Supporting Information

Halogen bonding in mono- and dihydrated halobenzene

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Contents:

Table S1. Cartesian coordinates of the different optimised XPh-H_2O structures in xyz format. The title line provides the system.

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15
FPh-H2O-Hbonded
C   0.17711700   0.79791300  -0.00004400
C  -1.01943000   1.51478700  -0.00020800
C  -2.24690800   0.85221500  -0.00015600
C  -2.28608400  -0.54187800   0.00005700
C  -1.10277700  -1.27900900   0.00022100
C   0.09603300  -0.58510600   0.00016600
H   1.14830400   1.28455400  -0.00008600
H  -0.98694700   2.60003600  -0.00037600
H  -3.17128600   1.42112600  -0.00028400
H  -3.23926300  -1.06172100   0.00009800
H  -1.09781300  -2.36382900   0.00039000
O   3.38037100   0.63202400  -0.00030400
H   4.34044500   0.53069000  -0.00039200
H   3.00852400  -0.26225600  -0.00012100
F   1.24970700  -1.30648000   0.00033100
15
ClPh-H2O-Hbonded
C   1.34670900  -1.16888400   0.00375900
C   2.52900800  -0.43152300   0.00483900
C   2.48890000   0.96190900   0.00094700
C   1.26048500   1.62030800  -0.00400100
C   0.06583800   0.90035700  -0.00512000
C   0.13308700  -0.48884900  -0.00122800
H   1.36182700  -2.25384800   0.00667500
H   3.48200100  -0.95196400   0.00873200
H   3.41248100   1.53251000   0.00176400
H   1.22302400   2.70549700  -0.00703500
H  -0.89490500   1.40752900  -0.00865700
O  -3.17012300   1.42047100   0.00218300
H  -4.10743700   1.65141800   0.03059600
H  -3.12673000   0.45301200   0.00484000
Cl  -1.34902600  -1.42751900  -0.00291400
15
BrPh-H2O-Hbonded
C  -1.47324300  -1.16979900   0.02771900
C  -2.77759600  -0.68001000   0.03095900
C  -3.01680100   0.69260300   0.00309300
C  -1.94152500   1.57806000  -0.02785500
C  -0.62826000   1.10887700  -0.03156500
C  -0.41705700  -0.26520000  -0.00370100
H  -1.27910400  -2.23698100   0.04920000
H  -3.60759500  -1.37993200   0.05523900
H  -4.03494500   1.06915000   0.00556400
H  -2.11727700   2.64946700  -0.04965900
H   0.20886700   1.80053100  -0.05378900
Br   1.35139000  -0.94082300  -0.00948000
O   2.40402300   2.39287800   0.00739800
H   2.60377000   1.44526400   0.03617500
H   3.22233300   2.85110600   0.23799900
15
IPh-H2O-Hbonded
C  -1.63081600  -1.25984500   0.01145100
C  -2.99770500  -0.98319400   0.01143600
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```
C  -3.44862000   0.33564000   0.00054400
C  -2.52930500   1.38290600  -0.01020100
C  -1.15681200   1.12751800  -0.01008800
C  -0.73040900  -0.19757200   0.00060800
H  -1.27739900  -2.28559600   0.01948300
H  -3.70727600  -1.80518300   0.01971400
H  -4.51367600   0.54600600   0.00016300
H  -2.87400700   2.41257700  -0.01915200
H  -0.44493400   1.94795800  -0.01744500
I   1.34155800  -0.63025200  -0.00187300
O   1.55690500   3.03484100  -0.02127700
H   2.01608200   2.18131500  -0.01210100
H   2.20541000   3.69483900   0.25634500
15
AtPh-H2O-Hbonded
C  -1.86692900  -1.31406800   0.06829200
C  -3.25664000  -1.18830500   0.06884000
C  -3.84910900   0.07134700  -0.00092000
C  -3.05020700   1.21101000  -0.07148200
C  -1.65736400   1.10689900  -0.07285400
C  -1.09062900  -0.16149900  -0.00263500
H  -1.40520200  -2.29450200   0.12157000
H  -3.87213200  -2.08137600   0.12361300
H  -4.93081800   0.16391100  -0.00083700
H  -3.50585600   2.19523100  -0.12694900
H  -1.04003100   1.99951300  -0.12496600
At   1.10859400  -0.37432200  -0.00765200
O   0.82776000   3.37836500   0.00081000
H   1.36421400   2.57184900  -0.03736100
H   1.16253800   3.88352500   0.75343600
15
BrPh-H2O-Xbonded
C  -1.36605100  -1.20509600   0.00001900
C  -2.75914200  -1.17876600   0.00003200
C  -3.44456200   0.03462800   0.00003400
C  -2.72536500   1.22824000   0.00002200
C  -1.33200600   1.21517800   0.00000800
C  -0.66064600  -0.00461500   0.00000600
H  -0.82881300  -2.14785000   0.00001700
H  -3.30853500  -2.11568800   0.00004200
H  -4.53000800   0.04987100   0.00004400
H  -3.24816900   2.18028400   0.00002300
H  -0.76873500   2.14260600  -0.00000200
Br   1.22255300  -0.03484700  -0.00001200
O   4.28517300  -0.02985600  -0.00005600
H   4.67005000   0.40607000  -0.77163900
H   4.67008700   0.40579200   0.77166600
15
IPh-H2O-Xbonded
C  -1.71737400  -1.20126300   0.00000400
C  -3.11194300  -1.17710600   0.00001900
C  -3.79620700   0.03720900   0.00002600
C  -3.08038000   1.23319600   0.00001900
C  -1.68561900   1.22079300   0.00000500
C  -1.01111700   0.00069200  -0.00000200
H  -1.18643400  -2.14774400  -0.00000100
H  -3.66172800  -2.11375500   0.00002400
H  -4.88178000   0.05140200   0.00003700
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```
H  -3.60550400   2.18391600   0.00002500
H  -1.13012100   2.15313500   0.00000000
O   4.17572900  -0.00206400   0.00005200
H   4.58707200   0.40793100  -0.77258300
H   4.58692000   0.40767900   0.77290200
I   1.10003000  -0.03032400  -0.00002400
15
AtPh-H2O-Xbonded
C  -2.03331400  -1.19990600  -0.00064600
C  -3.42866400  -1.18324600   0.00234100
C  -4.11887900   0.02764800   0.00631600
C  -3.40885200   1.22704400   0.00735700
C  -2.01339300   1.22072700   0.00453500
C  -1.33253000   0.00472100   0.00050600
H  -1.50046600  -2.14558200  -0.00398700
H  -3.97408700  -2.12261000   0.00143600
H  -5.20458900   0.03655100   0.00854300
H  -3.93880800   2.17523700   0.01042000
H  -1.46504200   2.15753600   0.00549400
O   3.88758400  -0.00091100   0.00813300
H   4.34891500   0.46495700  -0.70219500
H   4.33367300   0.24628800   0.82932800
At   0.87427700  -0.01631800  -0.00395900
```

Table S2. Cartesian coordinates of the different optimised XPh-$(H_2O)_2$ structures in xyz format. The title line provides the system.

```
18
IPh-(H2O)2-type1
C  -1.09833700  -0.23615700   0.00000100
C  -1.87730500  -1.39171700  -0.00000600
C  -3.26723400  -1.27594100   0.00000000
C  -3.86753500  -0.01791700   0.00001200
C  -3.07359500   1.12765000   0.00001800
C  -1.68136000   1.02994400   0.00001300
I   1.01018700  -0.40988300  -0.00000900
O   4.04060700  -0.41718400   0.00002900
H  -1.40947300  -2.37109400  -0.00001600
H  -3.87804100  -2.17404200  -0.00000500
H  -4.94986900   0.06878800   0.00001600
H  -3.53445400   2.11109600   0.00002700
H  -1.06765700   1.92652800   0.00001700
H   4.45575000  -0.82597800  -0.77179600
H   4.45565600  -0.82593500   0.77192700
O   0.80946400   3.17953900  -0.00002000
H   1.42552700   3.92382700   0.00004200
H   1.35426600   2.37659500  -0.00003400
18
AtPh-(H2O)2-type1
C  -1.36654800  -0.20078600  -0.00000300
C  -2.08230100  -1.39596200   0.00001800
C  -3.47704700  -1.35629100   0.00000300
C  -4.14454000  -0.13265600  -0.00003300
C  -3.41363100   1.05396500  -0.00005300
C  -2.01741000   1.03113500  -0.00003700
At   0.84286400  -0.27325600   0.00001700
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```
O   3.83351400  -0.28415000  -0.00008100
H  -1.56498500  -2.35036500   0.00004600
H  -4.03847100  -2.28620500   0.00001900
H  -5.23004800  -0.10459900  -0.00004600
H  -3.92690100   2.01122300  -0.00008100
H  -1.45704300   1.96196400  -0.00005100
H   4.27133900  -0.66770700  -0.77249800
H   4.27155500  -0.66794900   0.77209400
O   0.32092200   3.35978100   0.00001700
H   0.89256200   4.13873300   0.00016300
H   0.91195800   2.59017100   0.00004500
18
BrPh-(H2O)2-type2
C   0.77346200  -0.34861900  -0.00000200
C   2.14705300  -0.56476800   0.00000700
C   2.99915000   0.53843300   0.00000900
C   2.48156700   1.83371900   0.00000200
C   1.10194500   2.02859500  -0.00000700
C   0.24090700   0.93339900  -0.00000900
Br  -0.39734600  -1.84146400  -0.00000400
O  -3.21405100   0.35918600   0.00001300
H   2.54457700  -1.57439500   0.00001200
H   4.07332400   0.37869100   0.00001600
H   3.15389400   2.68626500   0.00000400
H   0.66600300   3.02284100  -0.00001100
H  -0.82921000   1.09735200  -0.00001700
H  -2.92713200  -0.15358200   0.76942200
H  -2.92712600  -0.15360400  -0.76937900
O  -2.14385900   2.97940200   0.00000300
H  -2.74585200   3.73416700  -0.00005600
H  -2.70259000   2.18026200   0.00000500
18
IPh-(H2O)2-type2
C   0.32313400  -0.83649800  -0.00000400
C   0.61910600  -2.19672500   0.00003200
C   1.95850500  -2.58718600   0.00005600
C   2.97512000  -1.63196100   0.00004600
C   2.65511100  -0.27563600   0.00001000
C   1.32135100   0.13048200  -0.00001600
I  -1.70334400  -0.21818500  -0.00003500
O  -0.32527300   3.22406300   0.00008700
H  -0.17227900  -2.93875300   0.00004100
H   2.20235400  -3.64547600   0.00008400
H   4.01406900  -1.94702400   0.00006600
H   3.42199200   0.49282500   0.00000300
H   1.09020600   1.18804500  -0.00004500
H  -0.71728700   2.77973800   0.76690500
H  -0.71734300   2.77975900  -0.76671500
O   2.50533300   3.03600300   0.00001200
H   3.03075100   3.84602600  -0.00004200
H   1.57032200   3.31324900   0.00004100
18
AtPh-(H2O)2-type2
C   0.69536900  -0.84823600   0.00006300
C   0.90681400  -2.22306300   0.00024100
C   2.22102200  -2.69355600   0.00040000
C   3.29301000  -1.80097300   0.00038200
C   3.05534600  -0.42787900   0.00020500
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C   1.74760100   0.05807700   0.00004500
At  -1.37830600  -0.07932700  -0.00019300
O   0.32511300   3.27420800   0.00057900
H   0.07370800  -2.91812000   0.00025700
H   2.40095000  -3.76466900   0.00053900
H   4.31123200  -2.17784900   0.00050600
H   3.86691900   0.29338400   0.00019200
H   1.58230100   1.12805100  -0.00008900
H  -0.09647700   2.85809300   0.76762500
H  -0.09678900   2.85812400  -0.76631400
O   3.13329000   2.87726400   0.00008500
H   3.71251600   3.64971900   0.00008400
H   2.21946300   3.21802200   0.00025900
18
FPh-(H2O)2-type3
C   1.10776300   0.84606800  -0.16473500
C   1.85845000  -0.14621400   0.45253300
C   1.50212500  -1.47676400   0.23158000
C   0.41575900  -1.78932500  -0.59041200
C  -0.32283400  -0.76620100  -1.18820500
C   0.01922100   0.56931300  -0.97715800
F   1.44420500   2.13377100   0.05674100
O  -1.46227500  -0.31515000   1.84894700
H   2.69825900   0.12851500   1.08222500
H   2.07742800  -2.26894900   0.70134000
H   0.14342300  -2.82657300  -0.75893400
H  -1.19455500  -0.99199000  -1.79318300
H  -0.57011900   1.37569200  -1.39954200
H  -0.93726600   0.44076600   2.14777000
H  -0.82711800  -0.90795200   1.41401400
O  -2.96508700   0.51095900  -0.43095300
H  -3.90417100   0.62568900  -0.23787600
H  -2.54773800   0.23313100   0.40795200
18
ClPh-(H2O)2-type3
C  -1.05307400   0.00295100  -0.24465100
C  -1.26624500   1.18956900   0.45517300
C  -0.31437600   2.20469000   0.36489100
C   0.83098800   2.03022000  -0.41562200
C   1.02568100   0.83466900  -1.10674500
C   0.08170900  -0.18898800  -1.02607000
Cl  -2.22196600  -1.28665200  -0.10037700
O   1.43772300  -0.56299700   1.89209500
H  -2.15954800   1.31016900   1.05955000
H  -0.47118500   3.13246200   0.90711600
H   1.57137400   2.82179400  -0.47805000
H   1.92932600   0.66621700  -1.68279200
H   0.25415200  -1.13478600  -1.52834300
H   0.58830500  -1.02604400   1.93754300
H   1.21569700   0.33226500   1.58780800
O   2.71200700  -1.58737400  -0.44545000
H   3.44982500  -2.17888000  -0.25025400
H   2.36954000  -1.28581200   0.41881300
18
BrPh-(H2O)2-type3
C   0.09436700   0.66180200  -0.16424300
C   0.69654600   1.67545200   0.57461700
C   2.08864400   1.73567500   0.61927800
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C   2.85735300   0.78662300  -0.05399700
C   2.23079500  -0.21802200  -0.78952500
C   0.83995500  -0.28165900  -0.86130600
Br  -1.79774500   0.59190900  -0.25850100
O  -0.44078900  -1.85504300   1.78277300
H   0.08900600   2.40714000   1.09705300
H   2.56904800   2.52533500   1.18926100
H   3.94095200   0.83228700  -0.00639200
H   2.81489800  -0.97276200  -1.30663300
H   0.35590300  -1.07987100  -1.41424100
H  -1.13783800  -1.31955600   1.37079700
H   0.27682700  -1.23006700   1.96488100
O   0.51434800  -3.25869200  -0.49434200
H   0.38591700  -4.21518600  -0.46484900
H   0.19192100  -2.91349600   0.36127300
18
IPh-(H2O)2-type3
C   0.03712500   0.60454300  -0.23378500
C   0.37354000   1.76199700   0.46868700
C   1.67977400   2.24565400   0.38526300
C   2.63081000   1.57888500  -0.39056000
C   2.27497000   0.42486100  -1.08717200
C   0.97152300  -0.06998000  -1.01472700
I  -1.91273100  -0.18209900  -0.04293700
O   1.87317000  -1.10441100   1.89430300
H  -0.36553100   2.27436900   1.07582000
H   1.95096800   3.14436400   0.93133900
H   3.64766600   1.95526900  -0.44453200
H   3.01089200  -0.12889800  -1.66052200
H   0.71859100  -0.99364400  -1.52375500
H   0.90444300  -1.13365800   1.87850800
H   2.09499600  -0.19971700   1.61850100
O   2.64507100  -2.52276900  -0.45700400
H   3.01630500  -3.39624000  -0.27909700
H   2.44402600  -2.12891300   0.41476500
18
AtPh-(H2O)2-type3
C   0.53164500   0.64440400  -0.23319500
C   0.91440700   1.78881300   0.46489000
C   2.23925500   2.22018000   0.37608500
C   3.16028300   1.51391900  -0.40092500
C   2.75664200   0.37296100  -1.09303800
C   1.43414800  -0.06966600  -1.01480700
At  -1.53384800  -0.09637500  -0.02460700
O   2.32033100  -1.12193100   1.89409000
H   0.19977000   2.33336100   1.07331900
H   2.54792200   3.10894100   0.91870700
H   4.19113100   1.84947100  -0.45951700
H   3.46814500  -0.21078600  -1.66763900
H   1.14526100  -0.98453700  -1.52074800
H   1.35121800  -1.10516900   1.88389700
H   2.58243700  -0.23229600   1.60470000
O   2.99418900  -2.59407700  -0.45403000
H   3.33429000  -3.47929200  -0.27201800
H   2.82249900  -2.18342200   0.41631700
18
FPh-(H2O)2-dimer
C  -0.50887100  -0.68167600  -0.24323500
```

C	-1.77886600	-1.21421600	-0.09660300
C	-2.82854100	-0.33471100	0.16452300
C	-2.58735300	1.03492700	0.27228800
C	-1.29256600	1.52938300	0.11682600
C	-0.22482800	0.66965100	-0.14561200
F	0.51663100	-1.54805100	-0.49515100
O	2.87842600	1.66055700	-0.24820400
H	-1.93030700	-2.28458000	-0.18788300
H	-3.83503700	-0.72409500	0.28331300
H	-3.40809100	1.71552800	0.47590300
H	-1.10141300	2.59491900	0.19909300
H	0.79012400	1.04047800	-0.27608000
H	3.16815700	0.77597400	0.04846200
H	3.51377600	1.94611600	-0.91638700
O	3.13265000	-0.99490700	0.58125500
H	3.09176400	-1.13950000	1.53584900
H	2.29889600	-1.33773500	0.22055900