

# Supplementary Material

## Halogen bonding with the halogenabenzene bird Structure, halobenzene and halocyclopentadiene

Emma L. Cates and Tanja van Mourik

School of Chemistry, University of St Andrews, North Haugh, St Andrews KY16 9ST (UK)

### Contents

Section S1. Calculation of counterpoise-corrected interaction energies

Section S2. Supplementary figures

Section S3. Cartesian coordinates of optimised structures

## Section S1. Calculation of counterpoise-corrected interaction energies

The counterpoise (CP)-corrected interaction energy  $\Delta E^{CP}$  follows from:

$$\Delta E^{CP} = E_{AB}^{\{AB\}}(AB) - E_A^{\{AB\}}(AB) - E_B^{\{AB\}}(AB) - E_A^{def} - E_B^{def} \quad (1)$$

where the subscripts indicate the system (dimer AB or monomer A or B); the superscripts in curly brackets indicate the basis set used for the calculation (the dimer basis set {AB} or the monomer basis sets {A} or {B}); and the letters in round brackets indicate the geometry used for the calculation (the dimer geometry AB or the optimised monomer geometries A or B). The deformation energy  $E_A^{def}$  follows from:

$$E_A^{def} = E_A^{\{A\}}(AB) - E_A^{\{A\}}(A) \quad (2)$$

with a similar expression for  $E_B^{def}$ .

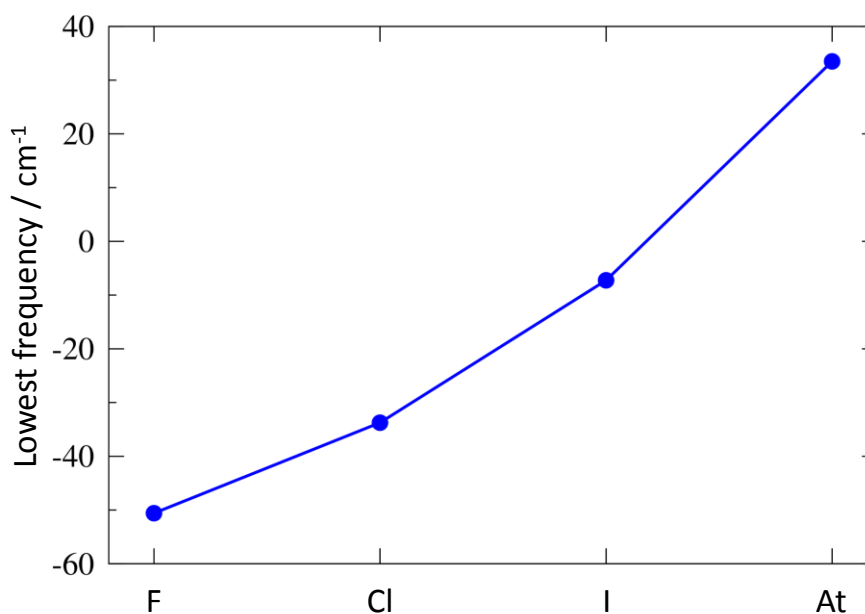
The BSSE (basis set superposition error) is defined as:

$$BSSE = E_A^{\{AB\}}(AB) + E_B^{\{AB\}}(AB) - E_A^{\{A\}}(AB) - E_B^{\{B\}}(AB) \quad (3)$$

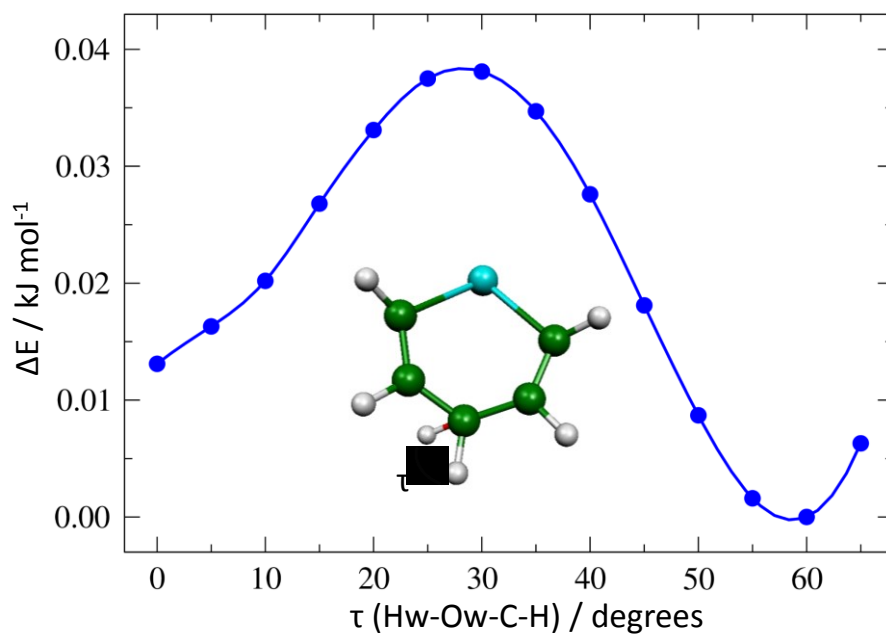
For single-point CP-corrected interaction energies, the “vertical” CP-corrected energy  $\Delta E^{CP}(vert)$  (*i.e.* excluding deformation energies) was calculated:

$$\Delta E^{CP}(vert) = E_{AB}^{\{AB\}}(AB) - E_A^{\{AB\}}(AB) - E_B^{\{AB\}}(AB) \quad (4)$$

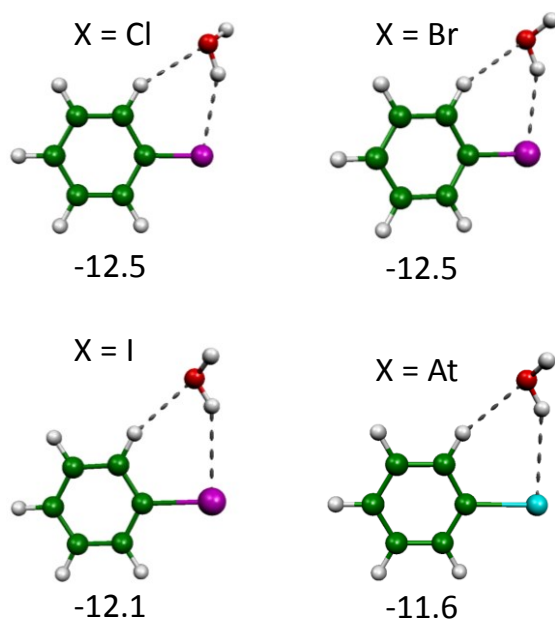
## Section S2. Supplementary figures



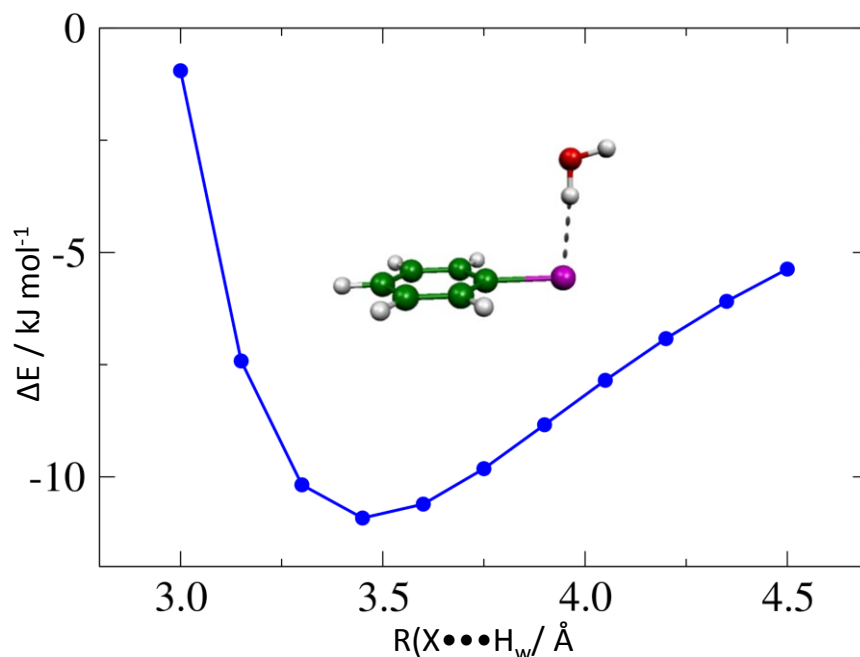
**Figure S2.1** Values of the lowest vibrational frequency in the Xbird-H<sub>2</sub>O (below) structures.



**Figure S2.2** Relaxed rotational energy profile for varying the torsion angle  $\tau$  in the Atbird-H<sub>2</sub>O (below) structure. The inset shows the definition of  $\tau$ . Energies  $\Delta E$  are relative to the lowest energy (for  $\tau = 60^\circ$ ). Energies are not counterpoise-corrected.



**Figure 2.3** Optimised structures of the H-bonded halobenzene...H<sub>2</sub>O and halobenzene...NH<sub>3</sub> structures. Interaction energies (in kJ/mol) are given as well.



**Figure S2.4.** Relative energies obtained through a rigid scan by increasing the X...H<sub>w</sub> distance in 10 steps of 0.15 Å starting from 3.0 Å in a perpendicular Cl-benzene...H<sub>2</sub>O complex with the water molecule located above the chlorine atom and acting as a hydrogen-bond donor (as shown in the inset).

### Section S3. Cartesian coordinates of optimised structures

The first line contains the number of atoms. The second line identifies the structure and level of theory used for the optimisation (penta = cyclopentadiene; avtz = aug-cc-pVTZ-PP for I, At and aug-cc-pVTZ for all other atoms; 631pgs = 6031+G\*). The following linear are the Cartesian coordinates.

```

11
Clbird-mpw2plyp-avtz.xyz
C  0.33368200 -1.42457000  0.27082500
C  0.33355100  1.42473800  0.27036400
C -0.99676400  1.21707700  0.05419500
C -1.60401900 -0.00011600 -0.30396000
C -0.99664600 -1.21715300  0.05457800
H  0.80554100 -2.04853900  1.01019100
H  0.80530500  2.04885300  1.00967900
H -1.64095200  2.05414700  0.29664300
H -2.65994800 -0.00019900 -0.51584200
H -1.64075600 -2.05420000  0.29730100
Cl  1.28894000  0.00000500 -0.24552800
11
Brbird-mpw2plyp-avtz.xyz
C -0.09243500 -1.50048400  0.33072700
C -0.09244100  1.50049100  0.33072300
C -1.39658100  1.22750600  0.04140800
C -1.96328300 -0.00000300 -0.35109800
C -1.39657400 -1.22751200  0.04140900
H  0.28733300 -2.15987400  1.09262000

```

H 0.28731400 2.15985900 1.09264400  
H -2.08219300 2.04424700 0.24187600  
H -3.00634300 -0.00000600 -0.62127800  
H -2.08218500 -2.04425400 0.24188200  
Br 1.03554200 0.00000100 -0.12590700

11

Ibird-mpw2plyp-avtz.xyz

C 0.42915900 1.58090000 0.34892600  
C 0.42916000 -1.58090200 0.34892400  
C 1.71045300 -1.24015400 0.02771600  
C 2.24412300 0.00000100 -0.37896500  
C 1.71045100 1.24015600 0.02771600  
H 0.12478900 2.29992400 1.09098700  
H 0.12479600 -2.29991700 1.09099700  
H 2.43294500 -2.03312100 0.20042500  
H 3.27925400 0.00000200 -0.68041600  
H 2.43294300 2.03312200 0.20042700  
I -0.89688300 0.00000000 -0.07827000

11

Atbird-mpw2plyp-avtz.xyz

C -0.74726600 -1.63313100 0.34076400  
C -0.74725300 1.63312200 0.34077000  
C -2.01435500 1.24691800 0.02081400  
C -2.53606200 0.00000700 -0.38216500  
C -2.01435800 -1.24691300 0.02082200  
H -0.48242900 -2.36166400 1.08999000  
H -0.48243000 2.36161200 1.09004400  
H -2.75274900 2.02961300 0.17890500  
H -3.57015700 0.00000600 -0.68817300  
H -2.75276900 -2.02959100 0.17892500  
At 0.68701500 0.00000000 -0.04583200

14

Clbird-h2o-mpw2plyp-avtz.xyz

C -1.72318600 -0.98128400 -0.15431900  
Cl 0.03529800 -1.16927100 0.06729700  
C 0.56686300 0.31502000 0.94955200  
C -0.11268700 1.41628500 0.47673300  
C -1.19621800 1.41876800 -0.40201100  
C -2.05417600 0.29494900 -0.46680500  
H -2.32886300 -1.76213300 0.26934200  
H 0.85871100 0.14002500 1.97379700  
H 0.19024400 2.35939900 0.91741900  
H -1.57403400 2.36578000 -0.74884100  
H -3.10532900 0.47314300 -0.65852700  
O 3.33153400 0.08219500 -0.48872800  
H 2.49565000 0.33239700 -0.06938100  
H 3.32769600 0.52900400 -1.33693300

14

Brbird-h2o-mpw2plyp-avtz.xyz

C -1.77756800 -0.79682700 -0.17091900  
Br 0.12397200 -0.95087100 0.05402800  
C 0.55405600 0.73567500 0.92920900  
C -0.25416500 1.74094700 0.44608500  
C -1.35135400 1.64378600 -0.41185400  
C -2.14850300 0.47391100 -0.46021000  
H -2.37230800 -1.58989500 0.24617800  
H 0.88513300 0.64414300 1.95281700  
H -0.03718800 2.71910200 0.86379700

H -1.80147600 2.56130300 -0.75317800  
H -3.21002700 0.61273800 -0.63363300  
O 3.28302700 0.47794400 -0.51244800  
H 3.33652300 0.93299400 -1.35462100  
H 2.46131000 0.79160200 -0.10661400

14

Ibird-h2o-mpw2plyp-avtz.xyz

C -1.77433400 -0.94919500 -0.04328000  
I 0.30739600 -0.74484300 0.03600500  
C 0.33139600 1.24965100 0.77292500  
C -0.75401700 1.95198400 0.29552700  
C -1.85757100 1.52535100 -0.44957700  
C -2.39410000 0.21516400 -0.36081100  
H -2.21682400 -1.81371600 0.41963200  
H 0.75059500 1.39115400 1.75896600  
H -0.77088900 2.98940700 0.61998500  
H -2.52776000 2.29209100 -0.80378500  
H -3.47344200 0.14172900 -0.45486600  
O 3.11931200 0.96965500 -0.41246200  
H 2.29746800 1.42684600 -0.17892400  
H 3.38614300 1.33421300 -1.25831100

14

Atbird2-h2o-mpw2plyp-avtz.xyz

C -0.01049800 1.57392300 -0.71922600  
C 1.20669600 2.03606100 -0.26085200  
C 2.24015900 1.41681800 0.44347300  
C 2.56433300 0.03670000 0.34255000  
C 1.78564600 -1.02877400 0.04091800  
At -0.34086100 -0.52683000 -0.02947000  
H -0.37366100 1.80653500 -1.71242700  
H 2.10843400 -1.94961700 -0.41301600  
H 3.62327500 -0.19385800 0.42233300  
H 3.03499800 2.06004600 .78649000  
H 1.39803700 3.06466400 -0.56056800  
O -2.76205800 1.47404200 0.54002800  
H -1.95406000 1.92275600 0.24438500  
H -3.48541900 2.06934200 0.33638100

15

Clbird-nh3-mpw2plyp-avtz.xyz

C -1.42567000 -1.27704200 -0.03781700  
Cl 0.30518300 -0.94003800 0.21708100  
C 0.34792200 0.71040800 0.92641100  
C -0.56821100 1.52327600 0.31753300  
C -1.57083000 1.12597400 -0.58005100  
C -2.08263700 -0.18614000 -0.51617000  
H -1.81489600 -2.12271800 0.50089300  
H 0.70358000 0.75689300 1.94220600  
H -0.56832000 2.55235300 0.65826300  
H -2.17429800 1.88767300 -1.04434800  
H -3.12973500 -0.33536800 -0.75125100  
N 3.33714100 0.08587800 -0.52292900  
H 3.37040700 0.06272700 -1.53274300  
H 2.63216400 0.76321900 -0.25901900  
H 4.22955600 0.43587500 -0.20331300

15

Brbird-nh3-mpw2plyp-avtz.xyz

C -1.50629200 -1.19082900 -0.01404600  
Br 0.35163200 -0.72810000 0.09922100

C 0.23706600 1.08499100 0.78006300  
C -0.84111700 1.73645800 0.24739700  
C -1.87659800 1.21000100 -0.54113900  
C -2.26881600 -0.14020900 -0.42002900  
H -1.81480300 -2.06037300 0.53915200  
H 0.66550400 1.24036700 1.75693700  
H -0.93956700 2.76960900 0.56533000  
H -2.59571800 1.90223600 -0.94704700  
H -3.32219000 -0.36141000 -0.55467100  
N 3.28237500 0.48240900 -0.47843800  
H 3.52520800 0.43886200 -1.45856200  
H 2.61310400 1.23339500 -0.36352800  
H 4.11927100 0.74147400 0.02526000

15

Ibird-nh3-mpw2plyp-avtz.xyz

C -1.62048700 -1.17064800 0.07950800  
I 0.39089700 -0.60342200 0.03824800  
C 0.06603000 1.40129900 0.64242700  
C -1.13198000 1.86960900 0.17411400  
C -2.16981600 1.20281500 -0.49964900  
C -2.45847800 -0.16646600 -0.29820700  
H -1.88717500 -2.05558600 0.63079000  
H 0.54309400 1.71968200 1.55631400  
H -1.32890200 2.90409900 0.44397600  
H -2.97540400 1.81529000 -0.87188400  
H -3.50760900 -0.44275100 -0.35044400  
N 3.17476600 0.83154800 -0.37610000  
H 3.62346700 0.73275100 -1.27647300  
H 2.57943000 1.64925100 -0.41798000  
H 3.90056700 1.01814900 0.30210600

15

Atbird-nh3-mpw2plyp-avtz.xyz

C -1.71570400 -1.14809600 0.06680900  
C -2.60842700 -0.18627000 -0.28367300  
C -2.41927700 1.20417500 -0.48130600  
C -1.42757600 1.96041000 0.16145400  
C -0.16938100 1.63925200 0.60131300  
At 0.35369900 -0.44719000 0.02579600  
H -1.94191200 -2.05655300 0.59855700  
H 0.25033800 2.00463700 1.52810700  
H -1.71379900 2.97780700 0.42108800  
H -3.27894300 1.75161000 -0.83448400  
H -3.64090600 -0.52344000 -0.32499400  
N 2.97884600 1.20828700 -0.37643100  
H 2.32617300 1.98308800 -0.37853000  
H 3.68398100 1.40533200 0.32048600  
H 3.44090700 1.19383600 -1.27546300

17

trinitro-Ibird-mpw2plyp-avtz.xyz

C 0.00603400 1.45991900 -0.00000100  
N 0.64469400 2.71151300 0.00000100  
O -0.00466300 3.74582400 0.00000100  
C -1.33097600 1.24496800 -0.00000200  
C -1.96434500 0.00001100 -0.00000200  
N -3.41685900 0.00001600 -0.00000300  
O -3.98712500 1.08565000 -0.00000600  
I 1.50925400 -0.00000700 0.00000000  
C 0.00601900 -1.45991900 0.00000000

N 0.64466500 -2.71152000 0.00000300  
O 1.89810900 -2.64874200 0.00000500  
C -1.33098900 -1.24495300 -0.00000100  
O -0.00470500 -3.74582300 0.00000500  
O -3.98713300 -1.08561400 -0.00000200  
O 1.89813800 2.64872100 0.00000400  
H -1.95671200 -2.12903800 0.00000000  
H -1.95668800 2.12906000 -0.00000200

20

trinitro-Ibird-h2o-mpw2plyp-avtz.xyz

C 0.03268800 -1.40332500 -0.00000200  
I 1.21299100 0.33583800 -0.00000300  
C -0.56986300 1.44132300 0.00000000  
C -1.83495100 0.96242800 0.00000200  
C -2.19969600 -0.38815000 0.00000200  
N -3.61958400 -0.68827500 0.00000400  
O -4.40259000 0.25623100 0.00000500  
N 0.89766500 -2.50679800 -0.00000500  
O 2.11760200 -2.20671600 -0.00000900  
C -1.32211400 -1.47142600 0.00000000  
O 0.46344900 -3.64970400 -0.00000400  
O -3.95499000 -1.86830700 0.00000500  
N -0.21606500 2.80410100 -0.00000200  
O -1.07314600 3.67478400 -0.00000200  
O 1.01980600 3.01453900 -0.00000400  
H -2.62772600 1.69985500 0.00000200  
H -1.74938400 -2.46646400 0.00000000  
O 4.17182100 -0.22382900 0.00002600  
H 5.08539900 0.06733800 -0.00000900  
H 4.19709400 -1.18441900 0.00001200

21

trinitro-Ibird-nh3-mpw2plyp-avtz.xyz

C -0.04541600 -1.41604700 0.00001400  
C -1.40181700 -1.42225900 0.00000300  
C -2.22793900 -0.29896700 -0.00000100  
N -3.65981200 -0.53138500 -0.00000900  
O -4.05140700 -1.69430000 -0.00001200  
I 1.22789800 0.25926300 0.00000100  
C -0.50915600 1.44495200 0.00001100  
N -0.09334600 2.79012400 0.00000600  
O 1.15145900 2.94518700 -0.00000400  
N 0.76656600 -2.55963400 0.00000800  
O 0.27916200 -3.68163900 0.00001100  
C -1.79788700 1.03215300 0.00000300  
O -4.39785400 0.44897900 -0.00001100  
O 1.99945200 -2.31684400 0.00000300  
O -0.90810000 3.70125400 0.00001000  
N 4.25283100 -0.18786100 -0.00002200  
H -2.55344500 1.80751300 0.00000100  
H -1.87444500 -2.39653800 0.00000100  
H 4.77931400 0.10463000 0.81232600  
H 4.77926600 0.10453300 -0.81243700  
H 4.23861300 -1.19989000 0.00003700

14

tricyano-Ibird-mpw2plyp-avtz.xyz

C 0.05947300 1.54508100 0.20783100  
C 0.05943100 -1.54508500 0.20783400  
C 1.38746400 -1.24614700 0.17330800



C	2.01218800	-0.00003100	-0.05471800
C	1.38749800	1.24610400	0.17330800
H	2.04122900	-2.06691100	0.44749400
H	2.04128600	2.06684900	0.44749500
I	-1.18938300	0.00001500	-0.52888800
C	-0.58264000	-2.65250400	0.76827800
C	3.43149000	-0.00005200	-0.17515300
C	-0.58256700	2.65251800	0.76827400
N	-1.15497200	-3.56890700	1.19545900
N	4.58421300	-0.00005200	-0.28773400
N	-1.15485000	3.56895000	1.19546000

17

tricyano-Ibird-h2o-mpw2plyp-avtz.xyz

C	1.13095300	1.32560700	0.16058400
C	1.23107100	2.64673000	0.61298800
N	1.26783000	3.75488500	0.95958300
C	2.12912400	0.40983900	0.03588900
C	2.01724300	-0.99120700	-0.12835400
C	3.21931200	-1.72097400	-0.34963200
N	4.19512700	-2.31446200	-0.54386300
I	-0.81160800	0.65788600	-0.32840700
C	-0.40983100	-1.29205800	0.39356800
C	-1.48366400	-1.93555000	1.00575500
N	-2.44317600	-2.42029000	1.45111100
C	0.87168400	-1.72833900	0.22599400
H	1.02990600	-2.76971900	0.48375800
H	3.13193800	0.79790500	0.17298800
O	-3.38689300	-0.53860100	-0.78604800
H	-3.85394900	-0.75053100	-1.59706100
H	-3.57136300	-1.26203500	-0.17432800

18

tricyano-Ibird-nh3-mpw2plyp-avtz.xyz

C	1.09579900	1.33959800	0.17928800
C	1.17442000	2.66504000	0.62497700
N	1.18344400	3.77505700	0.96826300
C	2.11934700	0.45635500	0.03052700
C	2.03304900	-0.94718000	-0.14088300
C	3.24481800	-1.65348100	-0.38310400
N	4.22850600	-2.22794700	-0.59508000
I	-0.83842200	0.63920500	-0.31931300
C	-0.38290400	-1.29579200	0.40987900
C	-1.41452900	-1.95888200	1.07334400
N	-2.32937700	-2.47660800	1.57203100
C	0.90756900	-1.70532000	0.22848900
H	1.08940900	-2.74224700	0.48879000
H	3.11623200	0.86409500	0.15206700
N	-3.30563700	-0.63637900	-0.92599500
H	-4.06941000	0.01657100	-1.04470300
H	-3.25082300	-1.19043200	-1.77102700
H	-3.55299800	-1.26672100	-0.17115100

14

Clbird-h2o-below-mpw2plyp-avtz-min.xyz

C	0.86920200	0.20339100	-1.42595200
Cl	0.91236400	1.09871600	0.12288200
C	0.99610100	-0.17552900	1.37878500
C	0.18134900	-1.22047700	1.07157400
C	-0.48566600	-1.42282600	-0.15464100
C	0.07138100	-0.89164900	-1.33912200

H 1.68379600 0.41080200 -2.09597700  
H 1.88186700 -0.15702900 1.98837800  
H 0.14111500 -2.01127000 1.81137100  
H -1.13906200 -2.27489000 -0.24176300  
H -0.04775000 -1.45568400 -2.25636300  
O -2.81704800 0.86155100 0.06957800  
H -2.14425200 0.17211600 -0.00289900  
H -3.14371600 0.78792400 0.96776400

14

Clbird-h2o-below-mpw2plyp-avtz-ts.xyz

C -0.91433200 0.05163700 1.41397100  
Cl -0.80843800 1.14325500 0.00001600  
C -0.91440600 0.05160700 -1.41391100  
C -0.18670500 -1.07827300 -1.21765700  
C 0.40043200 -1.48644100 0.00001100  
C -0.18664300 -1.07824800 1.21770000  
H -1.75135600 0.22755800 2.06509100  
H -1.75146100 0.22751700 -2.06499400  
H -0.15752000 -1.76519000 -2.05502200  
H 0.98799700 -2.38954500 0.00000400  
H -0.15741600 -1.76515000 2.05507700  
O 2.71367500 0.84140700 -0.00014900  
H 2.09206400 0.10172300 -0.00008700  
H 3.58166400 0.43480400 0.00017700

14

Brbird-h2o-below-mpw2plyp-avtz-min.xyz

C 0.47965100 -0.40521000 -1.53670800  
Br 1.03928300 0.57408900 0.02887800  
C 0.58693500 -0.67604700 1.42941100  
C -0.56905100 -1.33326000 1.14568100  
C -1.30595900 -1.31228600 -0.05856800  
C -0.65745800 -1.10713300 -1.29801700  
H 1.24165600 -0.58802200 -2.27314600  
H 1.40347900 -0.99942000 2.05069100  
H -0.89640800 -2.02536000 1.91440000  
H -2.23658900 -1.85567500 -0.07600400  
H -1.04658100 -1.64630100 -2.15497400  
O -2.60264900 1.68513900 0.06000500  
H -2.23482900 0.79228700 0.02280200  
H -2.98914000 1.75189400 0.93467900

14

Brbird-h2o-below-mpw2plyp-avtz-ts.xyz

C -0.51147900 -0.56206900 1.48782200  
Br -1.02310700 0.55487700 0.00000600  
C -0.51151800 -0.56211800 -1.48778700  
C 0.64292600 -1.22820100 -1.22773700  
C 1.33858200 -1.30846600 0.00000500  
C 0.64295900 -1.22816100 1.22776400  
H -1.29856200 -0.82140400 2.17316700  
H -1.29861900 -0.82147500 -2.17310300  
H 1.00677300 -1.84209700 -2.04472800  
H 2.27407500 -1.84400200 0.00000100  
H 1.00682700 -1.84203000 2.04476500  
O 2.37897900 1.80105100 -0.00008600  
H 2.14011000 0.86452100 -0.00005700  
H 3.33747500 1.81146900 0.00003600

14

Ibird-h2o-below-mpw2plyp-avtz-min.xyz

C 0.06217800 -0.57208800 -1.63724600  
I 1.00967000 0.31264600 0.02165600  
C 0.15141300 -0.94468500 1.47779100  
C -1.11410300 -1.30887100 1.13741700  
C -1.82605000 -1.08549100 -0.06429600  
C -1.18450600 -1.01173900 -1.32434800  
H 0.68788600 -0.90408200 -2.44706600  
H 0.82102000 -1.46618700 2.13953400  
H -1.60879000 -1.93392800 1.87561200  
H -2.85504100 -1.40848300 -0.07472500  
H -1.72658800 -1.44277500 -2.16106800  
O -2.50934900 2.09615800 0.12048200  
H -2.32195100 1.14918000 0.06476800  
H -2.96786500 2.20402000 0.95539700

14

Ibird-h2o-below-mpw2plyp-avtz-ts.xyz

C -0.07599500 -0.77403200 1.56736200  
I -1.00015500 0.28503600 0.00000300  
C -0.07602000 -0.77408700 -1.56733300  
C 1.19050900 -1.14189700 -1.24021600  
C 1.86605200 -1.04365400 0.00000300  
C 1.19052900 -1.14185400 1.24023700  
H -0.71393900 -1.21889900 2.31082500  
H -0.71397600 -1.21897900 -2.31077200  
H 1.72176100 -1.65982800 -2.03364400  
H 2.90289400 -1.34119500 0.00000000  
H 1.72179300 -1.65975800 2.03367400  
O 2.26366600 2.20180000 -0.00006400  
H 2.20707400 1.23634800 -0.00004600  
H 3.20281800 2.39413100 -0.00001100

14

Atbird-h2o-below-mpw2plyp-avtz-min-cl.xyz

C 0.33930000 -0.77688600 1.63764400  
At -0.80836500 0.14274100 -0.00378100  
C 0.32622500 -0.87503700 -1.59773700  
C 1.61198600 -1.10251400 -1.22254900  
C 2.26753700 -0.89887700 0.01509200  
C 1.62197800 -1.02333700 1.26983800  
H -0.21644300 -1.27918500 2.41097000  
H -0.23561800 -1.43511300 -2.32612800  
H 2.20805900 -1.58517200 -1.99342600  
H 3.33011400 -1.08539000 0.01762700  
H 2.22616500 -1.45198900 2.06554900  
O 2.39026900 2.34910400 0.03161400  
H 2.39389000 1.38169700 0.03655000  
H 2.88056900 2.58923800 -0.75639800

14

Atbird-h2o-below-mpw2plyp-avtz-min-cs.xyz

C 0.35551800 -0.82694100 1.61652200  
At -0.80036700 0.12569200 0.00000200  
C 0.35550400 -0.82699500 -1.61649700  
C 1.64497400 -1.03362600 -1.24668500  
C 2.29191600 -0.85059800 0.00000400  
C 1.64498500 -1.03358400 1.24670500  
H -0.19309200 -1.36808000 2.36850500  
H -0.19311400 -1.36815900 -2.36845700  
H 2.25483200 -1.47737800 -2.02984800  
H 3.35840800 -1.01417700 0.00000200

H 2.25485000 -1.47731000 2.02987700  
O 2.17889600 2.40611200 -0.00005500  
H 2.29004900 1.44494300 -0.00004100  
H 3.07070900 2.75789600 -0.00003600

11

Clpenta-mpw2plyp-avtz.xyz

C -0.26397700 0.00000000 0.58176300  
H -0.49795500 0.00000100 1.64539100  
C 0.58094500 -1.18062800 0.20739900  
H 0.25424700 -2.19956700 0.31824100  
C 1.76349600 -0.73617200 -0.23749500  
H 2.59276200 -1.34677700 -0.55447200  
C 0.58094600 1.18062800 0.20739800  
H 0.25424700 2.19956800 0.31823800  
C 1.76349700 0.73617200 -0.23749300  
H 2.59276400 1.34677600 -0.55446900  
Cl -1.86738300 0.00000000 -0.25308000

11

Brpenta-mpw2plyp-avtz.xyz

C 0.33277900 -0.00000100 0.68880500  
H 0.12998400 -0.00000200 1.75690000  
C 1.14170000 -1.17960700 0.25221000  
H 0.82897700 -2.19881900 0.39532200  
C 2.27854900 -0.73527200 -0.30234500  
H 3.07388500 -1.34669100 -0.69541400  
C 1.14170000 1.17960700 0.25221300  
H 0.82897700 2.19881800 0.39532800  
C 2.27854600 0.73527300 -0.30234900  
H 3.07388100 1.34669400 -0.69542000  
Br -1.45643900 0.00000000 -0.13394100

11

Ipenta-mpw2plyp-avtz.xyz

C 0.77919000 -0.00000100 0.76799100  
H 0.58113700 -0.00000100 1.83566800  
C 1.55585000 -1.17779700 0.28605700  
H 1.26116800 -2.19787600 0.45871600  
C 2.64530900 -0.73332600 -0.36201200  
H 3.40510400 -1.34607100 -0.81819900  
C 1.55585000 1.17779600 0.28605800  
H 1.26116800 2.19787600 0.45871800  
C 2.64530900 0.73332600 -0.36201200  
H 3.40510400 1.34607200 -0.81819700  
I -1.22646700 0.00000000 -0.09081500

11

Atpenta-mpw2plyp-avtz.xyz

C -1.18860400 0.00000000 0.81323900  
H -0.98422400 0.00000100 1.87864700  
C -1.94162900 1.17646500 0.30469800  
H -1.65798400 2.19684800 0.49353200  
C -3.00075900 0.73262800 -0.39551300  
H -3.73740000 1.34596600 -0.88744000  
C -1.94162800 -1.17646500 0.30469900  
H -1.65798300 -2.19684800 0.49353300  
C -3.00075800 -0.73262800 -0.39551300  
H -3.73739900 -1.34596700 -0.88744100  
At 0.92018000 0.00000000 -0.05741700

14

Clpenta-h2o-mpw2plyp-avtz.xyz

C 1.75799000 0.26847200 0.60261000  
C 1.84131100 -0.38290500 -0.71564300  
C 0.75752300 -1.14726400 -0.90142000  
C -0.09583400 -1.07850600 0.32915400  
C 0.62110500 -0.09986200 1.21131900  
Cl -1.79533600 -0.57281600 -0.03423400  
H -0.18797400 -2.05163000 0.80884000  
H 0.50549300 -1.74202700 -1.76159400  
H 2.65139900 -0.24695000 -1.41240000  
H 0.26152300 0.19787600 2.18086000  
H 2.50381900 0.93609000 1.00212400  
O -0.41365300 2.84081800 -0.34655900  
H 0.03434000 2.09364200 0.05978600  
H -1.23123800 2.46472400 -0.67928100

14

Brpenta-h2o-mpw2plyp-avtz.xyz

C -2.06935700 -0.95221900 -0.72937000  
C -2.20723800 -0.26865100 0.56580500  
C -1.03280300 -0.30280400 1.21513600  
C -0.05104400 -1.06083200 0.37876900  
C -0.81367500 -1.40266900 -0.86108700  
Br 1.54434500 0.02340800 -0.02913400  
H 0.35009200 -1.93420300 0.88657300  
H -0.79985100 0.10462700 2.18338300  
H -3.11620000 0.18699700 0.92298800  
H -0.38484800 -1.93295600 -1.69290300  
H -2.86209800 -1.05774000 -1.45085800  
O -1.10419600 2.85594200 -0.32260000  
H -0.22796800 2.92245300 -0.70714300  
H -1.13291200 1.96706700 0.04293200

14

Ipenta-h2o-mpw2plyp-avtz.xyz

C 2.98842900 -0.73243400 0.70302100  
C 2.98835800 0.73284500 0.70282000  
C 2.02215100 1.17604700 -0.11980900  
C 1.33165800 -0.00007000 -0.72073300  
C 2.02226500 -1.17595600 -0.11948600  
I -0.78738700 -0.00011400 -0.20200600  
H 1.31566300 -0.00021900 -1.80686700  
H 1.76149400 2.19668900 -0.33889700  
H 3.65971800 1.34634500 1.28076900  
H 1.76170300 -2.19668200 -0.33829100  
H 3.65984700 -1.34571100 1.28114000  
O -3.82693600 0.00002800 0.68193400  
H -3.96361600 -0.76027000 1.25106900  
H -3.96497800 0.76306200 1.24706400

14

Atpenta-h2o-mpw2plyp-avtz.xyz

C 3.22623500 -0.73040800 0.71633700  
C 3.22585300 0.73263400 0.71553800  
C 2.27074200 1.17448400 -0.12413800  
C 1.58687100 -0.00010100 -0.72389400  
C 2.27136000 -1.17367500 -0.12286000  
At -0.61815200 -0.00046600 -0.13158900  
H 1.52666000 -0.00071400 -1.80743000  
H 2.01645500 2.19549600 -0.34944000  
H 3.88659800 1.34737700 1.30431800  
H 2.01760300 -2.19506200 -0.34705400

H 3.88730200 -1.34416400 1.30578600  
O -3.58232500 -0.00005200 0.72404500  
H -3.80470500 -0.75264000 1.27639300  
H -3.81474300 0.77213300 1.24427300

15

Clpenta-nh3-mpw2plyp-avtz.xyz

C -2.41752300 0.53961500 -0.18873600  
C -1.37467900 1.57674200 -0.26577600  
C -0.20448200 1.06800900 0.14275800  
C -0.43356500 -0.35126100 0.57171600  
C -1.88020100 -0.59931500 0.26746300  
Cl 0.65855900 -1.52330600 -0.27960700  
H -0.21613500 -0.48677200 1.62988700  
H 0.75845300 1.54661000 0.20335400  
H -1.54289100 2.58590300 -0.60416600  
H -2.36680100 -1.54492800 0.42967700  
H -3.44895900 0.68796200 -0.46355400  
N 3.27053900 1.04113800 0.07807900  
H 2.88182900 0.12600600 -0.11043700  
H 3.68385400 1.37248500 -0.78269400  
H 4.02407100 0.91822800 0.74014300

15

Brpenta-nh3-mpw2plyp-avtz.xyz

C 2.74549600 -0.73391800 0.65898300  
C 2.74523700 0.73543200 0.65798300  
C 1.74646200 1.17776200 -0.12063200  
C 1.03907100 -0.00047400 -0.70955700  
C 1.74687600 -1.17766000 -0.11902700  
Br -0.87987700 -0.00052000 -0.26770500  
H 1.06309100 -0.00121100 -1.79697100  
H 1.47046600 2.19745500 -0.32456800  
H 3.44093800 1.34798900 1.20755400  
H 1.47123700 -2.19772500 -0.32157000  
H 3.44141100 -1.34548000 1.20939000  
N -3.92869500 0.00080000 0.66087000  
H -4.48717500 0.81702300 0.45440100  
H -4.49174400 -0.81203400 0.45343100  
H -3.75054000 -0.00028200 1.65543500

15

Ipenta-nh3-mpw2plyp-avtz.xyz

C 3.00671700 -0.73210700 0.65839400  
C 3.00671800 0.73206900 0.65842700  
C 2.02762700 1.17463300 -0.15056600  
C 1.32376700 0.00001600 -0.73596900  
C 2.02762300 -1.17463100 -0.15061700  
I -0.78783000 0.00000700 -0.15944500  
H 1.27885300 0.00004000 -1.82134600  
H 1.76396600 2.19583100 -0.36411800  
H 3.68522200 1.34596200 1.22769200  
H 1.76395800 -2.19581800 -0.36421400  
H 3.68521900 -1.34602600 1.22763200  
N -3.77224500 -0.00002200 0.65482400  
H -3.85154100 -0.00257100 1.66220400  
H -4.25921800 0.81654200 0.31259500  
H -4.26044600 -0.81406700 0.30836800

15

Atpenta-nh3-mpw2plyp-avtz.xyz

C 3.23217600 -0.73060700 0.68386500

C	3.23218100	0.73057800	0.68388200
C	2.27502900	1.17223400	-0.15587600
C	1.58479100	0.00000900	-0.74807400
C	2.27502100	-1.17223400	-0.15590600
At	-0.62080400	0.00000400	-0.10844300
H	1.50071700	0.00002400	-1.83001900
H	2.02169400	2.19410600	-0.37933400
H	3.89197300	1.34557900	1.27361500
H	2.02167700	-2.19410000	-0.37938700
H	3.89196100	-1.34562800	1.27358400
N	-3.51018200	-0.00001800	0.70991800
H	-3.59321800	-0.00215300	1.71709100
H	-3.99466100	0.81678100	0.36445700
H	-3.99568900	-0.81469800	0.36091400

12

Clbenzene-mpw2plyp-avtz.xyz

C	0.17541900	1.20953700	0.00000100
C	-0.50350300	-0.00000200	-0.00000100
C	0.17542000	-1.20953800	-0.00000100
C	1.56468900	-1.20177300	0.00000100
C	2.26192200	0.00000000	0.00000300
C	1.56468600	1.20177500	0.00000300
H	-0.37558200	2.13619300	0.00000100
H	-0.37557700	-2.13619600	-0.00000200
H	2.09956200	-2.13924900	0.00000200
H	3.34082900	0.00000300	0.00000400
H	2.09956100	2.13925000	0.00000400
Cl	-2.24827000	0.00000000	-0.00000300

12

Brbenzene-mpw2plyp-avtz.xyz

C	-0.77921000	-1.20975300	0.00009000
C	-0.10018400	0.00000000	0.00000800
C	-0.77921000	1.20975200	0.00009000
C	-2.16891100	1.20172900	0.00025300
C	-2.86583900	0.00000000	0.00033100
C	-2.16891200	-1.20172800	0.00025300
H	-0.23269500	-2.13898300	0.00002700
H	-0.23269600	2.13898300	0.00002800
H	-2.70371300	2.13929800	0.00031700
H	-3.94481200	0.00000100	0.00045700
H	-2.70371400	-2.13929700	0.00031600
Br	1.79974900	0.00000000	-0.00020900

12

Ibenzene-mpw2plyp-avtz.xyz

C	1.24183800	1.20920400	0.00000400
C	0.55823600	-0.00000400	0.00000100
C	1.24183900	-1.20920500	0.00000200
C	2.63198400	-1.20149200	0.00000500
C	3.32898200	0.00000100	0.00000800
C	2.63197800	1.20149600	0.00000700
H	0.70205700	2.14254000	0.00000400
H	0.70206900	-2.14254700	0.00000000
H	3.16652600	-2.13936800	0.00000500
H	4.40804900	0.00000600	0.00001100
H	3.16652300	2.13937000	0.00001000
I	-1.54630900	0.00000000	-0.00000400

12

Atbenzene-mpw2plyp-avtz.xyz

C	1.69732900	1.20899600	0.00000500
C	1.01437700	-0.00000200	0.00000300
C	1.69733100	-1.20899600	0.00000500
C	3.08802100	-1.20145200	0.00000900
C	3.78492700	0.00000100	0.00001100
C	3.08801800	1.20145400	0.00000800
H	1.15984200	2.14382800	0.00000300
H	1.15985000	-2.14383200	0.00000300
H	3.62260300	-2.13939400	0.00001000
H	4.86403700	0.00000400	0.00001400
H	3.62260000	2.13939500	0.00001000
At	-1.18410500	0.00000000	-0.00000300

15

Clbenzene-h2o-mpw2plyp-avtz.xyz

C	1.27561900	1.61984000	0.00068400
C	0.08438100	0.90326400	0.00020200
C	0.14740000	-0.48167600	0.00126300
C	1.35599900	-1.16097300	0.00300500
C	2.53581800	-0.42756900	0.00371200
C	2.49883800	0.96132200	0.00244600
Cl	-1.33699900	-1.41508000	-0.00157700
H	-0.86825400	1.40899100	0.00009600
H	1.37076700	-2.23897500	0.00333300
H	3.48223900	-0.94636600	0.00488000
H	3.41789100	1.52660800	0.00252600
H	1.24031200	2.69856200	-0.00084000
O	-3.26961200	1.39584600	-0.05876900
H	-4.08679000	1.49695900	0.43217300
H	-3.05862500	0.45857000	-0.01308800

15

Brbenzene-h2o-mpw2plyp-avtz.xyz

C	2.71382900	1.25648000	0.00022800
C	1.32469300	1.21724500	-0.00001000
C	0.68221900	-0.01321200	-0.00015400
C	1.40491500	-1.19838500	-0.00006700
C	2.79354800	-1.14502600	0.00017100
C	3.45090500	0.07888800	0.00031900
Br	-1.21554300	-0.07930900	-0.00048100
H	0.74839100	2.12854200	-0.00008500
H	0.89004300	-2.14572700	-0.00018600
H	3.35913900	-2.06446200	0.00023800
H	4.52934500	0.11472200	0.00050300
H	3.21718400	2.21143200	0.00034000
O	-4.40717400	0.02410100	0.00099500
H	-4.58050500	0.57949200	0.76360900
H	-4.58285900	0.58306800	-0.75846000

15

Ibenzene-h2o-mpw2plyp-631pgs.xyz

C	-3.09561600	1.22918500	0.00000500
C	-1.69864700	1.22093200	0.00000200
C	-1.01929200	0.00060600	0.00000000
C	-1.72376300	-1.20542300	-0.00000100
C	-3.12060400	-1.18457400	0.00000200
C	-3.80954500	0.02956000	0.00000400
I	1.10634500	-0.02383200	-0.00000400
H	-1.14868600	2.15430800	0.00000200
H	-1.19322800	-2.14996900	-0.00000300
H	-3.66704100	-2.12154300	0.00000100



H	-4.89367200	0.04078500	0.00000600
H	-3.62260000	2.17725500	0.00000600
O	4.18255500	-0.01602200	0.00000300
H	4.61665600	0.37443800	-0.77123200
H	4.61664100	0.37430300	0.77131500

15

Atbenzene-h2o-mpw2plyp-avtz.xyz

C	-3.40654300	1.22273800	0.00001600
C	-2.01592600	1.21663800	0.00001800
C	-1.33546500	0.00450200	-0.00000600
C	-2.03595300	-1.19619100	-0.00003100
C	-3.42647300	-1.17906800	-0.00003200
C	-4.11446900	0.02762900	-0.00000900
At	0.86486500	-0.01591300	-0.00000300
H	-1.47199800	2.14821400	0.00003700
H	-1.50758600	-2.13667600	-0.00004900
H	-3.96876700	-2.11275500	-0.00005100
H	-5.19368800	0.03658100	-0.00001000
H	-3.93328900	2.16530400	0.00003400
O	3.97041900	-0.01027000	0.00002600
H	4.40374400	0.37861800	-0.76253100
H	4.40371700	0.37802000	0.76290400

16

Clbenzene-nh3-mpw2plyp-avtz.xyz

C	-1.15060700	1.67142300	-0.00002300
C	-0.02547200	0.85466100	-0.00002800
C	-0.20809200	-0.51998500	-0.00000700
C	-1.47169100	-1.09134700	0.00001900
C	-2.58380400	-0.25868000	0.00002500
C	-2.42671600	1.12188500	0.00000400
Cl	1.19158000	-1.57307300	-0.00001300
H	0.96965900	1.27382800	-0.00004600
H	-1.57973100	-2.16409100	0.00003600
H	-3.57171800	-0.69351100	0.00004500
H	-3.29347300	1.76466400	0.00000800
H	-1.02207500	2.74322900	-0.00003900
N	3.44784400	1.37196200	0.00002200
H	4.00802800	1.58668500	0.81326700
H	3.28769500	0.37325900	0.00000100
H	4.00814100	1.58670300	-0.81314100

16

Brbenzene-nh3-mpw2plyp-avtz.xyz

C	-2.76906400	1.19848400	0.00002000
C	-1.37942600	1.20727700	0.00001900
C	-0.69201200	0.00075000	0.00000300
C	-1.37538400	-1.20807200	-0.00001200
C	-2.76504600	-1.20393400	-0.00001200
C	-3.46511900	-0.00389100	0.00000400
Br	1.20736300	0.00399400	0.00000300
H	-0.83543100	2.13835600	0.00003200
H	-0.82827500	-2.13732700	-0.00002500
H	-3.29822200	-2.14265100	-0.00002400
H	-4.54420200	-0.00570300	0.00000400
H	-3.30538100	2.13541000	0.00003200
N	4.41180700	-0.00503500	-0.00002100
H	4.80055500	0.92761500	-0.00049700
H	4.77349400	-0.48156300	0.81427600
H	4.77342700	-0.48236500	-0.81387900

16

Ibenzene-nh3-mpw2plyp-avtz.xyz

C	-3.10249900	1.20039100	-0.00033700
C	-1.71235800	1.20610600	-0.00029200
C	-1.01997200	0.00005000	-0.00008100
C	-1.71166800	-1.20640300	0.00009200
C	-3.10181100	-1.20147800	0.00004400
C	-3.80042700	-0.00074200	-0.00017100
I	1.08873000	0.00059200	0.00000100
H	-1.17429100	2.14104700	-0.00041900
H	-1.17305500	-2.14103000	0.00026000
H	-3.63612900	-2.13975100	0.00017400
H	-4.87966300	-0.00105800	-0.00020800
H	-3.63734900	2.13835900	-0.00050400
N	4.23810700	-0.00139100	0.00047000
H	4.61014900	0.93791500	-0.02276000
H	4.60639900	-0.45209300	0.82659700
H	4.60691700	-0.49256100	-0.80201800

16

Atbenzene-nh3-mpw2plyp-avtz.xyz

C	3.42434000	1.20017000	-0.00017700
C	2.03365500	1.20499200	-0.00015900
C	1.33931800	0.00002600	-0.00001700
C	2.03292400	-1.20537100	0.00010700
C	3.42361400	-1.20139100	0.00008900
C	4.12238800	-0.00082100	-0.00005300
At	-0.86850900	0.00043100	0.00001100
H	1.49875500	2.14213800	-0.00025600
H	1.49743000	-2.14218100	0.00021800
H	3.95800300	-2.13976000	0.00018600
H	5.20172200	-0.00115100	-0.00006700
H	3.95930200	2.13821000	-0.00028800
N	-3.94409700	-0.00181900	0.00005000
H	-4.31484300	0.93837800	-0.00001900
H	-4.31295000	-0.47263700	-0.81463300
H	-4.31293100	-0.47250900	0.81481600

15

Clbenzene-h2o-mpw2plyp-avtz-Hbonded.xyz

C	-2.49884000	0.96132400	-0.00245900
C	-1.27562100	1.61984100	-0.00063700
C	-0.08438300	0.90326400	-0.00013900
C	-0.14740300	-0.48167600	-0.00124600
C	-1.35600200	-1.16097200	-0.00304800
C	-2.53582100	-0.42756800	-0.00376900
Cl	1.33699600	-1.41507900	0.00161100
O	3.26964500	1.39583700	0.05873200
H	0.86825400	1.40898900	0.00001100
H	-1.37077100	-2.23897400	-0.00341000
H	-3.48224200	-0.94636300	-0.00498400
H	-3.41789200	1.52661000	-0.00255000
H	-1.24031300	2.69856300	0.00092200
H	3.05862500	0.45856900	0.01304200
H	4.08665300	1.49697600	-0.43248900

15

Brbenzene-h2o-mpw2plyp-avtz-Hbonded.xyz

C	-3.02043900	0.71814400	0.00303200
C	-1.94330900	1.59499400	-0.01192000
C	-0.63795900	1.11551800	-0.01335300

C	-0.43915600	-0.25675500	0.00026300
C	-1.49858800	-1.15148100	0.01531900
C	-2.79559400	-0.65268700	0.01676200
Br	1.33808400	-0.95081800	-0.00479000
O	2.53373400	2.37282800	-0.05345700
H	0.19893100	1.79583800	-0.02332200
H	-1.31551400	-2.21382500	0.02524200
H	-3.62742200	-1.34036700	0.02822200
H	-4.02951900	1.10037400	0.00365500
H	-2.11139200	2.66112500	-0.02321100
H	2.56141400	1.41207500	-0.00741400
H	3.23094800	2.67438500	0.53150000

15

Ibenzene-h2o-mpw2plyp-avtz-Hbonded.xyz

C	-3.44270300	0.38840300	0.00150800
C	-2.50903400	1.41633700	-0.02076400
C	-1.14619000	1.13749200	-0.02123000
C	-0.73921800	-0.18986600	0.00071000
C	-1.65725200	-1.23159900	0.02318300
C	-3.01482400	-0.93292700	0.02356200
I	1.31985900	-0.65370500	-0.00409700
O	1.70912200	3.05668800	-0.05153300
H	-0.42651100	1.94094600	-0.03688700
H	-1.32459100	-2.25708900	0.03967300
H	-3.73402100	-1.73776700	0.04074200
H	-4.49776900	0.61510800	0.00129400
H	-2.83457600	2.44544200	-0.03867200
H	2.00243600	2.14079100	-0.01456000
H	2.24487600	3.51842900	0.59599600

15

Atbenzene-h2o-mpw2plyp-avtz-Hbonded.xyz

C	-3.84661800	0.12083100	0.00031600
C	-3.03446300	1.24687200	-0.03246100
C	-1.64838600	1.12272000	-0.03231900
C	-1.09555400	-0.14994300	0.00101900
C	-1.88991800	-1.28790600	0.03410200
C	-3.27303500	-1.14374100	0.03368000
At	1.09566100	-0.39148600	-0.00378300
O	0.95209900	3.40159700	-0.04350200
H	-1.02579600	2.00352600	-0.05592500
H	-1.44652900	-2.27058600	0.05942100
H	-3.89724200	-2.02419600	0.05909500
H	-4.92051500	0.22753500	-0.00052300
H	-3.47351500	2.23279500	-0.05918300
H	1.36086200	2.53085600	-0.00521100
H	1.38259500	3.91057600	0.64589900

15

Ibenzene-h2o-m062x-631pgs.xyz

C	-3.07677500	1.23034900	0.00000200
C	-1.68202000	1.21964800	0.00000000
C	-1.00519900	0.00071300	0.00000000
C	-1.71039400	-1.20200300	0.00000100
C	-3.10499400	-1.17993600	0.00000300
C	-3.79100000	0.03340000	0.00000400
I	1.10590400	-0.02738000	-0.00000400
H	-1.12792700	2.15287900	-0.00000200
H	-1.17833800	-2.14794200	0.00000100
H	-3.65349800	-2.11735000	0.00000500

H	-4.87660300	0.04609600	0.00000600
H	-3.60321000	2.18035800	0.00000300
O	4.12303600	-0.01037800	0.00001000
H	4.53235900	0.40355200	-0.77198300
H	4.53232700	0.40355600	0.77201800

15

Ibenzene-h2o-m062x-avtz.xyz

C	-3.06089100	1.24112400	-0.00001000
C	-1.67263700	1.21944700	-0.00000100
C	-1.00937500	0.00031100	0.00000200
C	-1.72050000	-1.19151300	-0.00000400
C	-3.10846900	-1.15797800	-0.00001400
C	-3.78128800	0.05539800	-0.00001600
I	1.08919500	-0.04519500	0.00001500
H	-1.11239600	2.14354300	0.00000400
H	-1.19732900	-2.13705300	-0.00000200
H	-3.66253500	-2.08682300	-0.00001900
H	-4.86217000	0.07680100	-0.00002400
H	-3.57766300	2.19124500	-0.00001200
O	4.22296300	0.01968200	-0.00003700
H	4.50994700	0.52467700	-0.76431900
H	4.51004300	0.52476900	0.76414900

15

Ibenzene-h2o-mpw2plyp-631pgs.xyz

C	-3.09561600	1.22918500	0.00000500
C	-1.69864700	1.22093200	0.00000200
C	-1.01929200	0.00060600	0.00000000
C	-1.72376300	-1.20542300	-0.00000100
C	-3.12060400	-1.18457400	0.00000200
C	-3.80954500	0.02956000	0.00000400
I	1.10634500	-0.02383200	-0.00000400
H	-1.14868600	2.15430800	0.00000200
H	-1.19322800	-2.14996900	-0.00000300
H	-3.66704100	-2.12154300	0.00000100
H	-4.89367200	0.04078500	0.00000600
H	-3.62260000	2.17725500	0.00000600
O	4.18255500	-0.01602200	0.00000300
H	4.61665600	0.37443800	-0.77123200
H	4.61664100	0.37430300	0.77131500