Supporting information

Table S1 Summary of main quantities written in bond.out file obtained after calculations in PolaBer.

q(A)	Atomic charge (EFIELD=0*)
alpha11, alpha22, alpha33, alpha12, alpha13,alpha23	Components of atomic polarizability tensors ($Bohr^3$)
alphaiso	Isotropic value of atomic polarizability
Vol	Atomic volume bounded by an isosurface of the electron density distribution (0.001 a.u.Isodensity Envelope, EFIELD=0)
D(A-B)	Bond length in Bohr
d1, d2	Distances between atom A and BCP and BCP and atom B, respectively. (EFIELD=0, Bohr)
Rho, delrho, elips	Electron density, Laplacian and bond ellipticity(EF=0)
bcharge	Bond charge calculated for EFIELD=0
polA, polB, bonpol	Projections of polarizabilities of atom A on A-B bond and atom B on A-B bond, respectively bondpol=polA+polB (total bond polarizability)
dipA, dipB, bonddip	Projections of dipole moments of atom A on A-B bond and atom B on A-B bond, respectively bonddip=polA+polB (total bond dipole moment)
chi	Crystal electric susceptibility, obtained from summation of atomic polarizabilities in the crystal unit cell as well as from anisotropic Lorentz correction
n	Crystal refractive indices calculated from the crystal susceptibility. An analysis of the optic indicatrix is also provided.

* values corresponding to calculations without external electric field applied

Example of bash scripts using Gaussian09 for molecular orbital calculations, AIMAll for QTAIM analysis and PolaBer for atomic polarizabilities.

General Jobfile:

- choose the number of processors (-nproc) and number of atoms (-naat) computed at one time by AIMAll
- have g09, aimqb and polaber in the path
- have polar.gjf and dipolar.inp in the working directory
- g09 produce wfn file for each field calculation (zero.wfn, xp.wfn, xm.wfn etc.)

```
g09 < polar.gjf > polar.out
for fname in zero xp xm yp ym zp zm
do
  aimqb.ish -nogui -nproc=12 -naat=8 $fname.wfn
done
polaber
```

*Gaussian input file for calculating water distributed atomic polarizabilities (**polar.gjf**).*

- Set the number of processor (Nproc) for the molecular orbital calculation
- Choose the Hamiltonian and the basis set (in green)

```
%chk=polar.chk
%Nproc=12
#b3lyp/6-311++g(2d,2p) opt out=wfn

B3LYP 6-31++G(2d,2p) H2O

0 1
O       0.000000    0.000000    0.200000
H       0.000000   -0.500000   -0.700000
H       0.000000    0.500000   -0.700000

zero.wfn
--link1--
%chk=polar.chk
%Nproc=12
#b3lyp chkbasis nosymm scf=tight geom=checkpoint out=wfn
field=x+50

x=50

0 1

xp.wfn
--link1--
....
....
....
....
--link1--
%chk=polar.chk
%Nproc=12
#b3lyp chkbasis nosymm scf=tight geom=checkpoint out=wfn
field=z-50

z=-50

0 1

zm.wfn
```