036122256230999
0.0956446360234594	0.6516274880261629	0.8513385199089007
0.0605863754311169	0.8446386045817874	0.2847613136376673
0.8290940454350167	0.3107184605452180	0.0505984815976203
0.0640772530017008	0.3169946029565370	0.8170213862303223
0.8574603247874265	0.0899805620903680	0.2764152781865175
0.8511947663238012	0.6484469264553994	0.0733491544942546
0.0755860538772581	0.8679654492957323	0.6164560772257341
0.6233724953920824	0.1004738294195058	0.8287689501888642
0.6167636698119235	0.3281525239901697	0.2233623866065383
0.5328884020331603	0.4595211857095021	0.3949217501193945
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