

## HS

bfgs converged in 157 scf cycles and 148 bfgs steps

(criteria: energy < 1.0E-04 Ry, force < 1.0E-05Ry/Bohr, cell < 5.0E-01kbar)

End of BFGS Geometry Optimization

Final enthalpy = -4090.8491729027 Ry

Begin final coordinates

new unit-cell volume = 12745.38178 a.u.^3 ( 1888.67070 Ang^3 )

density = 1.83229 g/cm^3

CELL\_PARAMETERS (angstrom)

8.814039804	0.000000000	0.035738397
0.000000000	13.651369837	0.000000000
-4.342536496	0.000000000	15.678970981

ATOMIC\_POSITIONS (crystal)

Co1	0.6406322674	0.5024247113	0.4561474679
Co1	0.3593677326	0.4975752887	0.5438525621
Co1	0.3593677326	0.0024247113	0.0438525321
Co1	0.6406322674	0.9975752887	0.9561474379
Co1	0.9946352330	0.6349076177	0.5932176532
Co1	0.0053647670	0.3650923823	0.4067823468
Co1	0.0053647670	0.1349076177	0.9067823468
Co1	0.9946352330	0.8650923823	0.0932176532
Cl	0.9149738192	0.7186093692	0.6935441684
Cl	0.0850261808	0.2813906308	0.3064558316
Cl	0.0850261808	0.2186093692	0.8064558316
Cl	0.9149738192	0.7813906308	0.1935441684
Cl	0.2581890935	0.6440186707	0.6240697097
Cl	0.7418109065	0.3559813293	0.3759302903
Cl	0.7418109065	0.1440186707	0.8759302903
Cl	0.2581890935	0.8559813293	0.1240697097
O	0.4832047592	0.3999792856	0.4809736798
O	0.5167952708	0.6000207144	0.5190263202
O	0.5167952708	0.8999792856	0.0190263202
O	0.4832047592	0.1000207144	0.9809736798
N	0.5108359650	0.5395902695	0.3302022711
N	0.4891640350	0.4604097305	0.6697976989
N	0.4891640350	0.0395902695	0.1697977289
N	0.5108359650	0.9604097305	0.8302023011
N	0.7689121983	0.6168565032	0.4287763945
N	0.2310878017	0.3831434968	0.5712236055

N	0.2310878017	0.1168565032	0.0712236055
N	0.7689121983	0.8831434968	0.9287763945
N	0.8837995842	0.6740226309	0.4769783772
N	0.1162004158	0.3259773691	0.5230216228
N	0.1162004158	0.1740226309	0.0230216228
N	0.8837995842	0.8259773691	0.9769783772
N	0.7921611473	0.4521232166	0.5683566708
N	0.2078388527	0.5478767834	0.4316433292
N	0.2078388527	0.9521232166	0.9316433292
N	0.7921611473	0.0478767834	0.0683566708
N	0.9200317947	0.5015326544	0.6179382848
N	0.0799682053	0.4984673456	0.3820617152
N	0.0799682053	0.0015326544	0.8820617152
N	0.9200317947	0.9984673456	0.1179382848
N	0.8936251388	0.3656558015	0.6824622147
N	0.1063748612	0.6343441985	0.3175377853
N	0.1063748612	0.8656558015	0.8175377853
N	0.8936251388	0.1343441985	0.1824622147
H	0.9243034065	0.3088642634	0.7261593605
H	0.0756965935	0.6911357366	0.2738406395
H	0.0756965935	0.8088642634	0.7738406395
H	0.9243034065	0.1911357366	0.2261593605
H	0.3517011285	0.4254134141	0.3097008201
H	0.6482988715	0.5745866159	0.6902992089
H	0.6482988715	0.9254133841	0.1902991799
H	0.3517011285	0.0745865859	0.8097007911
H	0.2217891616	0.4746311402	0.1579367007
H	0.7782108234	0.5253688898	0.8420632853
H	0.7782108234	0.9746311102	0.3420632853
H	0.2217891616	0.0253688598	0.6579367147
H	0.3215629573	0.6250288224	0.0987906951
H	0.6784370127	0.3749711776	0.9012093339
H	0.6784370127	0.1250288224	0.4012093049
H	0.3215629573	0.8749711776	0.5987906661
H	0.5440895597	0.7182922292	0.1912122892
H	0.4559104403	0.2817077708	0.8087877258
H	0.4559104403	0.2182922292	0.3087877258
H	0.5440895597	0.7817077708	0.6912122742
H	0.7405516338	0.8162700878	0.3114418718
H	0.2594483662	0.1837299122	0.6885581572
H	0.2594483662	0.3162700878	0.1885581282
H	0.7405516338	0.6837299122	0.8114418428
H	0.1074204580	0.8116658657	0.5141600885
H	0.8925795420	0.1883341343	0.4858399115

H	0.8925795420	0.3116658657	0.9858399115
H	0.1074204580	0.6883341343	0.0141600885
H	0.9436481314	0.8841542683	0.5212792069
H	0.0563518686	0.1158457317	0.4787207931
H	0.0563518686	0.3841542683	0.9787207931
H	0.9436481314	0.6158457317	0.0212792069
H	0.0179646673	0.8923063749	0.4295947337
H	0.9820353327	0.1076936251	0.5704052663
H	0.9820353327	0.3923063749	0.0704052663
H	0.0179646673	0.6076936251	0.9295947337
H	0.3193660642	0.2439941017	0.4292554328
H	0.6806339358	0.7560058683	0.5707445672
H	0.6806339358	0.7439941317	0.0707445672
H	0.3193660642	0.2560058983	0.9292554328
H	0.3739374920	0.0773268065	0.4917026775
H	0.6260625080	0.9226732085	0.5082973225
H	0.6260625080	0.5773267915	0.0082973225
H	0.3739374920	0.4226732085	0.9917026775
H	0.6089153446	0.0482423232	0.6138768186
H	0.3910846554	0.9517576918	0.3861231814
H	0.3910846554	0.5482423082	0.8861231814
H	0.6089153446	0.4517576918	0.1138768186
H	0.7964028925	0.1837313653	0.6658352300
H	0.2035971075	0.8162686637	0.3341647700
H	0.2035971075	0.6837313363	0.8341647700
H	0.7964028925	0.3162686347	0.1658352300
H	0.1934669920	0.5249111177	0.7397053530
H	0.8065330080	0.4750888823	0.2602946470
H	0.8065330080	0.0249111177	0.7602946470
H	0.1934669920	0.9750888823	0.2397053530
H	0.1745258274	0.4106963350	0.7910386774
H	0.8254741726	0.5893036650	0.2089613226
H	0.8254741726	0.9106963350	0.7089613226
H	0.1745258274	0.0893036650	0.2910386774
H	0.0668893490	0.5156741201	0.8085654468
H	0.9331106510	0.4843258799	0.1914345532
H	0.9331106510	0.0156741201	0.6914345532
H	0.0668893490	0.9843258799	0.3085654468
C	0.3908398796	0.4891707304	0.2801300164
C	0.6091601204	0.5108292696	0.7198700126
C	0.6091601204	0.9891707304	0.2198699836
C	0.3908398796	0.0108292696	0.7801299874
C	0.3189237104	0.5173438806	0.1966350368
C	0.6810762596	0.4826561194	0.8033649932

C	0.6810762596	0.0173438806	0.3033649632
C	0.3189237104	0.9826561194	0.6966350068
C	0.3738556558	0.6008168417	0.1639226440
C	0.6261443732	0.3991831583	0.8360773260
C	0.6261443732	0.1008168417	0.3360773560
C	0.3738556558	0.8991831583	0.6639226740
C	0.4984651691	0.6531946721	0.2152078008
C	0.5015348009	0.3468053279	0.7847921842
C	0.5015348009	0.1531946721	0.2847921842
C	0.4984651691	0.8468053279	0.7152078158
C	0.5657252143	0.6205374581	0.2983575776
C	0.4342747857	0.3794625419	0.7016423924
C	0.4342747857	0.1205374581	0.2016424224
C	0.5657252143	0.8794625419	0.7983576076
C	0.6983507030	0.6673887897	0.3572302274
C	0.3016492970	0.3326112103	0.6427697426
C	0.3016492970	0.1673887897	0.1427697726
C	0.6983507030	0.8326112103	0.8572302574
C	0.7703344814	0.7592640773	0.3590482163
C	0.2296655186	0.2407359227	0.6409517837
C	0.2296655186	0.2592640773	0.1409517837
C	0.7703344814	0.7407359227	0.8590482163
C	0.8862479536	0.7613671402	0.4360832463
C	0.1137520464	0.2386328598	0.5639167537
C	0.1137520464	0.2613671402	0.0639167537
C	0.8862479536	0.7386328598	0.9360832463
C	0.9943464759	0.8417286283	0.4772233708
C	0.0056535241	0.1582713717	0.5227766292
C	0.0056535241	0.3417286283	0.0227766292
C	0.9943464759	0.6582713717	0.9772233708
C	0.5240451302	0.3102126368	0.5117558993
C	0.4759548698	0.6897873632	0.4882441007
C	0.4759548698	0.8102126368	0.9882441007
C	0.5240451302	0.1897873632	0.0117558993
C	0.4243314023	0.2300893569	0.4807864048
C	0.5756686277	0.7699106581	0.5192135952
C	0.5756686277	0.7300893419	0.0192135952
C	0.4243314023	0.2699106581	0.9807864048
C	0.4551989124	0.1373441442	0.5163199960
C	0.5448010876	0.8626558408	0.4836800040
C	0.5448010876	0.6373441592	0.9836800040
C	0.4551989124	0.3626558408	0.0163199960
C	0.5878181803	0.1203333959	0.5842883439
C	0.4121818197	0.8796666041	0.4157116561

C	0.4121818197	0.6203333959	0.9157116561
C	0.5878181803	0.3796666041	0.0842883439
C	0.6914600021	0.1969651522	0.6137757039
C	0.3085399979	0.8030348778	0.3862242961
C	0.3085399979	0.6969651222	0.8862242961
C	0.6914600021	0.3030348478	0.1137757039
C	0.6639095289	0.2911579653	0.5775004786
C	0.3360904711	0.7088420347	0.4224995214
C	0.3360904711	0.7911579653	0.9224995214
C	0.6639095289	0.2088420347	0.0775004786
C	0.7776934216	0.3682102791	0.6077586490
C	0.2223065784	0.6317897209	0.3922413510
C	0.2223065784	0.8682102791	0.8922413510
C	0.7776934216	0.1317897209	0.1077586490
C	0.9799186340	0.4487349976	0.6875099384
C	0.0200813660	0.5512650324	0.3124900616
C	0.0200813660	0.9487349676	0.8124900616
C	0.9799186340	0.0512650024	0.1875099384
C	0.1121210107	0.4762702791	0.7608772618
C	0.8878789893	0.5237297509	0.2391227382
C	0.8878789893	0.9762702491	0.7391227382
C	0.1121210107	0.0237297209	0.2608772618

## BS1

bfgs converged in 151 scf cycles and 145 bfgs steps

(criteria: energy < 1.0E-04 Ry, force < 1.0E-05Ry/Bohr, cell < 5.0E-01kbar)

End of BFGS Geometry Optimization

Final enthalpy = -4090.8509100541 Ry

Begin final coordinates

new unit-cell volume = 12744.02226 a.u.^3 ( 1888.46924 Ang^3 )

density = 1.83248 g/cm^3

CELL\_PARAMETERS (angstrom)

8.814631061	-0.000049088	0.034059193
0.000170049	13.648057153	0.001052997
-4.345776783	0.001536681	15.680869179

ATOMIC\_POSITIONS (crystal)

Co1	0.6404306642	0.5025573919	0.4563032619
Co1	0.3591116546	0.4980673730	0.5441713723
Co1	0.3595246849	0.0024564167	0.0438647732
Co1	0.6406983631	0.9976070287	0.9561110345

Co2	0.9937917608	0.6349209848	0.5934186528
Co1	0.0054835021	0.3653173087	0.4067915518
Co1	0.0053686428	0.1349863672	0.9068367720
Co1	0.9948450733	0.8651725204	0.0931741634
Cl	0.9151747886	0.7184581783	0.6938912254
Cl	0.0847763856	0.2815866592	0.3063757383
Cl	0.0849809273	0.2185440878	0.8064319769
Cl	0.9150306553	0.7815567173	0.1934702108
Cl	0.2572434147	0.6430580113	0.6230566012
Cl	0.7419620441	0.3561237237	0.3760552368
Cl	0.7417989386	0.1440652843	0.8759443467
Cl	0.2583838794	0.8559685559	0.1240703754
O	0.4828469728	0.4001437054	0.4809651683
O	0.5169746209	0.6002476042	0.5191692898
O	0.5169229000	0.8999725420	0.0190125260
O	0.4832337566	0.1000596491	0.9809290741
N	0.5107119843	0.5395635120	0.3302745986
N	0.4892469836	0.4605304988	0.6699724193
N	0.4893845634	0.0395599784	0.1698126077
N	0.5107657585	0.9603765484	0.8301560481
N	0.7685995373	0.6168884611	0.4289391831
N	0.2311953440	0.3832914246	0.5712868222
N	0.2312554935	0.1168809578	0.0712493655
N	0.7689420427	0.8831414089	0.9287432223
N	0.8834283012	0.6739269192	0.4771157052
N	0.1162636840	0.3261662835	0.5230574824
N	0.1163111504	0.1740722608	0.0230724124
N	0.8839136846	0.8259972479	0.9769598006
N	0.7916363921	0.4521397630	0.5684006558
N	0.2082715819	0.5479749941	0.4314839281
N	0.2078618155	0.9521532886	0.9316960244
N	0.7922736202	0.0479585406	0.0683159000
N	0.9195119826	0.5014964155	0.6178630354
N	0.0802459329	0.4986417096	0.3819749970
N	0.0799252135	0.0015648233	0.8821284685
N	0.9202251013	0.9985732405	0.1178935991
N	0.8933585759	0.3655537013	0.6823993857
N	0.1066778043	0.6345121506	0.3174110888
N	0.1063010647	0.8656673813	0.8176229521
N	0.8936618292	0.1344126496	0.1824406107
H	0.9241303072	0.3087332318	0.7260885148
H	0.0759523079	0.6913278342	0.2737240587
H	0.0756019129	0.8088555875	0.7739442313
H	0.9242680768	0.1912020755	0.2261557611

H	0.3514472466	0.4254373529	0.3098510518
H	0.6484831773	0.5746756987	0.6905790894
H	0.6484736735	0.9253202370	0.1903193443
H	0.3516760188	0.0746168072	0.8095646434
H	0.2217127075	0.4744906283	0.1580089990
H	0.7784631686	0.5252257691	0.8422840212
H	0.7784053625	0.9744599323	0.3420866487
H	0.2214950196	0.0252087227	0.6578928843
H	0.3217841009	0.6247076231	0.0987236813
H	0.6785119090	0.3747840174	0.9013192323
H	0.6787326450	0.1249008671	0.4012365122
H	0.3210050320	0.8746020865	0.5988991582
H	0.5444101723	0.7179705796	0.1910852408
H	0.4558767524	0.2816594621	0.8088207581
H	0.4561912199	0.2182256821	0.3088322489
H	0.5436332880	0.7813741144	0.6913600752
H	0.7413067864	0.8159792885	0.3112592449
H	0.2594089221	0.1837731498	0.6885570214
H	0.2596187090	0.3162456978	0.1886559607
H	0.7403441414	0.6835455021	0.8116081131
H	0.1084184625	0.8113931087	0.5133717336
H	0.8924416939	0.1885720402	0.4858956863
H	0.8926202481	0.3117295662	0.9859656406
H	0.1074937144	0.6883230976	0.0142635150
H	0.9449663399	0.8833688461	0.5218579494
H	0.0561292248	0.1160586081	0.4786707229
H	0.0563571886	0.3842569523	0.9788358908
H	0.9437420186	0.6158237054	0.0214043227
H	0.0171509646	0.8925102651	0.4295386024
H	0.9820070024	0.1078224102	0.5703883193
H	0.9821534908	0.3923568360	0.0705288896
H	0.0180425034	0.6076034094	0.9297501294
H	0.3189998139	0.2441596745	0.4290327893
H	0.6807104782	0.7562958817	0.5708817541
H	0.6808388784	0.7439404564	0.0706759844
H	0.3192630732	0.2560702193	0.9292399731
H	0.3734058011	0.0774021992	0.4913723425
H	0.6263394276	0.9229424446	0.5082265456
H	0.6261681889	0.5772406297	0.0082551033
H	0.3737248860	0.4227500883	0.9917290628
H	0.6082466860	0.0481487354	0.6136367234
H	0.3915761419	0.9519319798	0.3858735749
H	0.3910006759	0.5481628692	0.8861561730
H	0.6087343813	0.4518384238	0.1139186104

H	0.7957891209	0.1836008771	0.6657753954
H	0.2041875047	0.8163901916	0.3338674294
H	0.2034428664	0.6836925971	0.8342762489
H	0.7963295068	0.3163451587	0.1658423675
H	0.1935730270	0.5245056353	0.7395125695
H	0.8066425611	0.4753230051	0.2603039293
H	0.8063511475	0.0249071910	0.7603590731
H	0.1937286951	0.9752643797	0.2396756006
H	0.1739699057	0.4105479137	0.7910958786
H	0.8255644515	0.5895220395	0.2089014822
H	0.8252914629	0.9106408243	0.7090979303
H	0.1746219825	0.0894456418	0.2910332800
H	0.0668564151	0.5159386656	0.8082989186
H	0.9330784568	0.4844586160	0.1914013415
H	0.9328428048	0.0156484642	0.6914926471
H	0.0671516417	0.9843407484	0.3085059347
C	0.3906974770	0.4891239327	0.2802247081
C	0.6093066144	0.5108729413	0.7200913584
C	0.6093707053	0.9890919257	0.2198855087
C	0.3907214624	0.0107769379	0.7800588965
C	0.3188907703	0.5172016832	0.1966829425
C	0.6812533021	0.4825805064	0.8035573239
C	0.6813073294	0.0172270420	0.3033861198
C	0.3186384984	0.9824909408	0.6966147047
C	0.3739899920	0.6005768105	0.1638933728
C	0.6262323342	0.3990806450	0.8362077673
C	0.6264144673	0.1007127004	0.3361026754
C	0.3734309376	0.8989046647	0.6639879880
C	0.4986575166	0.6529548017	0.2151474653
C	0.5015642287	0.3467776400	0.7848763245
C	0.5017969397	0.1531290845	0.2848228667
C	0.4980869537	0.8465436117	0.7152969455
C	0.5657744338	0.6204080522	0.2983577920
C	0.4343321577	0.3795242994	0.7017426607
C	0.4345049469	0.1205052732	0.2016680293
C	0.5655469505	0.8793376306	0.7983857329
C	0.6983638922	0.6672814725	0.3572378100
C	0.3017126206	0.3327054724	0.6428233682
C	0.3018391373	0.1673845946	0.1428067645
C	0.6982754216	0.8325315512	0.8572623251
C	0.7707440377	0.7590425733	0.3589655707
C	0.2296645068	0.2408248699	0.6409698190
C	0.2298202373	0.2592640408	0.1410275358
C	0.7702623855	0.7406279256	0.8591376624



C	0.8864800600	0.7611405864	0.4360846141
C	0.1137357816	0.2387881955	0.5639287373
C	0.1138607058	0.2614023046	0.0639983241
C	0.8862931465	0.7385890050	0.9361412941
C	0.9947900701	0.8414523391	0.4771650697
C	0.0055458393	0.1584559787	0.5227745041
C	0.0057189563	0.3417929395	0.0228884708
C	0.9944229435	0.6582283180	0.9773348851
C	0.5235957074	0.3103383208	0.5116939283
C	0.4762134041	0.6900044120	0.4882555740
C	0.4760546164	0.8101930496	0.9882443913
C	0.5240125728	0.1898434819	0.0117281726
C	0.4238960440	0.2302060829	0.4806083882
C	0.5758657058	0.7701678834	0.5192480913
C	0.5758081641	0.7300393582	0.0191793225
C	0.4242266423	0.2699760453	0.9807794662
C	0.4546744247	0.1374032408	0.5160798402
C	0.5451086193	0.8628991570	0.4836053186
C	0.5448861034	0.6372779853	0.9836535773
C	0.4550341672	0.3627284910	0.0163396891
C	0.5872316108	0.1202925548	0.5840971853
C	0.4126185745	0.8798506279	0.4155262990
C	0.4121691911	0.6202729700	0.9157288980
C	0.5876641188	0.3797425062	0.0843138378
C	0.6908904346	0.1968945531	0.6136832586
C	0.3090318772	0.8031816512	0.3860131436
C	0.3084940211	0.6969286193	0.8862790286
C	0.6913695129	0.3031073079	0.1137823509
C	0.6633889293	0.2911641163	0.5774906599
C	0.3365004731	0.7089934160	0.4223628429
C	0.3361080119	0.7911440036	0.9225410960
C	0.6638738605	0.2089075869	0.0774838839
C	0.7772111556	0.3681747489	0.6077724144
C	0.2227170472	0.6319087181	0.3920886759
C	0.2223016525	0.8682227972	0.8923067593
C	0.7777225486	0.1318543232	0.1077314289
C	0.9796112601	0.4486615265	0.6874135340
C	0.0202928333	0.5514632224	0.3124058469
C	0.0199799924	0.9487539893	0.8125752863
C	0.9800583374	0.0513600623	0.1874762294
C	0.1119287395	0.4761742177	0.7607549177
C	0.8879664091	0.5239317818	0.2390815885
C	0.8876940240	0.9762535431	0.7392091005
C	0.1123128576	0.0238397740	0.2608477971

## BS2

bfgs converged in 151 scf cycles and 147 bfgs steps

(criteria: energy < 1.0E-04 Ry, force < 1.0E-05Ry/Bohr, cell < 5.0E-01kbar)

End of BFGS Geometry Optimization

Final enthalpy = -4090.8506826749 Ry

Begin final coordinates

new unit-cell volume = 12748.20634 a.u.^3 ( 1889.08925 Ang^3 )

density = 1.83188 g/cm^3

CELL\_PARAMETERS (angstrom)

8.815335410	-0.001546610	0.034764677
-0.002613833	13.647440347	0.000060169
-4.344865418	0.000535367	15.685135531

ATOMIC\_POSITIONS (crystal)

Co1	0.6405855364	0.5025117123	0.4561289057
Co1	0.3593578510	0.4975418033	0.5438536396
Co1	0.3586157589	0.0024090207	0.0439845195
Co2	0.6416627835	0.9977143021	0.9559750949
Co1	0.9947898231	0.6350878082	0.5931153106
Co1	0.0052145889	0.3649924959	0.4068233776
Co1	0.0055656021	0.1352483307	0.9065634546
Co1	0.9945142325	0.8649612470	0.0931927476
Cl	0.9153154462	0.7189316401	0.6933562580
Cl	0.0848064821	0.2811311810	0.3066325734
Cl	0.0846873061	0.2186363388	0.8062126797
Cl	0.9151024580	0.7812679267	0.1936108021
Cl	0.2583217962	0.6439951418	0.6239662993
Cl	0.7416944504	0.3560157190	0.3760367552
Cl	0.7422255522	0.1431883504	0.8768277326
Cl	0.2581126986	0.8559013981	0.1238966347
O	0.4831671594	0.3999954201	0.4810031566
O	0.5167821237	0.6000335250	0.5189989494
O	0.5167816299	0.9004365539	0.0188272490
O	0.4832665519	0.0995611864	0.9812381309
N	0.5108304007	0.5396410080	0.3302048190
N	0.4891689981	0.4603448723	0.6698098409
N	0.4882984789	0.0396165411	0.1698218302
N	0.5116109626	0.9604010969	0.8302214029
N	0.7689270410	0.6169615156	0.4287530904
N	0.2310687728	0.3830583762	0.5712214870

N	0.2306707188	0.1170781959	0.0711505585
N	0.7689304438	0.8827723914	0.9289500656
N	0.8838443952	0.6741576598	0.4769266968
N	0.1161401752	0.3258862258	0.5230313274
N	0.1159418128	0.1742803709	0.0229090932
N	0.8836491681	0.8257191270	0.9770947837
N	0.7921505299	0.4522553381	0.5683098438
N	0.2078249669	0.5478234146	0.4316513973
N	0.2074360647	0.9521767944	0.9317962672
N	0.7923477454	0.0476523695	0.0683934545
N	0.9200362421	0.5017002342	0.6178695561
N	0.0799384388	0.4983826495	0.3820910753
N	0.0796939114	0.0016226898	0.8821918979
N	0.9200693168	0.9982663797	0.1179339615
N	0.8936040779	0.3657950596	0.6823780432
N	0.1063866063	0.6342838110	0.3175670389
N	0.1064744037	0.8658834310	0.8175469089
N	0.8935851754	0.1340971353	0.1824978852
H	0.9242217599	0.3090019257	0.7260657051
H	0.0756923179	0.6910838126	0.2738659550
H	0.0760213958	0.8091482081	0.7737740970
H	0.9241321434	0.1908664288	0.2262322546
H	0.3516790636	0.4254084899	0.3096915759
H	0.6482993610	0.5745843661	0.6903811353
H	0.6473603689	0.9254185018	0.1902728486
H	0.3526038887	0.0746209553	0.8098294550
H	0.2218806086	0.4745959643	0.1579618937
H	0.7781225336	0.5253031998	0.8420896694
H	0.7776938161	0.9748102848	0.3419087386
H	0.2221108230	0.0252561805	0.6582015829
H	0.3217439227	0.6250107723	0.0988283648
H	0.6783104064	0.3748094984	0.9011397449
H	0.6781592076	0.1253054471	0.4010142711
H	0.3214727478	0.8747278796	0.5990570060
H	0.5442913298	0.7183127441	0.1912189749
H	0.4558238589	0.2815120821	0.8086853276
H	0.4555392217	0.2185200582	0.3086973467
H	0.5440177649	0.7814347219	0.6913270473
H	0.7406971016	0.8163949946	0.3114149147
H	0.2593498648	0.1835544466	0.6884694362
H	0.2586491949	0.3163845356	0.1886010687
H	0.7416303253	0.6837262755	0.8112715491
H	0.1077899813	0.8118544588	0.5137420850
H	0.8922652919	0.1881950883	0.4860652504

H	0.8921005155	0.3119309341	0.9859921841
H	0.1082534849	0.6882637672	0.0137049320
H	0.9441668641	0.8841123675	0.5214106755
H	0.0559163929	0.1158842559	0.4785402998
H	0.0558709107	0.3842251128	0.9784774517
H	0.9446413486	0.6161293864	0.0217052215
H	0.0175916576	0.8926802893	0.4294923196
H	0.9822339378	0.1073814928	0.5703739030
H	0.9821245473	0.3927561524	0.0702814074
H	0.0176708692	0.6072403953	0.9296731141
H	0.3193072522	0.2439193901	0.4293521475
H	0.6806205797	0.7560910501	0.5706949829
H	0.6808049489	0.7444457206	0.0706423302
H	0.3192836374	0.2555742395	0.9293861989
H	0.3739148622	0.0772374457	0.4918205620
H	0.6261077672	0.9227802939	0.5082281346
H	0.6263232705	0.5777044081	0.0083147879
H	0.3738618585	0.4223404331	0.9916803545
H	0.6089628056	0.0482102032	0.6139033224
H	0.3911862772	0.9518193508	0.3860675258
H	0.3911599708	0.5483874543	0.8863247514
H	0.6090130603	0.4516237273	0.1136712003
H	0.7965102948	0.1837804335	0.6657524995
H	0.2036671890	0.8162573080	0.3341419596
H	0.2034402862	0.6837935554	0.8344214114
H	0.7966056611	0.3161770332	0.1656408206
H	0.1934929506	0.5251229458	0.7396397745
H	0.8064903405	0.4749695492	0.2603358028
H	0.8064590019	0.0249604793	0.7602631195
H	0.1937035992	0.9751338452	0.2397178118
H	0.1745548171	0.4108164713	0.7908699262
H	0.8255204723	0.5892274028	0.2090367045
H	0.8257505454	0.9108362627	0.7088837609
H	0.1740741019	0.0891069428	0.2912588394
H	0.0669585958	0.5157699910	0.8084709682
H	0.9330845244	0.4842145158	0.1915285758
H	0.9332799621	0.0160081867	0.6915683760
H	0.0668176458	0.9837204115	0.3083933340
C	0.3908534225	0.4891835097	0.2801364260
C	0.6091483617	0.5107752984	0.7199047688
C	0.6083606466	0.9892252720	0.2198354901
C	0.3915263688	0.0108026294	0.7802468071
C	0.3190040928	0.5173351712	0.1966551186
C	0.6810275017	0.4825654776	0.8033676085

C	0.6804966743	0.0174884866	0.3032524103
C	0.3192983879	0.9825539308	0.6968361988
C	0.3739964490	0.6008125947	0.1639465247
C	0.6260772456	0.3990325708	0.8360249583
C	0.6256891223	0.1010147954	0.3359438776
C	0.3740105119	0.8990109424	0.6641218812
C	0.4986029852	0.6532203305	0.2152194606
C	0.5014942248	0.3466374562	0.7847196454
C	0.5010298115	0.1533709474	0.2847146210
C	0.4986521931	0.8466176862	0.7153275142
C	0.5657809996	0.6205935072	0.2983609594
C	0.4342530826	0.3793462465	0.7016042163
C	0.4335805547	0.1206493170	0.2016265355
C	0.5662099013	0.8793427061	0.7984025582
C	0.6983990812	0.6674839972	0.3572196156
C	0.3016050221	0.3325016995	0.6427349281
C	0.3010259606	0.1675319089	0.1427607511
C	0.6987389520	0.8324278879	0.8572511362
C	0.7704180867	0.7593860417	0.3590190268
C	0.2295673935	0.2406022740	0.6409057252
C	0.2290438649	0.2594235230	0.1409445799
C	0.7710167856	0.7406360394	0.8589848936
C	0.8863282944	0.7615109306	0.4360241085
C	0.1136431710	0.2385127669	0.5639005723
C	0.1133641917	0.2615930094	0.0638551311
C	0.8866840584	0.7385001859	0.9360889212
C	0.9945000906	0.8418965564	0.4771118581
C	0.0054837727	0.1581373501	0.5227761728
C	0.0053508883	0.3419825248	0.0227056411
C	0.9948435258	0.6581794443	0.9772373504
C	0.5240161700	0.3102207893	0.5117771161
C	0.4759530492	0.6898153212	0.4882167332
C	0.4759979298	0.8105776948	0.9882136566
C	0.5240417631	0.1894340911	0.0118400421
C	0.4242920935	0.2300468519	0.4808548999
C	0.5756739721	0.7699770869	0.5191723922
C	0.5758173054	0.7304810362	0.0191581700
C	0.4242848361	0.2695378043	0.9808599069
C	0.4551817810	0.1372928015	0.5163980719
C	0.5448334425	0.8627355376	0.4836275016
C	0.5449815908	0.6376792333	0.9836982847
C	0.4551669660	0.3623503213	0.0163039477
C	0.5878456333	0.1203165265	0.5843203228
C	0.4122419290	0.8797195108	0.4156670100

C	0.4122464585	0.6205367112	0.9158378894
C	0.5878817229	0.3794704205	0.0841709065
C	0.6915017101	0.1969937143	0.6137516036
C	0.3085901417	0.8030502041	0.3861970831
C	0.3084926645	0.6971063205	0.8863808271
C	0.6915782452	0.3028709745	0.1136651968
C	0.6639143008	0.2912042660	0.5774776097
C	0.3361104113	0.7088439687	0.4224834531
C	0.3360509132	0.7913727166	0.9225641526
C	0.6639787317	0.2086055729	0.0774987276
C	0.7776792493	0.3683198468	0.6077017939
C	0.2223122881	0.6317499533	0.3922458597
C	0.2222057134	0.8683698174	0.8923076242
C	0.7777475904	0.1315585966	0.1077862906
C	0.9799234941	0.4489001340	0.6874175691
C	0.0200707598	0.5511788001	0.3125366545
C	0.0200598129	0.9489015849	0.8125406071
C	0.9798991361	0.0510220042	0.1875286769
C	0.1121528317	0.4764213469	0.7607679797
C	0.8878626815	0.5236277373	0.2391886791
C	0.8879805228	0.9764462445	0.7391377196
C	0.1120426627	0.0234871581	0.2609016466

## BS3

bfgs converged in 154 scf cycles and 148 bfgs steps

(criteria: energy < 1.0E-04 Ry, force < 1.0E-05Ry/Bohr, cell < 5.0E-01kbar)

End of BFGS Geometry Optimization

Final enthalpy = -4090.8505393184 Ry

Begin final coordinates

new unit-cell volume = 12747.65955 a.u.^3 ( 1889.00823 Ang^3 )

density = 1.83196 g/cm^3

CELL\_PARAMETERS (angstrom)

8.812622629	0.002061708	0.037306259
0.003066045	13.644959483	0.000778059
-4.338938714	-0.000182728	15.690918198

ATOMIC\_POSITIONS (crystal)

Co1	0.6415864439	0.5022047177	0.4558108070
Co2	0.3584441498	0.4977618218	0.5441769432
Co1	0.3593114907	0.0025833474	0.0439005323
Co1	0.6406826591	0.9974319982	0.9560958834

Co1	0.9942613473	0.6353765203	0.5933914673
Co2	0.0057693752	0.3646002130	0.4066141175
Co1	0.0052835935	0.1353062844	0.9069445545
Co1	0.9947345192	0.8647248459	0.0930622427
Cl	0.9152637547	0.7192380919	0.6935629478
Cl	0.0847247697	0.2807725220	0.3064089590
Cl	0.0849011285	0.2192847584	0.8068037527
Cl	0.9151329397	0.7806541890	0.1931530548
Cl	0.2576714930	0.6432505556	0.6231153422
Cl	0.7423436654	0.3567373404	0.3769032849
Cl	0.7416928752	0.1440605018	0.8760688791
Cl	0.2583218771	0.8559596292	0.1239390459
O	0.4830909679	0.4004113063	0.4812807885
O	0.5169145513	0.5995663735	0.5187090264
O	0.5167632575	0.9000013836	0.0189775305
O	0.4832256875	0.1000133638	0.9810204572
N	0.5119546804	0.5396677756	0.3300939605
N	0.4880610498	0.4603101370	0.6699045008
N	0.4889339754	0.0397803184	0.1698108335
N	0.5110578079	0.9602333080	0.8301910266
N	0.7694270697	0.6171288429	0.4288269263
N	0.2305853173	0.3828532631	0.5711802308
N	0.2309130887	0.1171183829	0.0712657922
N	0.7690781095	0.8828993061	0.9287403334
N	0.8840790284	0.6743219967	0.4770706290
N	0.1159267874	0.3256590450	0.5229348089
N	0.1160465689	0.1743340334	0.0230933134
N	0.8839446972	0.8256901567	0.9769106311
N	0.7921736900	0.4523959213	0.5683480479
N	0.2078413117	0.5475863811	0.4316542579
N	0.2078214199	0.9523695785	0.9317582470
N	0.7921586889	0.0476433131	0.0682464888
N	0.9198259707	0.5018937899	0.6178981704
N	0.0801791694	0.4980888878	0.3821117932
N	0.0800728977	0.0019085264	0.8822052761
N	0.9199071454	0.9981045704	0.1178041087
N	0.8932992742	0.3660674767	0.6825098551
N	0.1066802768	0.6339195789	0.3175009041
N	0.1065201368	0.8660057775	0.8176765297
N	0.8934746682	0.1340194998	0.1823193477
H	0.9238470992	0.3093278475	0.7262534877
H	0.0761293511	0.6906570995	0.2737517489
H	0.0759443088	0.8092560349	0.7739612971
H	0.9240667758	0.1907750041	0.2260306680

H	0.3528510971	0.4254828730	0.3095553325
H	0.6471434091	0.5745058231	0.6904406564
H	0.6480748112	0.9255043175	0.1903860791
H	0.3519049338	0.0745037355	0.8096148522
H	0.2228837028	0.4749708402	0.1579651787
H	0.7770832687	0.5250455693	0.8420429259
H	0.7776264845	0.9747436968	0.3420527806
H	0.2223470104	0.0252546940	0.6579528298
H	0.3226637607	0.6255279364	0.0989968399
H	0.6773376921	0.3744755502	0.9010119255
H	0.6776553968	0.1252435522	0.4010762763
H	0.3223395410	0.8747641936	0.5989271453
H	0.5451227579	0.7186833064	0.1913803389
H	0.4549090365	0.2812964559	0.8086222062
H	0.4552296611	0.2185610219	0.3086609649
H	0.5447808740	0.7814567702	0.6913397385
H	0.7418192453	0.8164559195	0.3114139220
H	0.2582320406	0.1835124837	0.6885811437
H	0.2590457396	0.3166181220	0.1884947526
H	0.7409875138	0.6834094481	0.8115015998
H	0.1079413430	0.8120205981	0.5140783554
H	0.8920835886	0.1879583228	0.4859194451
H	0.8923409567	0.3121503487	0.9859861515
H	0.1076761996	0.6878788451	0.0140094573
H	0.9440107616	0.8842679180	0.5215313852
H	0.0560164863	0.1157102675	0.4784743237
H	0.0562158853	0.3844024512	0.9786332934
H	0.9438087079	0.6156233674	0.0213677842
H	0.0180463260	0.8928675237	0.4298175022
H	0.9819644720	0.1071112470	0.5701821579
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H	0.0179428314	0.6071080725	0.9296791674
H	0.3193547865	0.2443008138	0.4295182584
H	0.6806475243	0.7556860549	0.5704759738
H	0.6805408666	0.7438337268	0.0705216788
H	0.3194422865	0.2561776460	0.9294720431
H	0.3740737774	0.0775340719	0.4918358348
H	0.6259230307	0.9224498279	0.5081550864
H	0.6258700466	0.5771603848	0.0080298850
H	0.3741183223	0.4228568814	0.9919547822
H	0.6091716761	0.0483556856	0.6137861794
H	0.3908154207	0.9516252116	0.3862064421
H	0.3908301118	0.5482372660	0.8860270023
H	0.6091659087	0.4517869982	0.1139514092



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H	0.2034466918	0.8160575697	0.3343106672
H	0.2034002959	0.6839086103	0.8342714275
H	0.7965954678	0.3161162558	0.1657104397
H	0.1931214845	0.5252655513	0.7396667539
H	0.8068804262	0.4747023538	0.2603532887
H	0.8068147692	0.0254995260	0.7604572701
H	0.1931667872	0.9745157508	0.2395519229
H	0.1737112987	0.4112657946	0.7912286786
H	0.8262533392	0.5887094945	0.2087940879
H	0.8258737988	0.9112916457	0.7090850765
H	0.1741127744	0.0887248966	0.2909225901
H	0.0660881822	0.5165501188	0.8083037454
H	0.9338986958	0.4834403480	0.1917105744
H	0.9336507254	0.0163095557	0.6917391446
H	0.0663247144	0.9837111061	0.3082662775
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C	0.6080419983	0.5106766634	0.7199572279
C	0.6088561467	0.9893209519	0.2198948879
C	0.3911288048	0.0106876235	0.7801065328
C	0.3200155784	0.5176304985	0.1966602115
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C	0.6805897357	0.0175077632	0.3033315943
C	0.3193932686	0.9824975389	0.6966725372
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C	0.6250546071	0.3988111321	0.8359679528
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C	0.3007675954	0.3323823250	0.6427701498
C	0.3013473482	0.1676596001	0.1427541721
C	0.6986465530	0.8323557447	0.8572494288
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C	0.3084612193	0.8028070421	0.3862618007
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C	0.3360228885	0.7912737304	0.9225235961
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C	0.9797094630	0.0508496735	0.1873551489
C	0.1115190191	0.4768312225	0.7608520183
C	0.8884647132	0.5231483799	0.2391663993
C	0.8882428591	0.9768378069	0.7393129483
C	0.1117389247	0.0231805185	0.2606934837

