

Supplementary Data file 1: Structure Coordinates for the lattice and relaxed ion positions BHP system, all coordinates are in Angstrom.

Lattice:

70.529399999999954	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.2373600000000007	0.0000000000000000
-2.6403143518737733	0.0000000000000000	7.7315366989292231

Ion Positions:

Br	3.3487468513	6.7543507026	5.9708021379
Br	5.3805919854	1.4970148019	3.4935042114
Br	4.0637270781	2.5515450813	7.3591806632
Br	4.7043162851	5.5256809189	2.1072441299
Br	7.2442919250	4.7201147853	5.3979571405
Br	1.4447056161	3.5379567613	4.0861905517
Br	0.1224996602	0.5287166668	7.9579095361
Br	8.5566939484	7.5439282876	1.5325366082
Br	15.3155965333	6.9698889855	5.2198111456
Br	17.3284698315	1.7136958991	2.7410769726
Br	16.0589982075	2.8767840944	6.6121030213
Br	16.6736204807	5.8424370100	1.3384764344
Br	19.2202804120	4.9870314921	4.6198966565
Br	13.4417221138	3.7266972988	3.3064920499
Br	12.1260904922	0.8564213721	7.1735292647
Br	20.5484303428	7.8796318090	0.7902866997
Br	27.1467334813	6.8340165781	4.6725748754
Br	28.9480785067	1.7607886326	2.0270435517
Br	27.8005306871	2.9236056826	6.3378507164
Br	28.5215418468	6.0489059608	1.2876102507
Br	25.4663423289	3.6300601144	2.5521259886
Br	23.9597156892	0.4136569109	6.5344914360
Br	32.2381803873	7.8552961979	0.8537308153
C	8.8383107110	0.3690871656	5.1939348416
C	-0.1221490075	7.8588704336	4.3163788320

C	-1.4219226438	4.4782198873	8.1848929156
C	10.1833731721	3.6330338015	1.2979090342
C	7.8330706063	0.5493847204	6.3075278170
C	0.8953486192	7.6833750413	3.2102312891
C	-0.4070125353	4.6360543788	7.0738163891
C	9.1991394969	3.4606709531	2.4321229149
C	20.7703163422	0.7537984580	4.4305894395
C	11.8553727134	8.0548305611	3.4986053884
C	10.5530531206	4.7792559583	7.3854131477
C	22.2032778325	4.0337829930	0.5029373301
C	19.7685764903	0.8762902113	5.5545726645
C	12.8781827059	7.8762022173	2.4007960292
C	11.5661751161	4.9573754736	6.2779442373
C	21.2449331853	3.8405700543	1.6574279485
C	31.5656374021	0.9702892299	5.1400687578
C	23.7104149409	7.7349557760	2.9106374502
C	22.7241936916	4.6720086202	5.9242692146
C	30.3541216228	0.0901121389	4.9183568254
C	24.6849559830	7.5896494962	1.7662072425
C	24.2184904315	4.4782333328	6.0733066908
C	35.7229411542	4.1632435271	3.2777604265
C	36.1076430968	5.2386110886	4.2261359468
C	36.4756513648	3.8894691640	2.0849509977
C	37.4140631700	5.3035013903	4.8265529335
C	34.5972654260	3.3816161608	3.5146947289
C	35.1815180778	6.2016593151	4.6108695979
C	36.1263124448	2.7534022303	1.2742223381
C	37.7537139809	6.4163761053	5.6717635869
C	34.2271220034	2.2908478848	2.7050962724
C	35.5071464994	7.2976101863	5.4348275224
C	34.9982281376	1.9655867535	1.6173101122
C	36.7815126455	7.4163907862	5.9354293328

C	37.5374240691	4.7246400735	1.6425311130
C	38.3747639845	4.2678702712	4.6714580559
C	36.8885350141	2.4680372897	0.1139684375
C	39.0446218266	6.4735042151	6.2600441117
C	38.2493398795	4.4323948748	0.4946341895
C	39.6113775376	4.3426484207	5.2786053066
C	37.9330604639	3.2844079692	-0.2755261093
C	42.6003421280	5.4616095502	-1.6640518468
H	9.1908489977	7.5635895166	5.1405686937
H	-0.5280803161	0.6462397766	4.3322450481
H	-1.8389519477	3.4581099299	8.2090781348
H	10.5491193667	4.6707411193	1.2417914330
H	9.7149488737	1.0078687177	5.3764173104
H	-0.9572958798	7.1557654292	4.1747913509
H	-2.2498727136	5.1894950932	8.0418352618
H	11.0570959241	2.9841169717	1.4578902218
H	8.4047110212	0.6266378718	4.2136603194
H	0.3220547583	7.6621742146	5.3067510740
H	1.6686545681	4.6764874842	1.4405728970
H	7.0860161218	3.3832700060	8.0580519028
H	8.2296031368	0.2341261258	7.2862621337
H	0.5041645535	7.9652619383	2.2189758442
H	-0.8055771114	4.3542054729	6.0855360641
H	9.6186712240	3.7757165559	3.4013174832
H	7.5003102201	1.5963902617	6.3955080410
H	1.2580352398	6.6439872009	3.1511205024
H	-0.0324138075	5.6708028926	7.0079417688
H	8.8615725939	2.4158129172	2.5287266002
H	6.0362384370	0.1421827263	5.2864276747
H	2.6771635169	8.1524926893	4.2273720423
H	1.3713325460	4.1488216042	8.0889816095
H	7.3904222044	3.8798591060	1.4364081890

H	6.0366337771	7.9016563464	6.9317672046
H	2.6641636675	0.3639034781	2.5737367851
H	1.3511993402	3.7000530668	6.4356181873
H	7.4122475324	4.3509182230	3.0839792155
H	6.8475501613	6.9728061095	5.7928982379
H	1.8338425028	1.2981203119	3.6988295860
H	0.5140472117	2.7745291378	7.5628960112
H	8.2104893985	5.2810852230	1.9373516838
H	21.1909715393	7.9745875187	4.3853304471
H	11.4837452724	0.8545784437	3.5308735649
H	10.1560864956	3.7516549774	7.4000139194
H	22.5354355619	5.0823195036	0.4287734471
H	21.6066822319	1.4486156829	4.5973323853
H	10.9931666806	7.3967353248	3.3158647964
H	9.7034551558	5.4607544035	7.2301441430
H	23.0955905520	3.4059457685	0.6453505259
H	20.3105712707	0.9776352345	3.4539362748
H	12.2800546566	7.8198778177	4.4886113632
H	13.6357714100	4.9847160354	0.6427346212
H	19.0946673060	3.7658885733	7.2731606828
H	20.1949185037	0.5827118688	6.5274201442
H	12.4910496252	8.1724872742	1.4122818511
H	11.1646511668	4.6748240939	5.2910723508
H	21.6680897803	4.1796634716	2.6170468178
H	19.3759580706	1.9019305977	5.6475547985
H	13.2276544478	6.8331485060	2.3309592022
H	11.9280804850	5.9966372450	6.2144610624
H	20.9466769124	2.7852876329	1.7697434901
H	17.9948213746	0.3680016226	4.5426994008
H	14.6589747920	8.3185695007	3.4340117497
H	13.3570294026	4.4912810046	7.2829117235
H	19.4127846522	4.1952477138	0.6746831721

H	18.0255589304	8.1391046381	6.1915248859
H	14.6634190772	0.5489468057	1.7855766510
H	13.3303264944	4.0262994249	5.6329168748
H	19.4321817541	4.6627763273	2.3260344737
H	18.8728562538	7.2438426645	5.0505913305
H	13.8320808932	1.4734326699	2.9128230157
H	12.5063128920	3.1097868081	6.7732366620
H	20.1896530981	5.6235152349	1.1750226049
H	32.4987715884	8.6207486104	5.1853485719
H	23.3575659186	0.5373761208	3.0037015134
H	22.1967621693	3.7212538591	5.7437635346
H	31.4440230013	1.5147721519	6.0888557233
H	22.8266340444	7.1049702998	2.7313105209
H	22.5161261068	5.3394750900	5.0749370107
H	31.6519301844	1.7152767173	4.3330151784
H	24.1653403236	7.4462521090	3.8724285974
H	24.9327115812	5.1428561241	-0.9082172477
H	30.1853069709	-0.5979118584	5.7676538482
H	24.2586091414	7.9154762577	0.8032607473
H	24.6676711160	4.0259028911	5.1685838172
H	29.4522898518	0.7098799530	4.8096096915
H	25.0355737474	6.5506917881	1.6515860741
H	24.7296446928	5.4337282887	6.2681940106
H	31.0176610492	-0.2732923773	2.8861476432
H	26.4782764436	8.0279612454	2.7834719145
H	24.0531025439	3.8456968392	8.1003943286
H	29.5422202937	7.2874983338	3.2717851397
H	26.4829095900	0.2061957284	1.1226122047
H	25.5572220012	3.5476250413	7.3897134887
H	30.9466562668	6.5858067179	3.8475951545
H	25.6769347880	1.1763542554	2.2327363403
H	24.2494512203	2.5690997834	6.9951447808

H	33.3278296389	1.7159108173	2.9350090772
H	34.7277023336	-0.2072805201	5.6588378338
H	34.7009373664	1.1146014236	0.9945831145
H	37.0475132494	0.0304319955	6.5710201348
H	37.7815414329	5.6244456513	2.2113643408
H	38.1190524531	3.3928546663	4.0690368064
H	36.5991270232	1.6060291854	-0.4952261032
H	41.9328380170	-0.9013911590	-0.8434924455
H	39.0496587889	5.1014113838	0.1660250341
H	40.3268326469	3.5245645915	5.1501483094
H	38.5019342548	3.0626341409	-1.1820694973
H	43.5876986079	5.5137715953	-1.1958018923
H	33.6939874545	4.7362694482	6.8539442532
N	6.6087808718	7.9635530848	6.0585325001
N	2.0947312963	0.3073635704	3.4500587729
N	0.7835868002	3.7622143611	7.3126799143
N	7.9742907585	4.2899030859	2.2031768307
N	18.5901104935	8.2231423501	5.3145433091
N	14.0859474883	0.4840211439	2.6548840965
N	12.7675373891	4.0962734723	6.5125281947
N	19.9880252654	4.6236853259	1.4386226356
N	30.4791926554	7.5083416592	3.6740071199
N	25.9063115069	0.1838733834	1.9983819217
N	24.5305432755	3.5674653032	7.2099952202
O	33.8270813819	3.6111445386	4.6613992416
O	33.8585875927	6.1141673897	4.1669142162
O	32.9180023247	5.1448149025	6.3875049934
O	31.6001316545	4.9747946230	4.2092325607
P	32.9384530201	4.9517983762	4.8208076576
Pb	4.3606944146	4.1072667445	4.7576282443
Pb	5.6752898974	-0.0580942575	0.8928132548
Pb	16.3455433906	4.3565196543	3.9630878220

Pb	17.6634026121	0.2462063404	0.1081093238
Pb	28.0524181980	4.1051056921	3.6537975840
Pb	29.6201277194	0.0547469335	-0.4134755863

Lattice and relaxed positions for BP system, all coordinates are in angstrom:

Lattice:

80.529399999999954	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.2373600000000007	0.0000000000000000
-2.6403143518737733	0.0000000000000000	7.7315366989292231

Ion Positions:

Pb	4.3790960785	4.1397236935	4.9396390120
Pb	5.6998325411	-0.0196151674	1.0739693268
Br	3.3842144510	6.7848566805	6.1588204112
Br	5.4028237152	1.5288325435	3.6775567809
Br	4.0811439931	2.5917343483	7.5433432535
Br	4.7036091191	5.5728795550	2.2930859012
Br	7.2711139261	4.7639620989	5.5788371413
Br	1.4763499518	3.5580830629	4.2740560845
Br	0.1569119038	0.5624731391	8.1400697161
Br	8.5921549718	7.5934000297	1.7127487258
C	8.8690740992	0.4290296574	5.3608889940
C	-0.0962363618	7.8553581118	4.4965004963
C	-1.4177560670	4.5020203366	8.3618056174
C	10.1871000054	3.6877833540	1.4945833785
H	9.2408999554	7.6297081043	5.3232218818
H	-0.5147986850	0.6375669114	4.5078274928
H	-1.8359672096	3.4822908661	8.3729782767
H	10.5603016634	4.7239164440	1.4560904253
H	9.7357948760	1.0863022270	5.5246977208

H	-0.9232240858	7.1421166880	4.3571634064
H	-2.2449836551	5.2149544954	8.2223727376
H	11.0530401712	3.0294566913	1.6582934235
H	8.4248431200	0.6628016449	4.3794246868
H	0.3502221032	7.6680196633	5.4875724489
H	1.6687602092	4.6894344309	1.6214400749
H	7.1016007465	3.4539492816	8.2451121675
C	7.8677626528	0.6106083967	6.4783949941
C	0.9240233291	7.6873422500	3.3916479587
C	-0.3973826842	4.6704528213	7.2571283411
C	9.1862389614	3.5082043654	2.6128149422
H	8.2729239369	0.3084528255	7.4578430105
H	0.5303116803	7.9633564358	2.3998736999
H	-0.7908605698	4.3944262529	6.2652759303
H	9.5924058749	3.8105182361	3.5918137645
H	7.5255442715	1.6554162528	6.5579013470
H	1.2961252491	6.6512575363	3.3349701741
H	-0.0256093497	5.7066902348	7.2006156502
H	8.8427215686	2.4639255148	2.6932321510
N	6.6494459185	8.0115033334	6.2429222595
N	2.1163787873	0.3221574856	3.6302489802
N	0.7952548567	3.7986886430	7.4957946752
N	7.9688757708	4.3460906991	2.3774285665
H	6.0675615368	0.1819515343	5.4733426539
H	2.7034700561	8.1719967627	4.4062675617
H	1.3822146796	4.1863826050	8.2718263165
H	7.3864297504	3.9387774441	1.6079906172
H	6.0844191129	7.9481501159	7.1213829364
H	2.6842827329	0.3850866731	2.7531307158
H	1.3631943157	3.7358606080	6.6187229969
H	7.4039956489	4.4101051782	3.2559585406
H	6.8933771137	7.0215001975	5.9789677973

H	1.8488893697	1.3099153039	3.8819746495
H	0.5281171881	2.8108225136	7.7475895645
H	8.2138026758	5.3357401191	2.1132745441
Pb	16.3742790991	4.1213747689	4.1164160937
Pb	17.6982522006	0.0024407736	0.2515331271
Br	15.3600160404	6.7452410123	5.3591281162
Br	17.3848961163	1.4960831145	2.8759551678
Br	16.0673833085	2.6286697847	6.7417556711
Br	16.6785402367	5.6179568748	1.4932273400
Br	19.2660042839	4.7413686600	4.7737996585
Br	13.4823168297	3.4989694595	3.4615484357
Br	12.1671652282	0.6237685204	7.3265298290
Br	20.5924861913	7.6190654256	0.9095278270
C	20.8478746224	0.4357701193	4.5521692158
C	11.8931736528	7.8162047355	3.6725220092
C	10.5711445098	4.5395720286	7.5392094669
C	22.1735172289	3.6903093056	0.7000734750
H	21.2316992025	7.6413021121	4.5034637877
H	11.5084674933	0.6110423319	3.7038157696
H	10.1885282971	3.5065561509	7.5695126927
H	22.5656799107	4.7197091720	0.6725854999
H	21.7071410225	1.1017093341	4.7199658192
H	11.0351705756	7.1478394657	3.5076452911
H	9.7117956366	5.2062619188	7.3745824824
H	23.0261179175	3.0151127370	0.8652985228
H	20.3980719758	0.6741432600	3.5743701291
H	12.3355836886	7.5914039186	4.6569608937
H	13.6529499652	4.7643966751	0.7925312271
H	19.0921448013	3.4708310334	7.4452572527
C	19.8483308619	0.5954693993	5.6742326264
C	12.9016594941	7.6418916386	2.5605684922
C	11.5796469467	4.7168205411	6.4277630854

C	21.1610216225	3.5201774904	1.8090927692
H	20.2596135244	0.2897335538	6.6500171974
H	12.4986128539	7.9355784321	1.5776852191
H	11.1776180343	4.4229156320	5.4445298358
H	21.5628564530	3.8108154876	2.7934109620
H	19.4940732096	1.6354193578	5.7640781964
H	13.2558026220	6.6006347355	2.4865434409
H	11.9316527524	5.7588811567	6.3545832553
H	20.8013042708	2.4806929708	1.8808766620
N	18.6390291170	7.9842303332	5.4352883116
N	14.1096351599	0.2552994046	2.7985898440
N	12.7893185256	3.8683978006	6.6656247231
N	19.9579738273	4.3772926370	1.5685522164
H	18.0549299580	0.1496631610	4.6647396777
H	14.6925694373	8.0932890120	3.5718486053
H	13.3716878986	4.2689340982	7.4387146079
H	19.3747860684	3.9804099976	0.7941906795
H	18.0742343521	7.9164577333	6.3136695918
H	14.6767337665	0.3202898817	1.9215421830
H	13.3561087282	3.8043081285	5.7883502372
H	19.3896604192	4.4449776531	2.4445692206
H	18.8919871123	6.9964192107	5.1716208452
H	13.8555918927	1.2438190043	3.0584665626
H	12.5371183304	2.8793731153	6.9254671782
H	20.2172023545	5.3647772279	1.3095136288
Pb	28.3596575134	4.1687469173	3.3486404570
Pb	29.6730762418	0.0591791649	-0.5382929962
Br	27.3890255014	6.8130950851	4.5694883919
Br	29.4109530997	1.5543055700	2.0955701248
Br	28.0481526686	2.6924091764	5.9789627277
Br	28.6508084052	5.6718002636	0.7206697037
Br	31.2513337233	4.8049920067	4.0266975999

Br	25.4715077974	3.5401371068	2.6923776519
Br	24.1289402541	0.6726704516	6.5398041787
Br	32.5513854800	7.6995644285	0.1094807189
C	32.9568842336	0.3986350006	3.8192488596
C	23.8965483820	7.8269539804	2.8967672807
C	22.5455643042	4.5758422634	6.7666502924
C	34.1539455961	3.7898792659	-0.0459432963
H	33.3178193539	7.5951848875	3.8432505040
H	23.4970035142	0.6159130006	2.9323128444
H	22.1625917399	3.5429487210	6.7926751876
H	34.4810183219	4.8348658235	-0.1758838577
H	33.8262097299	1.0556074540	3.9736746312
H	23.0477368311	7.1464290977	2.7337542650
H	21.6866124608	5.2438120693	6.6055177105
H	35.0449053431	3.1825423820	0.1726159018
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H	37.5393879356	3.4802217109	4.4413413114
H	42.8418002075	4.6100772365	0.4772062221
H	37.9731792275	0.7111664678	1.5487134522
H	36.7648908090	2.4079281553	5.4766235249
H	44.0618461965	4.6279960559	-0.7143002729
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C	46.1967551118	5.1334260082	4.4945417473
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C	47.6866413785	8.6669373017	7.7262679429
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H	43.4740555086	8.6690552650	5.8007570655
H	46.8780892255	1.5487120145	3.0284545397
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H	47.9986184117	6.9863171828	3.6082621746
H	48.4014352350	5.2901106457	5.9349638206
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H	49.8846931629	6.5814697548	2.0660189352
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