

## **Supporting Information**

### **Boronic Acids as Hydrogen Bond Donor Catalysts for Efficient Conversion of CO<sub>2</sub> into Organic Carbonate in Water**

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#### **Supporting information**

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## **1. General information**

All starting materials are commercially available and were used as received, unless otherwise indicated. Boronic acids were purchased from Sigma-Aldrich and Scientific Resources Pte Ltd. The epoxides were purchased from the VWR international. GC-MS were measured on SHIMADZO-QP2010. GC analyses were performed on a Agilent GC-6890 using a flame ionization detector. NMR spectra were recorded on a Bruker 400.

The calculations were carried out by performing DFT by use of the B3PW91functional with the 6-311++G (d, p) basis set as implemented in Gaussian 03 program package. Vibrational frequency calculations, from which the zero-point energies were derived, have been performed for each optimized stucture at the same level to indentify the natures of all the stationary points. All the bond lengths are in angstroms ( $\text{\AA}$ ). Structures were generated using CYLview.<sup>[1]</sup>

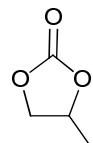
[1] CYLview, 1.0b; C. Y. Legault, Université de Sherbrooke, 2009 (<http://www.cylview.org>).

## **2. Experiments details of conversion of $\text{CO}_2$ with epoxide**

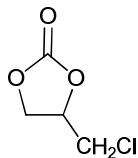
$\text{CO}_2$  fixation reactions were conducted in a 25 mL stainlesssteel reactor equipped with a magnetic stirrer and automatic temperature control system. Typically, in the reactor, an appropriate volume of  $\text{CO}_2$  (1.0 MPa) was added to a mixture of glycidyl phenyl ether (2 mmol), TBAI (5 mmol%), boronic acids (10 mmol%) and  $\text{H}_2\text{O}$  (2 mL) at room temperature. The temperature was then raised to 50 °C. After 4 h reaction, the reactor was cooled to 0 °C in ice bath, and the remaining  $\text{CO}_2$  was removed slowly. The product was then analyzed by GC.

Recyling experiments of B27: after reaction, the supported catalyst was filtrated from the reaction system and washed with methanol (3×2 mL), then dried for next run.

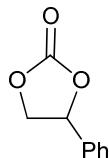
## **3. Characterization of cyclic carbonates**



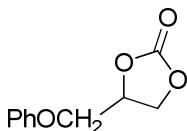
<sup>1</sup>H NMR ( $\text{CDCl}_3$ , TMS, 400 MHz):  $\delta$  4.86-4.94 (m, 1H), 4.60 (t,  $J$  = 8.0 Hz, 1H), 4.05 (t,  $J$  = 8.8 Hz, 1H), 1.49 (d,  $J$  = 6.0 Hz, 3H); <sup>13</sup>C NMR ( $\text{CDCl}_3$ , TMS, 100.4 MHz):  $\delta$  154.95 (C=O), 73.51, 70.46, 18.95.



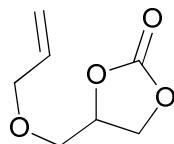
<sup>1</sup>H NMR (CDCl<sub>3</sub>, TMS, 400 MHz): δ 4.98 (m, 1H), 4.58 (t, 1H, *J* = 8.4 Hz), 4.39 (dd, 1H, *J* = 6.0 Hz), 3.80 (dd, 1H, *J* = 5.2 Hz), 3.71 (dd, 1H, *J* = 3.2 Hz); <sup>13</sup>C NMR (CDCl<sub>3</sub>, TMS, 100.4 MHz): δ 154.95 (C=O), 73.51, 70.46, 43.83.



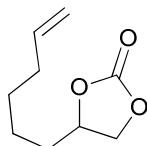
<sup>1</sup>H NMR (CDCl<sub>3</sub>, TMS, 400 MHz): δ 7.35-7.44 (m, 5H), 5.68 (t, 1H, *J* = 8.0 Hz), 4.80 (t, 1H, *J* = 8.4 Hz), 4.34 (t, 1H, *J* = 8.4 Hz); <sup>13</sup>C NMR (CDCl<sub>3</sub>, TMS, 100.4 MHz): δ 154.81 (C=O), 135.70, 129.63, 129.12, 125.81, 77.92, 71.10.



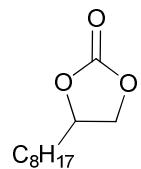
<sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ 7.31 (t, <sup>3</sup>*J* = 8.0 Hz, 2H), 7.02 (t, <sup>3</sup>*J* = 7.4 Hz, 1H), 6.91 (d, <sup>3</sup>*J* = 8.0 Hz, 2H), 5.03 (m, 1H), 4.62 (t, <sup>3</sup>*J* = 8.4 Hz, 1H), 4.55 (dd, <sup>3</sup>*J* = 8.4 Hz), 4.24 (dd, <sup>3</sup>*J* = 3.6 Hz, 1H), 4.15 (dd, <sup>3</sup>*J* = 4.4 Hz, 1H), <sup>13</sup>C NMR (CDCl<sub>3</sub>, TMS, 100.4 MHz): δ 157.71, 154.65, 129.62, 121.92, 114.57, 74.11, 68.84, 66.17.



<sup>1</sup>H NMR (CDCl<sub>3</sub>, 400MHz): δ 5.8–6.0 (t, 1H), 5.0-5.2 (d, 2H), 4.4-4.7 (3H), 4.0-4.1 (m, 2H), 3.5-3.8 (d, 2H). <sup>13</sup>C NMR (CDCl<sub>3</sub>, TMS, 100.4 MHz): δ 155.90, 133.88, 117.47, 72.05, 72.30, 68.92, 66.24 .



<sup>1</sup>H NMR (CDCl<sub>3</sub>, TMS, 400 MHz): δ 5.8–6.0 (t, 1H), 5.0–5.2 (d, 2H), 4.7 (m, 1H), 4.5 (dd, 1H), 4.04 (dd, 1H, *J* = 8.4 Hz), 2.4–2.7 (m, 2H), 2.1 (m, 2H), 1.43–1.55 (m, 4H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, TMS, 100.4 MHz): δ 155.2 (C=O), 139.2, 115.6, 70.4, 66.3, 36.5, 33.8, 29.6, 25.3.



<sup>1</sup>H NMR (CDCl<sub>3</sub>, TMS, 400 MHz): δ 4.6–4.8 (m, 1H), 4.50 (dd, 1H, *J* = 8.4 Hz), 4.04 (dd, 1H, *J* = 8.4 Hz), 1.6–1.9 (m, 2H), 1.1–1.6 (m, 12H), 0.86 (t, 2H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, TMS, 100.4 MHz): δ 155.2 (C=O), 77.1, 69.5, 34.0, 31.9, 29.4, 29.2, 29.2, 24.5, 22.7, 14.2.

#### 4. Supporting Tables

**Table S1** NBO charge at B atom and hydrogen bond lengths of **B19** and Propylene oxide in different solvents.

| Entry | Solvent          | NBO charge of B atom (e) <sup>*</sup> | H-bond 1 (Å) | H-bond 2 (Å) |
|-------|------------------|---------------------------------------|--------------|--------------|
| 1     | H <sub>2</sub> O | 1.119 (1.125)                         | 1.921        | 1.945        |
| 2     | Acetone          | 1.119 (1.125)                         | 1.925        | 1.952        |
| 3     | Dichloromethane  | 1.119 (1.125)                         | 1.934        | 1.961        |
| 4     | Tetrahydrofuran  | 1.119 (1.125)                         | 1.937        | 1.964        |
| 5     | Chloroform       | 1.119 (1.125)                         | 1.947        | 1.973        |
| 6     | Toluene          | 1.113 (1.118)                         | 1.981        | 1.984        |

\*NBO charge of B atom (e) is the number after formation of hydrogen bond, and pure boronic acid in parenthesis.

**Table S2** Compared with the other organocatalysts <sup>a</sup>

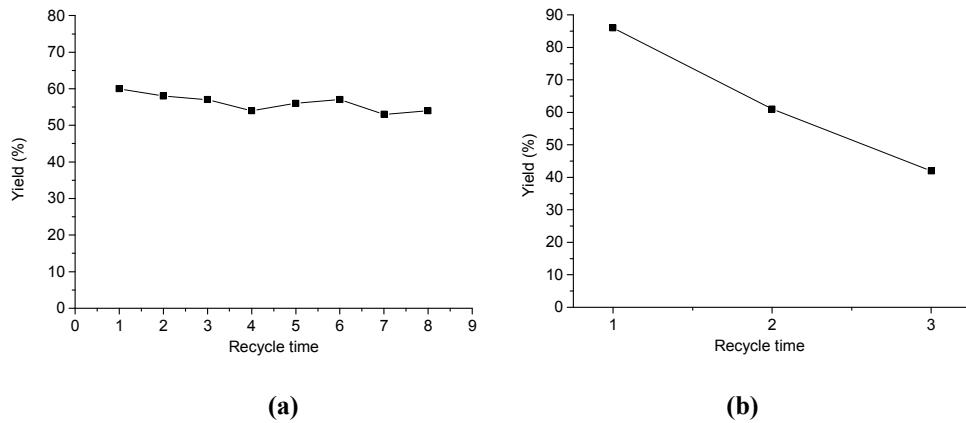
| Epoxide <sup>a</sup> | HBDs | Conditions  | Yield (%) | Reference                            |
|----------------------|------|---|-----------|--------------------------------------|
|                      |      | 40 °C, 1 bar, 18 h,<br>Epoxide: TBAI: HBD 10: 1: 1  | 91        | Mattson et al.<br>2014 <sup>1</sup>  |
|                      |      | 45 °C, 1 MPa, 18 h,<br>Epoxide: TBAI: HBD 20: 1: 1  | 52        | Kleij et al.<br>2012 <sup>2</sup>    |
|                      |      | 60 °C, 2 MPa, 5 h,<br>Epoxide: TBABr: HBD 100: 3: 3 | 50        | Tassaing et<br>al. 2015 <sup>3</sup> |
|                      |      | 45 °C, 1 bar, 20 h,<br>Epoxide: TBAI: HBD 25: 2: 2  | 85        | Hirose et al.<br>2016 <sup>4</sup>   |
|                      |      | 50 °C, 1 MPa, 7 h,<br>Epoxide: TBAI: HBD 20: 1: 2   | 88        | This work                            |

<sup>a</sup> Styrene oxide is chosen for compared because this epoxide is studied in all the references in this table and easily compared.

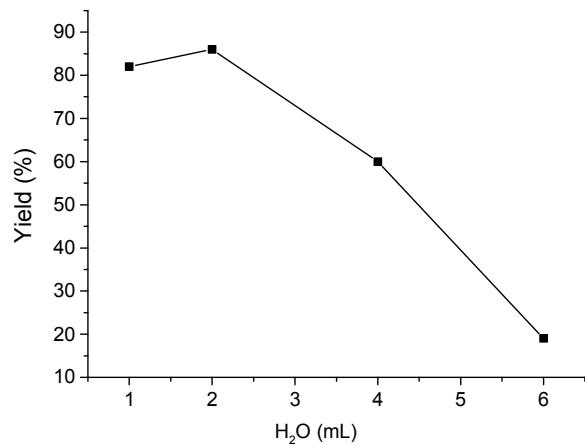
**References:**

1. A. M. Hardman-Baldwin and A. E. Mattson, *ChemSusChem* 2014, **7**, 3275.
2. C. J. Whiteoak, A. Nova, F. Maseras and A. W. Kleij, *ChemSusChem* 2012, **5**, 2032.
3. M. Alves, B. Grignard, S. Gennen, R. Mereau, C. Detrembleur, C. Jerome and T. Tassaing, *Catal. Sci. Technol.*, 2015, **5**, 4636.
4. L. Wang, G. Y. Zhang, K. Kodama and T. Hirose, *Green Chem.*, 2016, DOI: 10.1039/C5GC02697K.

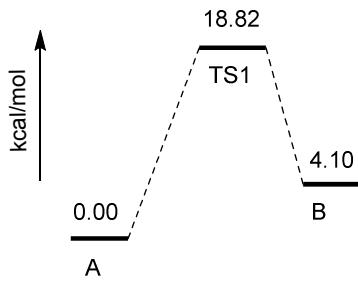
## 5. Supporting Figures



**Figure S1** Catalyst reusability test. **(a)** For catalyst **B27**. Reaction conditions: Glycidyl phenyl ether (2 mmol), nTBAI (5 mol%), B27 (0.11 g), H<sub>2</sub>O (2 mL), CO<sub>2</sub> pressure (1 MPa), Temperature (50 °C), Time (4 h). Recycling method: the supported catalyst was filtrated from the reaction system and washed with methanol (3×2 mL), then dried for next run. **(b)** For catalyst **B19**. Reaction conditions: Glycidyl phenyl ether (2 mmol), nTBAI (5 mol%), B27 (0.11 g), H<sub>2</sub>O (2 mL), CO<sub>2</sub> pressure (1 MPa), Temperature (50 °C), Time (4 h). Recycling method: the solid product was wahsed with hot water (3×4 mL) after reaction, then the catalyst was obtained by removing water and reused for next run.

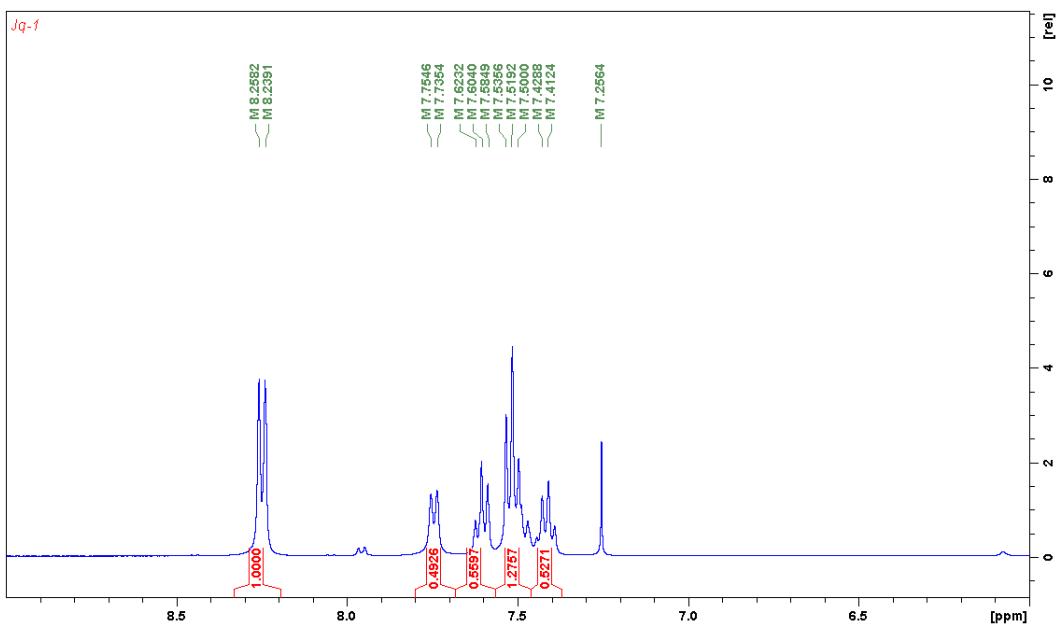


**Figure S2** The influence of H<sub>2</sub>O amount on the yield of product. Reaction conditions: Glycidyl phenyl ether (2 mmol), nTBAI (5 mol%), HBDs (10 mol%), CO<sub>2</sub> pressure (1 MPa), Temperature (50 °C), Time (4 h).

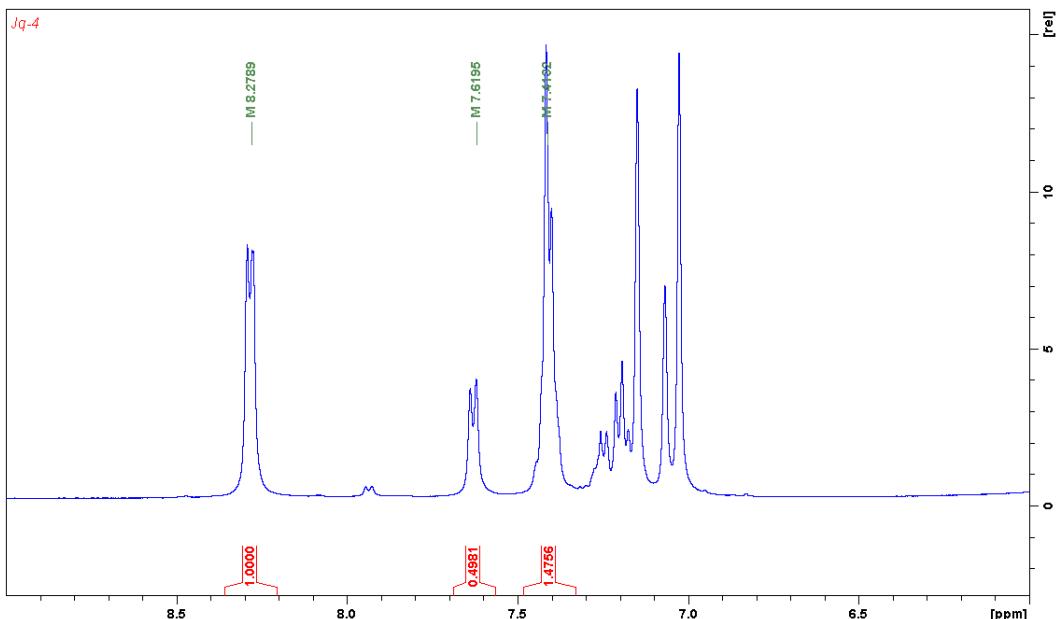


**Figure S3** Relative energies of ring-opening step for fixation of CO<sub>2</sub> with PO catalyzed by **B19** and TEAB, relative energies at the B3PW91/6-311++G (d, p) level.

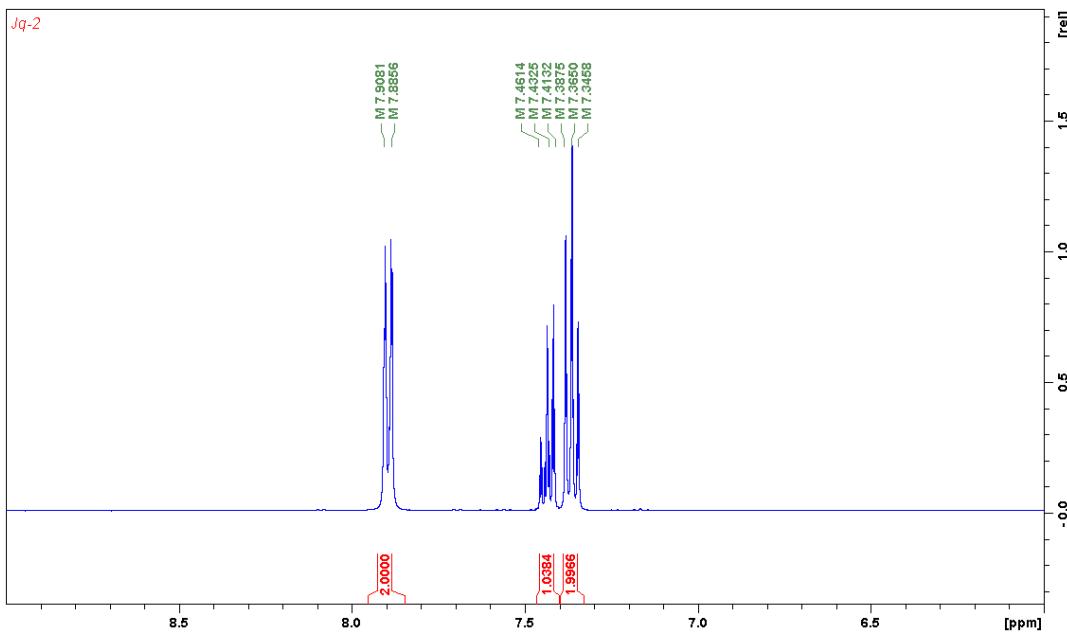
**Figure S4-S14**, the equilibrium of monomer-oligomer was studied by NMR in different solvents. Phenylboronic acid was used as the model compound for the NMR test. It is true that boronic acid monomer partially converted to oligomer and the equilibriums between monomer and oligomer were observed for phenylboronic acid in non-coordinating solvents, such as chloroform and toluene (Figure S4, 5 and 8, 9). While for coordinating solvents, such as acetone and acetonitrile, only monomeric boronic acid was observed (no equilibrium, even the samples were heated at 50 °C for 1 h, Figures S6, 7 and 10, 11). However, for catalyst B19, only boronic acid monomer was found in chloroform. It is possibly because of the steric hindrance of 2- and 6-substituents that blocks the formation of boronic acid oligomer (Figures S12). As expected, only monomeric B19 was observed in acetonitrile, even after heating at 50 °C for 1 h (Figure S13, 14).



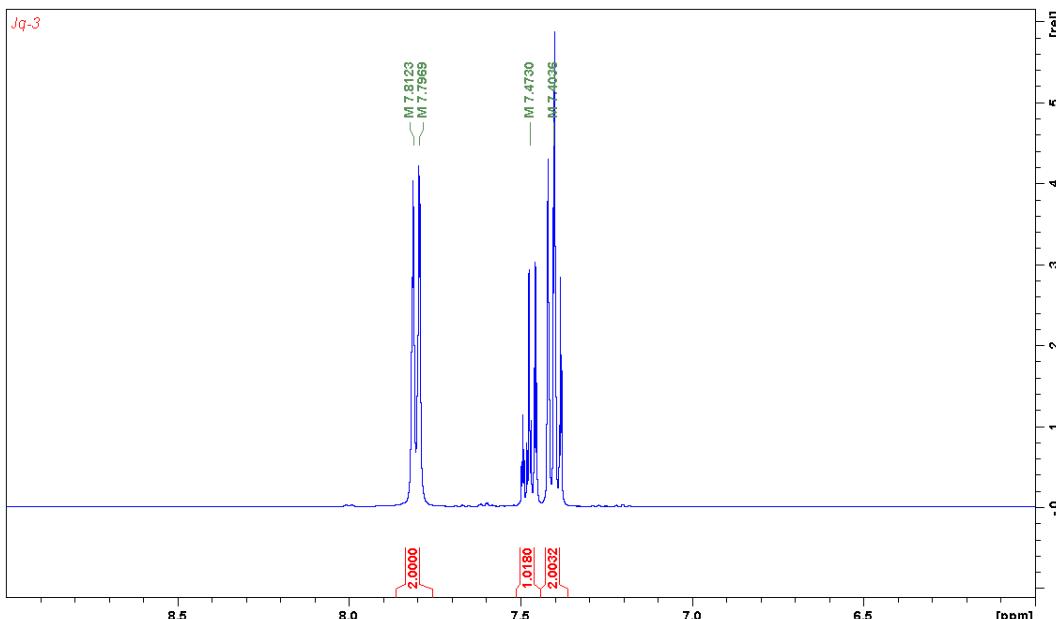
**Figure S4.**  $^1\text{H}$  NMR spectrum of phenylboronic acid in chloroform-d.



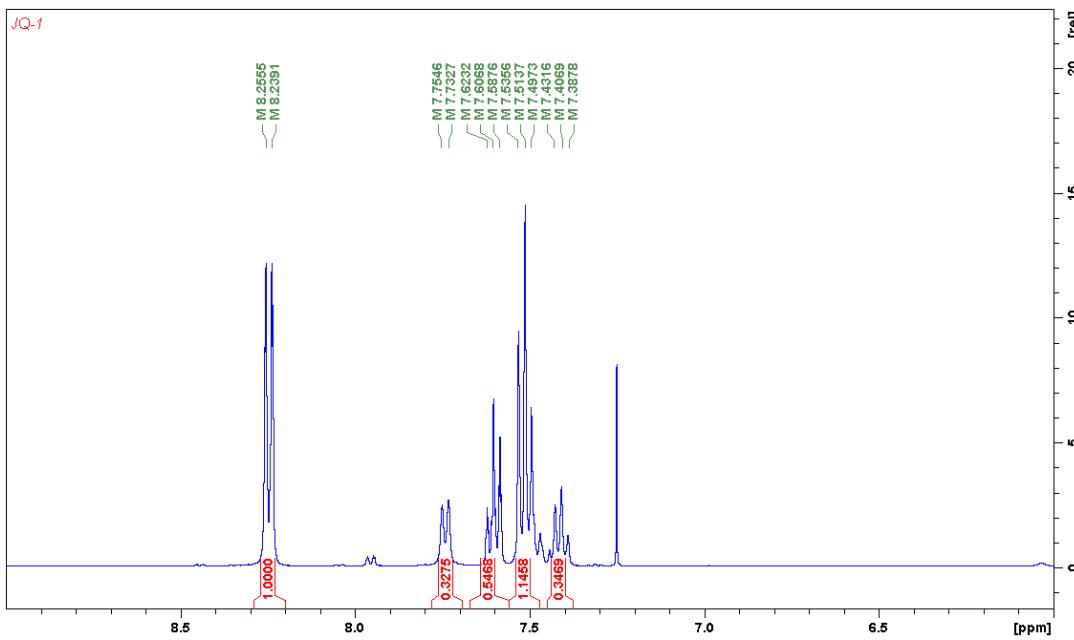
**Figure S5.**  $^1\text{H}$  NMR spectrum of phenylboronic acid in toluene-d8.



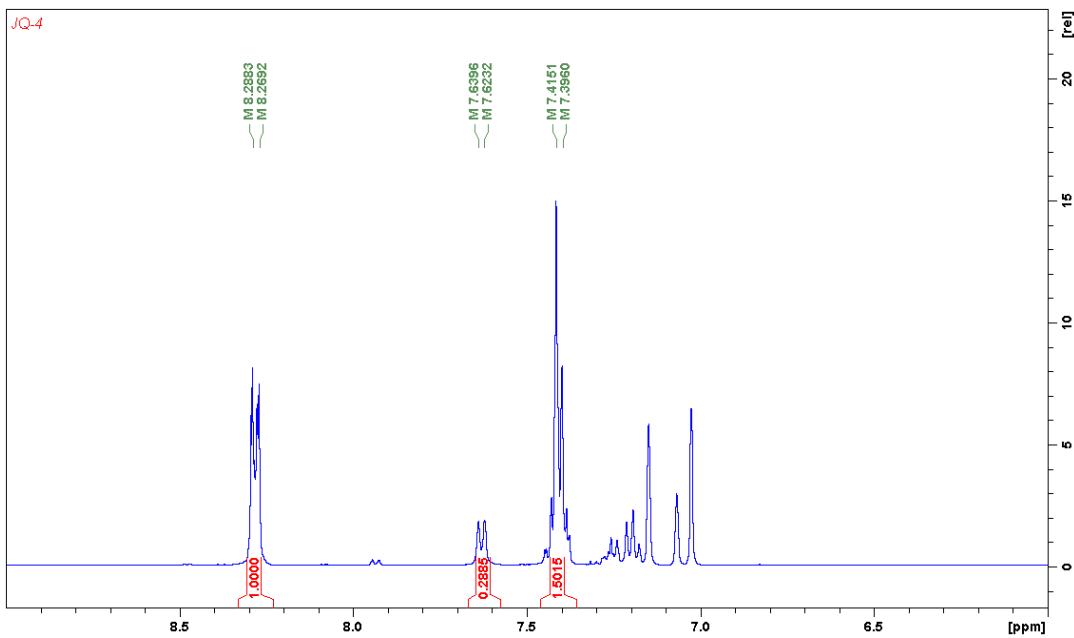
**Figure S6.**  $^1\text{H}$  NMR spectrum of phenylboronic acid in acetone-d6



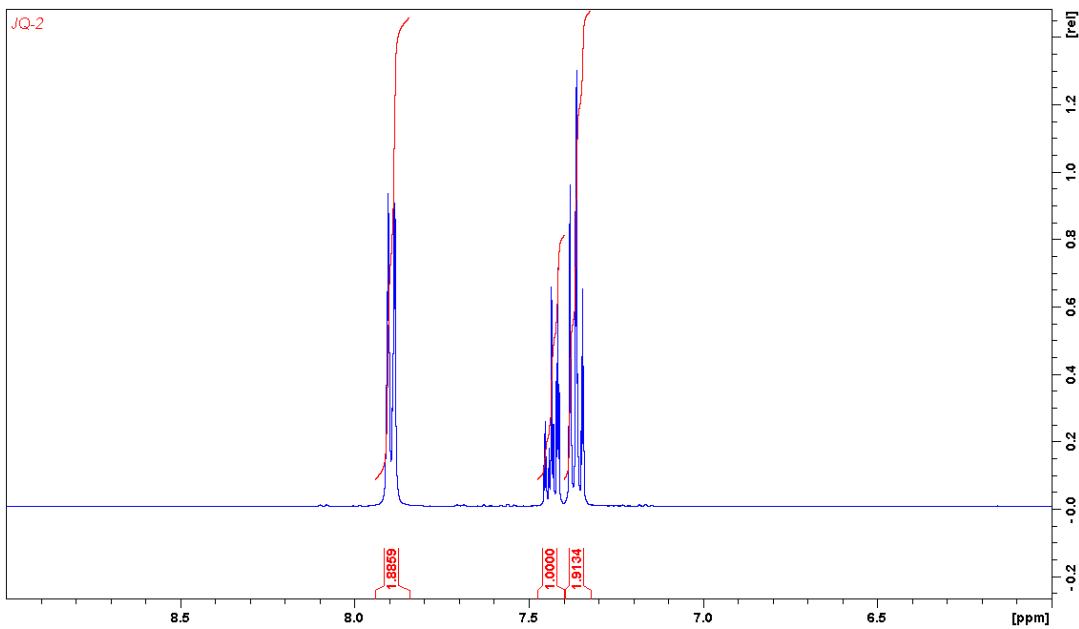
**Figure S7.**  $^1\text{H}$  NMR spectrum of phenylboronic acid in acetonitrile-d3.



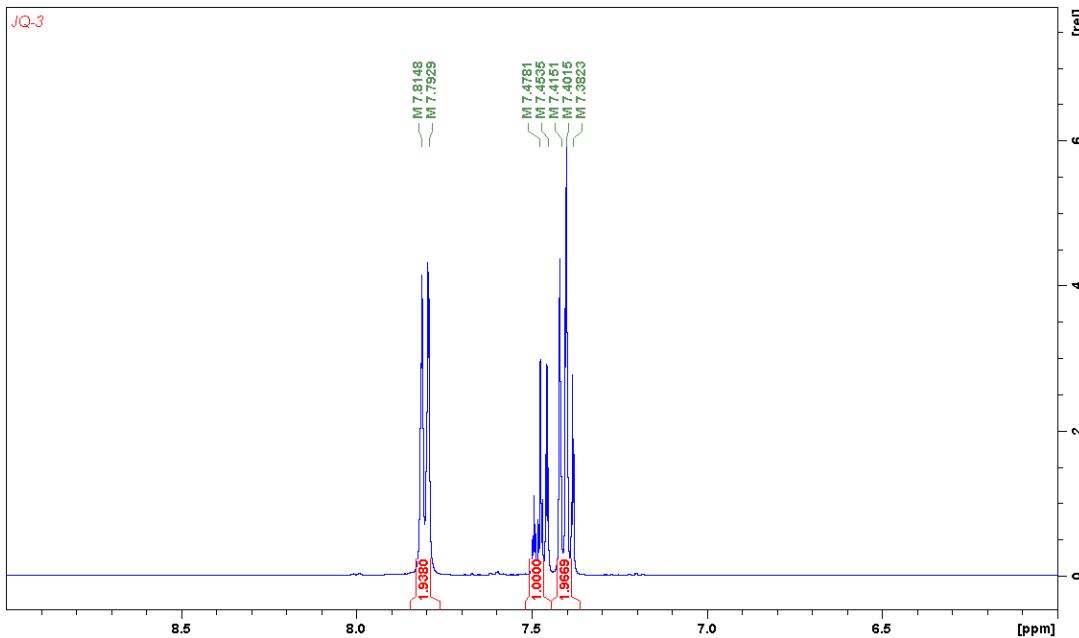
**Figure S8.** <sup>1</sup>H NMR spectrum of phenylboronic acid in chloroform-d after heating at 50 °C for 1 h.



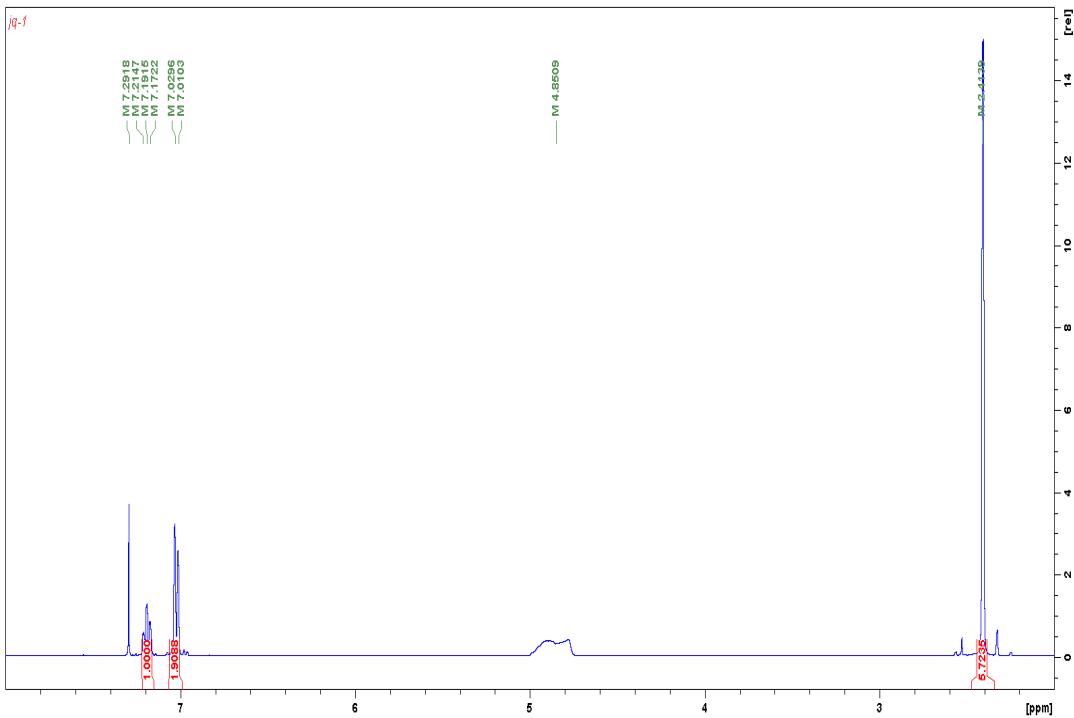
**Figure S9.** <sup>1</sup>H NMR spectrum of phenylboronic acid in toluene-d8 after heating at 50 °C for 1 h.



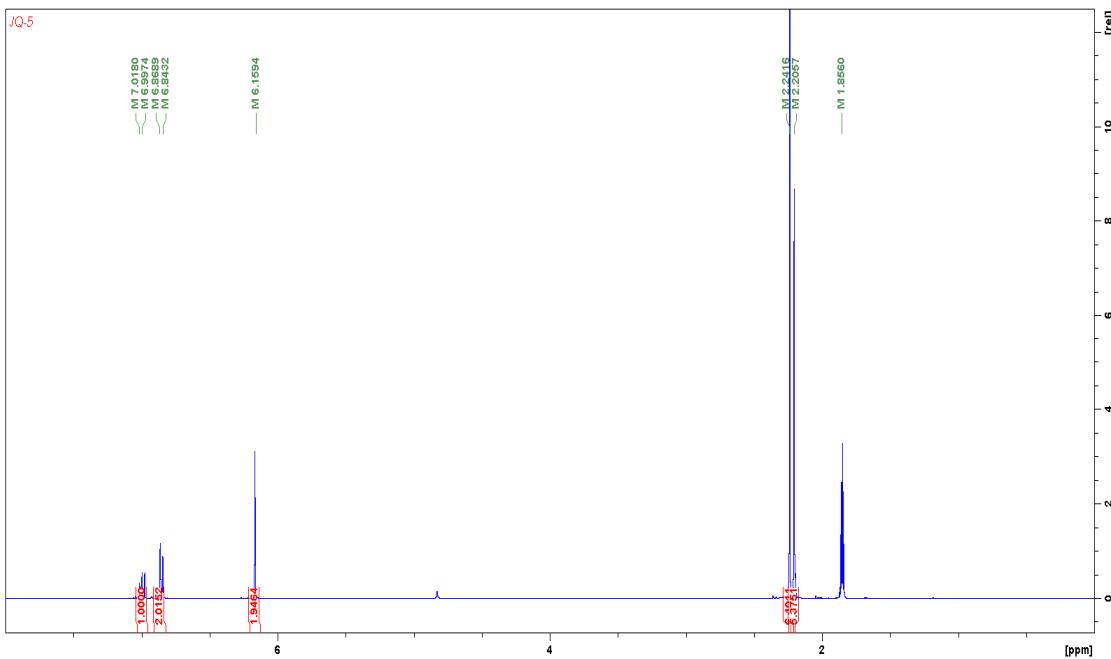
**Figure S10.** <sup>1</sup>H NMR spectrum of phenylboronic acid in acetone-d<sub>6</sub> after heating at 50 °C for 1 h.



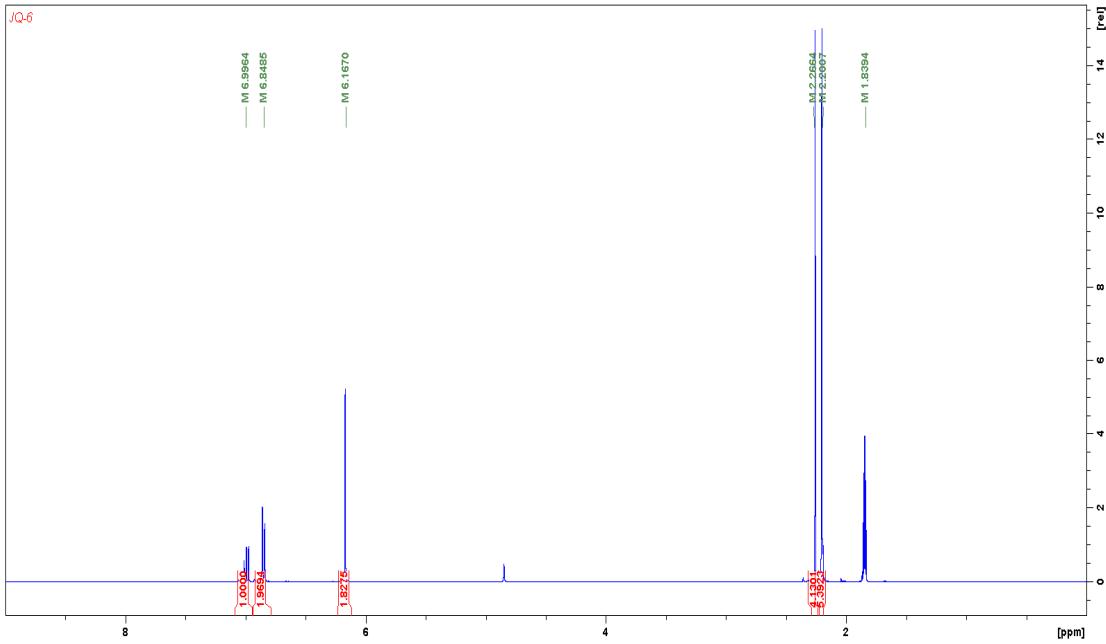
**Figure S11.** <sup>1</sup>H NMR spectrum of phenylboronic acid in acetonitrile-d<sub>3</sub> after heating at 50 °C for 1 h.



**Figure S12.**  $^1\text{H}$  NMR spectrum for commercial B19 in chloroform-d

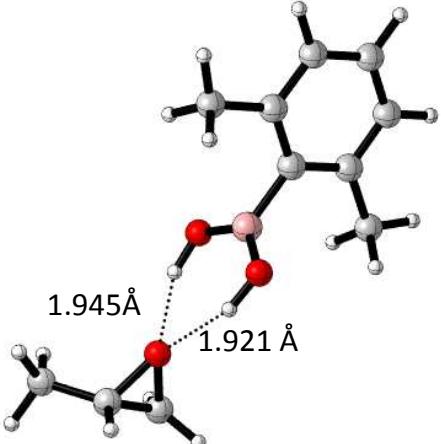


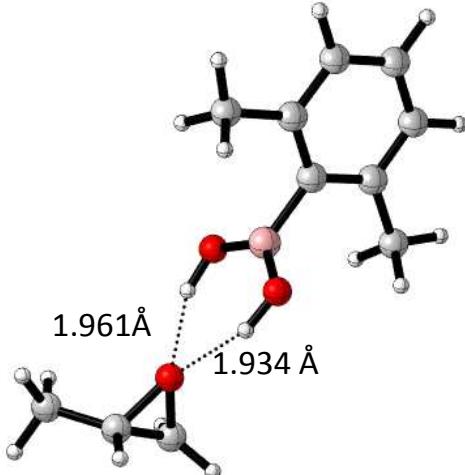
**Figure S13.**  $^1\text{H}$  NMR spectrum for commercial B19 in acetonitrile-d3.



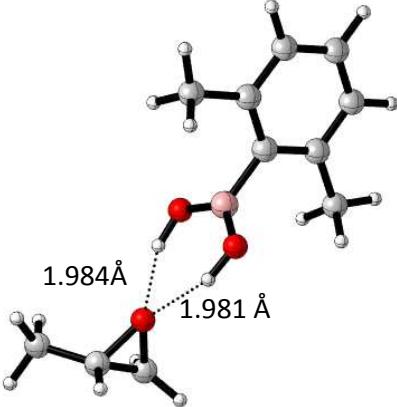
**Figure S14.**  $^1\text{H}$  NMR spectrum for commercial B19 in acetonitrile-d<sub>3</sub> after heating at 50 °C for 1 h.

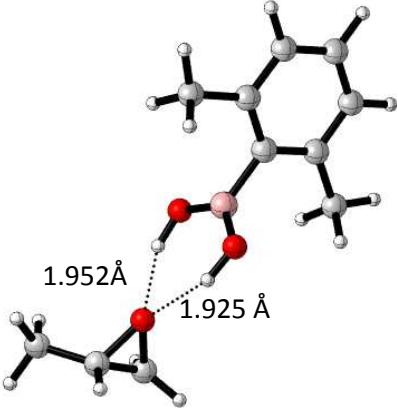
**6. Hydrogen bond and cartesian coordinates for the optimized geometries in Table S1**

| Solvent              | Hydrogen bond and cartesian coordinates for the optimized geometries               |             |             |
|----------------------|--|-------------|-------------|
| $\text{H}_2\text{O}$ |  |             |             |
|                      | C  | 2.40091600  | -1.16354100 |
|                      | C  | 1.61848800  | 0.00356400  |
|                      | C  | 2.25249600  | 1.26210500  |
|                      | C  | 3.64878700  | 1.33787600  |
|                      | C  | 4.41840800  | 0.18377100  |
|                      | C  | 3.79558100  | -1.05984300 |
|                      | H  | 4.13393900  | 2.30726500  |
|                      | H  | 5.50018200  | 0.25348800  |
|                      | H  | 4.39513400  | -1.95923600 |
|                      | B  | 0.04128100  | -0.09775300 |
|                      | O  | -0.67590400 | -0.04352600 |
|                      | H  | -1.63571300 | -0.11446000 |
|                      | O  | -0.56704500 | -0.23701000 |
|                      | H  | -1.53734000 | -0.29094900 |
|                      | C  | 1.74825900  | -2.52829200 |
|                      | H  | 1.27876700  | -2.78898900 |
|                      | H  | 0.96622400  | -2.56470100 |
|                      | H  | 2.47914700  | -3.30524900 |
|                      |  |             | -0.41146100 |

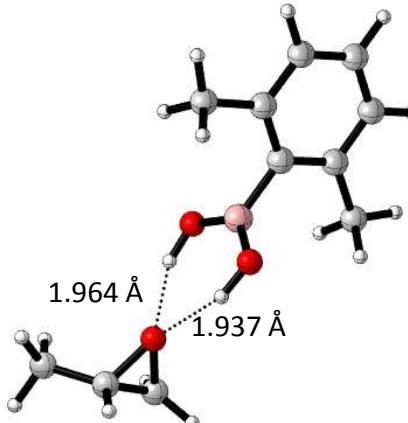
|                 |  |             |             |             |
|-----------------|--|-------------|-------------|-------------|
|                 | C  | 1.43711200  | 2.53180600  | 0.20313000  |
|                 | H  | 0.81786400  | 2.69557000  | -0.68478300 |
|                 | H  | 0.76186700  | 2.49216900  | 1.06330400  |
|                 | H  | 2.08143000  | 3.40466900  | 0.32391500  |
|                 | C  | -4.33111200 | -1.20998700 | 0.23718900  |
|                 | C  | -4.50858000 | 0.23973700  | 0.36921800  |
|                 | O  | -3.17551800 | -0.33137200 | 0.21982300  |
|                 | H  | -4.39416600 | -1.84725900 | 1.11274700  |
|                 | H  | -4.54077500 | -1.68455700 | -0.71610300 |
|                 | H  | -4.67462500 | 0.62511900  | 1.37171500  |
|                 | C  | -4.99734100 | 1.10143900  | -0.75907700 |
|                 | H  | -6.07871900 | 1.24017400  | -0.67175000 |
|                 | H  | -4.52745500 | 2.08758900  | -0.72309200 |
|                 | H  | -4.78251800 | 0.64156700  | -1.72590600 |
| Dichloromethane |  |             |             |             |
|                 | C  | 2.40049700  | -1.16616400 | -0.11318900 |
|                 | C  | 1.62460200  | 0.00514800  | 0.00895300  |
|                 | C  | 2.26535800  | 1.25993100  | 0.07478700  |
|                 | C  | 3.66172000  | 1.32811200  | 0.01906800  |
|                 | C  | 4.42499500  | 0.16973700  | -0.10216400 |
|                 | C  | 3.79538300  | -1.07043900 | -0.16859500 |

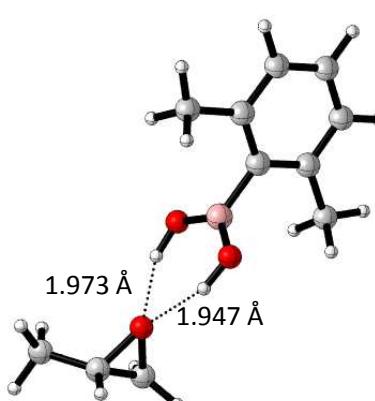
|  |   |             |             |             |
|--|---|-------------|-------------|-------------|
|  | H | 4.15204600  | 2.29516600  | 0.07022600  |
|  | H | 5.50714500  | 0.23347100  | -0.14547300 |
|  | H | 4.38989500  | -1.97352900 | -0.26450400 |
|  | B | 0.04736300  | -0.08759800 | 0.07287000  |
|  | O | -0.66878000 | -0.05597000 | -1.09730100 |
|  | H | -1.62815600 | -0.11948700 | -0.95019600 |
|  | O | -0.56386300 | -0.19727400 | 1.29583400  |
|  | H | -1.53336500 | -0.24945600 | 1.22395000  |
|  | C | 1.73923500  | -2.52672200 | -0.17429200 |
|  | H | 1.24547100  | -2.77103800 | 0.77203700  |
|  | H | 0.97560100  | -2.56605600 | -0.95681900 |
|  | H | 2.46923300  | -3.31215400 | -0.37941100 |
|  | C | 1.45636200  | 2.53366500  | 0.19804000  |
|  | H | 0.81350800  | 2.68257600  | -0.67556200 |
|  | H | 0.80565800  | 2.51037800  | 1.07759800  |
|  | H | 2.10554300  | 3.40700300  | 0.28562300  |
|  | C | -4.33114200 | -1.20794700 | 0.26070800  |
|  | C | -4.52433000 | 0.24219500  | 0.36619900  |
|  | O | -3.18678400 | -0.31694400 | 0.22309200  |
|  | H | -4.38470100 | -1.82982100 | 1.14807100  |
|  | H | -4.53873900 | -1.70292200 | -0.68273900 |
|  | H | -4.69201700 | 0.64423200  | 1.36208700  |
|  | C | -5.02651600 | 1.07779100  | -0.77599400 |
|  | H | -6.10908200 | 1.20693600  | -0.68809700 |
|  | H | -4.56686200 | 2.06926900  | -0.76012900 |
|  | H | -4.80955500 | 0.60309400  | -1.73514100 |

|         |   |  |             |
|---------|---|--|-------------|
|         |   |  |             |
| Toluene | C | -2.37876700  | -1.19318500 |
|         | C | -1.62449000  | -0.00219000 |
|         | C | -2.29219100  | 1.24180200  |
|         | C | -3.68559900  | 1.27849500  |
|         | C | -4.42470000  | 0.10217800  |
|         | C | -3.77204500  | -1.12615500 |
|         | H | -4.19323500  | 2.23745600  |
|         | H | -5.50552400  | 0.14257200  |
|         | H | -4.34768400  | -2.04471000 |
|         | B | -0.05057200  | -0.06007800 |
|         | O | 0.67452300   | -0.62463800 |
|         | H | 1.62977000   | -0.61786200 |
|         | O | 0.55818100   | 0.45609500  |
|         | H | 1.52543100   | 0.38048500  |
|         | C | -1.70743800  | -2.55022400 |
|         | H | -1.07884000  | -2.66694800 |
|         | H | -1.06183400  | -2.69354800 |
|         | H | -2.44883100  | -3.35186800 |
|         | C | -1.52622400  | 2.54553900  |
|         | H | -0.75692100  | 2.60997000  |
|         | H | -1.01889600  | 2.64673400  |
|         | H | -2.19540100  | 3.39929200  |
|         |   |  | 0.04349200  |

|         |   |             |             |             |  |
|---------|---|-------------|-------------|-------------|--|
|         | C   | 4.42419800  | -0.86709100 | -0.80661900 |  |
|         | C   | 4.53061500  | 0.43120200  | -0.13103800 |  |
|         | O   | 3.23002800  | -0.17066600 | -0.37611600 |  |
|         | H   | 4.54200800  | -0.93216400 | -1.88347200 |  |
|         | H   | 4.63652300  | -1.77423500 | -0.24891000 |  |
|         | H   | 4.70365900  | 1.30020500  | -0.76137600 |  |
|         | C   | 4.94707600  | 0.56638100  | 1.30597600  |  |
|         | H   | 6.02166500  | 0.76297000  | 1.36274000  |  |
|         | H   | 4.42627500  | 1.40124900  | 1.78167900  |  |
|         | H   | 4.73023500  | -0.34604300 | 1.86534900  |  |
|         |   |             |             |             |  |
| Acetone |  |             |             |             |  |
|         | C   | 2.40106800  | -1.16446300 | -0.11484700 |  |
|         | C   | 1.62096400  | 0.00417700  | 0.00887400  |  |
|         | C   | 2.25739100  | 1.26134300  | 0.07718000  |  |
|         | C   | 3.65372200  | 1.33438100  | 0.02282500  |  |
|         | C   | 4.42109700  | 0.17871800  | -0.10019000 |  |
|         | C   | 3.79583300  | -1.06365600 | -0.16941800 |  |
|         | H   | 4.14071400  | 2.30294900  | 0.07647000  |  |
|         | H   | 5.50303200  | 0.24626400  | -0.14255600 |  |
|         | H   | 4.39360300  | -1.96440500 | -0.26678300 |  |
|         | B   | 0.04373400  | -0.09410300 | 0.07223900  |  |
|         | O   | -0.67272400 | -0.04923800 | -1.09713100 |  |

|  |   |             |             |             |
|--|---|-------------|-------------|-------------|
|  | H | -1.63241600 | -0.11732400 | -0.95046400 |
|  | O | -0.56604800 | -0.22143700 | 1.29413300  |
|  | H | -1.53602200 | -0.27483200 | 1.22197900  |
|  | C | 1.74529500  | -2.52768200 | -0.17775100 |
|  | H | 1.26543000  | -2.78194800 | 0.77310600  |
|  | H | 0.97112700  | -2.56536800 | -0.94989300 |
|  | H | 2.47622300  | -3.30791000 | -0.39854300 |
|  | C | 1.44420900  | 2.53247900  | 0.20070300  |
|  | H | 0.81608800  | 2.69021200  | -0.68203800 |
|  | H | 0.77807500  | 2.49908700  | 1.06825100  |
|  | H | 2.09030400  | 3.40573100  | 0.30883200  |
|  | C | -4.33118600 | -1.20892600 | 0.24806300  |
|  | C | -4.51443600 | 0.24118300  | 0.36845700  |
|  | O | -3.17982000 | -0.32559000 | 0.22049900  |
|  | H | -4.38954600 | -1.83933200 | 1.12896800  |
|  | H | -4.54130000 | -1.69234900 | -0.70071700 |
|  | H | -4.67980300 | 0.63413900  | 1.36821000  |
|  | C | -5.00975800 | 1.09153200  | -0.76565900 |
|  | H | -6.09153000 | 1.22652300  | -0.67707600 |
|  | H | -4.54390500 | 2.07988400  | -0.73910500 |
|  | H | -4.79519500 | 0.62479700  | -1.7292     |

|                 |  |             |             |             |
|-----------------|--|-------------|-------------|-------------|
|                 | <br> |             |             |             |
| Tetrahydrofuran | C  | 2.40091800  | -1.16634500 | -0.11290200 |
|                 | C  | 1.62542600  | 0.00514300  | 0.00904400  |
|                 | C  | 2.26655800  | 1.25967500  | 0.07437800  |
|                 | C  | 3.66286500  | 1.32744300  | 0.01826900  |
|                 | C  | 4.42576400  | 0.16885000  | -0.10272500 |
|                 | C  | 3.79576500  | -1.07110500 | -0.16858000 |
|                 | H  | 4.15348600  | 2.29438100  | 0.06896500  |
|                 | H  | 5.50792800  | 0.23225200  | -0.14626800 |
|                 | H  | 4.38995600  | -1.97444300 | -0.26421600 |
|                 | B  | 0.04824400  | -0.08704900 | 0.07321700  |
|                 | O  | -0.66781500 | -0.05947700 | -1.09710200 |
|                 | H  | -1.62709900 | -0.12261400 | -0.95038700 |
|                 | O  | -0.56306000 | -0.19220600 | 1.29657200  |
|                 | H  | -1.53239200 | -0.24445800 | 1.22514600  |
|                 | C  | 1.73899200  | -2.52656700 | -0.17377200 |
|                 | H  | 1.24036900  | -2.76800900 | 0.77073900  |
|                 | H  | 0.97928700  | -2.56709100 | -0.96007600 |
|                 | H  | 2.46937700  | -3.31308900 | -0.37334800 |
|                 | C  | 1.45787300  | 2.53357500  | 0.19765200  |
|                 | H  | 0.81261200  | 2.68085500  | -0.67445600 |
|                 | H  | 0.80977500  | 2.51166300  | 1.07917300  |

|            |   |             |             |             |  |
|------------|---|-------------|-------------|-------------|--|
|            | H   | 2.10726400  | 3.40711300  | 0.28188300  |  |
|            | C   | -4.33299900 | -1.20713900 | 0.26434300  |  |
|            | C   | -4.52628500 | 0.24337300  | 0.36522900  |  |
|            | O   | -3.18893900 | -0.31617300 | 0.22414600  |  |
|            | H   | -4.38675800 | -1.82623700 | 1.15366700  |  |
|            | H   | -4.54044300 | -1.70521600 | -0.67753000 |  |
|            | H   | -4.69427500 | 0.64845400  | 1.35987300  |  |
|            | C   | -5.02837700 | 1.07551300  | -0.77957000 |  |
|            | H   | -6.11100300 | 1.20480900  | -0.69251500 |  |
|            | H   | -4.56883900 | 2.06708500  | -0.76658200 |  |
|            | H   | -4.81094800 | 0.59813900  | -1.73727700 |  |
|            |   |             |             |             |  |
| Chloroform |  |             |             |             |  |
|            | C   | 2.40027600  | -1.16793600 | -0.11102900 |  |
|            | C   | 1.62897300  | 0.00621900  | 0.00944200  |  |
|            | C   | 2.27439000  | 1.25836700  | 0.07180500  |  |
|            | C   | 3.67068200  | 1.32134700  | 0.01366000  |  |
|            | C   | 4.42947600  | 0.16010200  | -0.10574300 |  |
|            | C   | 3.79518600  | -1.07769100 | -0.16819400 |  |
|            | H   | 4.16458400  | 2.28678200  | 0.06154800  |  |
|            | H   | 5.51180600  | 0.21973200  | -0.15072700 |  |
|            | H   | 4.38613600  | -1.98332300 | -0.26243100 |  |
|            | B   | 0.05184800  | -0.08090300 | 0.07473700  |  |

|  |   |             |             |             |
|--|---|-------------|-------------|-------------|
|  | O | -0.66418900 | -0.06695200 | -1.09595800 |
|  | H | -1.62313200 | -0.12585700 | -0.94891900 |
|  | O | -0.56023300 | -0.16855700 | 1.29915700  |
|  | H | -1.52904600 | -0.22016000 | 1.22867400  |
|  | C | 1.73305700  | -2.52559800 | -0.16928700 |
|  | H | 1.22240900  | -2.75735100 | 0.77122300  |
|  | H | 0.98263500  | -2.56810100 | -0.96439900 |
|  | H | 2.46210500  | -3.31693100 | -0.35450300 |
|  | C | 1.46990000  | 2.53484500  | 0.19495700  |
|  | H | 0.81203700  | 2.67501700  | -0.66886400 |
|  | H | 0.83546500  | 2.52192300  | 1.08657800  |
|  | H | 2.12201500  | 3.40797200  | 0.26137400  |
|  | C | -4.33371000 | -1.20658700 | 0.27271500  |
|  | C | -4.53663700 | 0.24351200  | 0.36275700  |
|  | O | -3.19647700 | -0.30836900 | 0.22719000  |
|  | H | -4.38463200 | -1.81979400 | 1.16639200  |
|  | H | -4.53706200 | -1.71319100 | -0.66560300 |
|  | H | -4.70866400 | 0.65455700  | 1.35440200  |
|  | C | -5.04330500 | 1.06439200  | -0.78829500 |
|  | H | -6.12702400 | 1.18656100  | -0.70420000 |
|  | H | -4.59083100 | 2.05925700  | -0.78150700 |
|  | H | -4.82057900 | 0.58261200  | -1.74256800 |

**7. NBO charges and cartesian coordinates for all the optimized geometries in Scheme 3**

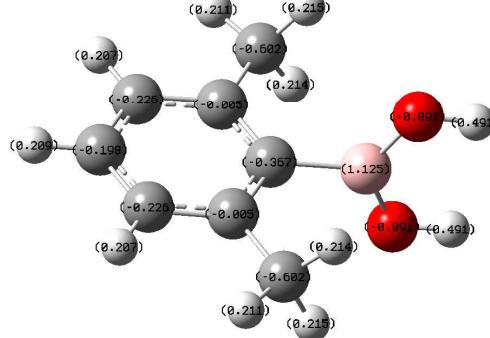
|    |   |             |             |             |
|----|---|-------------|-------------|-------------|
| B1 |   |             |             |             |
|    | C | -0.55649900 | -1.20371600 | -0.00755000 |
|    | C | 0.17032500  | -0.00000700 | -0.00004800 |
|    | C | -0.55649900 | 1.20370400  | 0.00739300  |
|    | C | -1.95131100 | 1.20779700  | 0.00778600  |
|    | C | -2.65202200 | 0.00000100  | 0.00006400  |
|    | C | -1.95130900 | -1.20779600 | -0.00775100 |
|    | H | -2.49302000 | 2.15088600  | 0.01446500  |
|    | H | -3.73972700 | 0.00000000  | 0.00011200  |
|    | H | -2.49302300 | -2.15088400 | -0.01434400 |
|    | B | 1.73962700  | -0.00000100 | -0.00005100 |
|    | O | 2.39427600  | 1.20554100  | -0.01626400 |
|    | H | 3.37348700  | 1.13176900  | -0.01035800 |
|    | O | 2.39430300  | -1.20552900 | 0.01635400  |
|    | H | 3.37351200  | -1.13174300 | 0.01047100  |
|    | H | -0.02205700 | -2.15003600 | -0.01302600 |
|    | H | -0.02205500 | 2.15002700  | 0.01286300  |
| B2 |   |             |             |             |
|    | C | -0.06558700 | 1.20027900  | 0.00926600  |

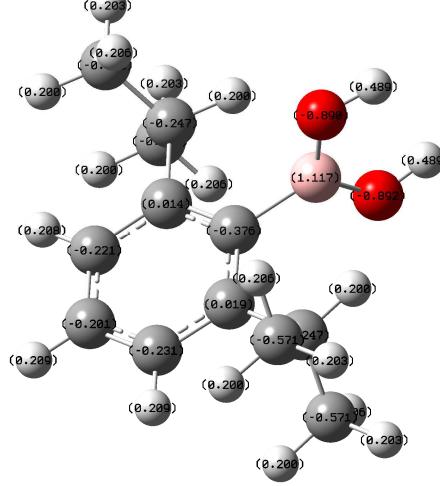
|     |   |             |             |             |
|-----|---|-------------|-------------|-------------|
|     | C | 0.66437100  | 0.00076500  | -0.00019800 |
|     | C | -0.06881600 | -1.19899900 | -0.01527700 |
|     | C | -1.46041500 | -1.19890500 | -0.02090600 |
|     | C | -2.18153900 | 0.00329900  | -0.00712100 |
|     | C | -1.45923200 | 1.20242800  | 0.00628300  |
|     | H | -1.99761700 | -2.14236800 | -0.03767600 |
|     | H | -1.99488300 | 2.14662900  | 0.01224600  |
|     | B | 2.22731300  | -0.00074000 | 0.00217600  |
|     | O | 2.87807100  | -1.21065700 | 0.02922600  |
|     | H | 3.84050400  | -1.16683000 | 0.03542900  |
|     | O | 2.88076700  | 1.20776600  | -0.02276800 |
|     | H | 3.84311800  | 1.16185100  | -0.02584200 |
|     | H | 0.46508700  | 2.14626000  | 0.01768400  |
|     | H | 0.46091000  | -2.14548300 | -0.02654600 |
|     | C | -3.69026800 | -0.00100800 | 0.01072100  |
|     | H | -4.06743800 | -0.27306200 | 1.00240200  |
|     | H | -4.09434500 | 0.98188000  | -0.23906800 |
|     | H | -4.09369100 | -0.72919200 | -0.69777700 |
| B10 |   |             |             |             |
|     | C | -1.82359900 | 1.45624000  | 0.03467400  |
|     | C | -0.47778400 | 1.04731900  | -0.00160000 |
|     | C | -0.25095500 | -0.33909700 | 0.02148500  |
|     | C | -1.30031300 | -1.25804100 | 0.03204400  |
|     | C | -2.62972200 | -0.83115200 | 0.02435100  |



|     |   |             |             |             |  |
|-----|---|-------------|-------------|-------------|--|
|     | C | -0.52925800 | 0.16287000  | -0.00242700 |  |
|     | C | -0.14660300 | 1.51553300  | 0.00054600  |  |
|     | C | 1.20416900  | 1.85989000  | 0.00049200  |  |
|     | C | 2.18944000  | 0.87560800  | -0.00394600 |  |
|     | C | 1.83432900  | -0.48307600 | -0.00695900 |  |
|     | H | 1.49915700  | 2.90394700  | 0.00566000  |  |
|     | H | 3.23832400  | 1.15508200  | -0.00442400 |  |
|     | B | -2.04128700 | -0.24626400 | 0.00112300  |  |
|     | O | -2.98553100 | 0.75101000  | 0.01259000  |  |
|     | H | -3.90319800 | 0.45750700  | 0.01371800  |  |
|     | O | -2.35570100 | -1.58338300 | -0.00743200 |  |
|     | H | -3.29640500 | -1.79140200 | -0.00544000 |  |
|     | H | 0.18988600  | -1.86660500 | -0.00933700 |  |
|     | H | -0.90355600 | 2.29079200  | 0.00505800  |  |
|     | N | 2.81608100  | -1.47709900 | -0.07164200 |  |
|     | H | 3.72288900  | -1.21078900 | 0.28717600  |  |
|     | H | 2.53300500  | -2.38306900 | 0.27622800  |  |
| B14 |   |             |             |             |  |
|     | C | -0.57262700 | 1.19164300  | 0.02340800  |  |
|     | C | 0.16412900  | 0.00000000  | -0.00000400 |  |
|     | C | -0.57262800 | -1.19164400 | -0.02341300 |  |
|     | C | -1.96433800 | -1.14298900 | -0.02472800 |  |
|     | C | -1.96433700 | 1.14299000  | 0.02473100  |  |
|     | H | -2.54488100 | -2.06083500 | -0.04612600 |  |
|     | H | -2.54488000 | 2.06083500  | 0.04613200  |  |

|     |   |             |             |             |  |
|-----|---|-------------|-------------|-------------|--|
|     | B | 1.73815600  | -0.00000100 | -0.00001200 |  |
|     | O | 2.37302700  | -1.21075900 | 0.04743400  |  |
|     | H | 3.33641000  | -1.18309800 | 0.05408100  |  |
|     | O | 2.37302700  | 1.21075900  | -0.04742800 |  |
|     | H | 3.33641000  | 1.18309900  | -0.05405400 |  |
|     | H | -0.07014400 | 2.15145700  | 0.04245300  |  |
|     | H | -0.07014500 | -2.15145700 | -0.04246200 |  |
|     | N | -2.66331000 | 0.00000000  | 0.00000400  |  |
| B15 |   |             |             |             |  |
|     | C | -0.58029100 | 1.20648400  | 0.02104100  |  |
|     | C | 0.15840900  | 0.01496000  | 0.00033800  |  |
|     | C | -0.57846800 | -1.17850200 | -0.02079400 |  |
|     | C | -1.97032800 | 1.15768100  | 0.02188700  |  |
|     | H | -2.56712500 | 2.06169300  | 0.04012200  |  |
|     | B | 1.72603600  | 0.00723800  | 0.00021600  |  |
|     | O | 2.36346000  | -1.20477500 | 0.04123600  |  |
|     | H | 3.32660300  | -1.17405200 | 0.04697800  |  |
|     | O | 2.36811300  | 1.21674200  | -0.04086000 |  |
|     | H | 3.33118200  | 1.18292100  | -0.04686700 |  |
|     | H | -0.06732600 | 2.16153200  | 0.03805200  |  |
|     | H | -0.05671400 | -2.13069300 | -0.03821100 |  |
|     | C | -2.59023300 | -0.08977600 | -0.00173300 |  |
|     | H | -3.67392200 | -0.16407900 | -0.00307400 |  |
|     | N | -1.91571400 | -1.24776100 | -0.02364600 |  |

|     |   |  |             |
|-----|---|--|-------------|
|     |   |  |             |
| B19 | C | 0.60631400   | 1.21968600  |
|     | C | -0.10221900  | 0.00002600  |
|     | C | 0.60620700   | -1.21970300 |
|     | C | 2.00541300   | -1.20520800 |
|     | C | 2.70320300   | -0.00010000 |
|     | C | 2.00552000   | 1.20506800  |
|     | H | 2.54955800   | -2.14417600 |
|     | H | 3.78799800   | -0.00014900 |
|     | H | 2.54974400   | 2.14399100  |
|     | B | -1.68181200  | 0.00005200  |
|     | O | -2.33130800  | -0.09324400 |
|     | H | -3.29538600  | -0.09546100 |
|     | O | -2.33127700  | 0.09336400  |
|     | H | -3.29535800  | 0.09552100  |
|     | C | -0.13089400  | 2.54187200  |
|     | H | -0.74309000  | 2.66720400  |
|     | H | -0.80253700  | 2.61661000  |
|     | H | 0.56529700   | 3.38111900  |
|     | C | -0.13111200  | -2.54182800 |
|     | H | -0.74256200  | -2.66745300 |
|     | H | -0.80348500  | -2.61619300 |
|     | H | 0.56497700   | -3.38110700 |
|     |   | -0.07825500  |             |

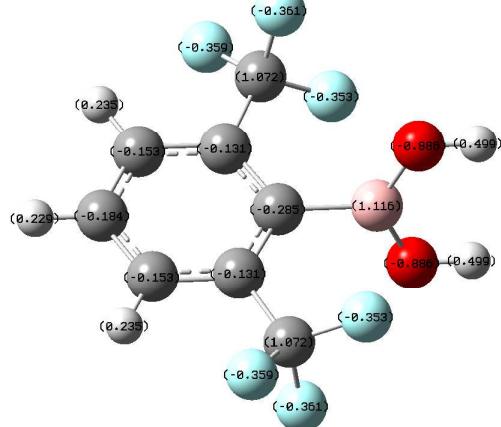
|     |   |  |             |
|-----|---|--|-------------|
|     |   |  |             |
| B20 | C | -1.21863400  | -0.53977600 |
|     | C | 0.00026700   | 0.17133600  |
|     | C | 1.21917400   | -0.53928700 |
|     | C | 1.20607600   | -1.93910600 |
|     | C | 0.00063200   | -2.63755000 |
|     | C | -1.20514200  | -1.93949100 |
|     | H | 2.14753100   | -2.48454900 |
|     | H | 0.00086600   | -3.72521400 |
|     | H | -2.14639700  | -2.48525000 |
|     | B | -0.00036700  | 1.75299500  |
|     | O | 0.09610300   | 2.41148800  |
|     | H | 0.07998900   | 3.38128100  |
|     | O | -0.09782200  | 2.41935000  |
|     | H | -0.08868200  | 3.38837400  |
|     | C | 2.56423500   | 0.21062500  |
|     | C | 3.34575000   | -0.14851200 |
|     | C | 3.32191600   | -0.12747600 |
|     | H | 2.32877000   | 1.30794500  |
|     | H | 2.76430500   | 0.11120500  |
|     | H | 4.31506900   | 0.40565300  |
|     | H | 3.56833300   | -1.24278500 |
|     | H |  | -1.24880900 |

|     |   |             |             |             |
|-----|---|-------------|-------------|-------------|
|     | H | 2.72319300  | 0.14753400  | 2.16976000  |
|     | H | 3.54377300  | -1.22125800 | 1.31211500  |
|     | H | 4.29066800  | 0.42718900  | 1.30530900  |
|     | C | -2.56397500 | 0.20965400  | -0.00600800 |
|     | C | -3.34180800 | -0.14879500 | 1.23415000  |
|     | C | -3.32514300 | -0.12969700 | -1.26175500 |
|     | H | -2.32887000 | 1.30706500  | 0.00404200  |
|     | H | -2.75782600 | 0.11184200  | 2.14949500  |
|     | H | -4.31124000 | 0.40504700  | 1.26445200  |
|     | H | -3.56393900 | -1.24313100 | 1.25689500  |
|     | H | -2.72910800 | 0.14482300  | -2.16516600 |
|     | H | -3.54673500 | -1.22359100 | -1.30410400 |
|     | H | -4.29419500 | 0.42459600  | -1.29643800 |
| B21 |   |             |             |             |
|     | C | 1.20191900  | -0.50130400 | 0.00512100  |
|     | C | 0.00000600  | 0.21927200  | -0.00000600 |
|     | C | -1.20186000 | -0.50138100 | -0.00512700 |
|     | C | -1.21638200 | -1.90168700 | -0.00497300 |
|     | C | 0.00009700  | -2.58058300 | 0.00000100  |
|     | C | 1.21653300  | -1.90160800 | 0.00497300  |
|     | H | -2.14334800 | -2.45754300 | -0.00946300 |

|     |  |             |             |             |
|-----|--|-------------|-------------|-------------|
|     | H  | 0.00013200  | -3.66493800 | 0.00000300  |
|     | H  | 2.14353600  | -2.45740300 | 0.00946600  |
|     | B  | -0.00002900 | 1.79737300  | 0.00000200  |
|     | O  | -0.07430600 | 2.44442900  | 1.20595300  |
|     | H  | -0.08026900 | 3.40820100  | 1.16335400  |
|     | O  | 0.07403800  | 2.44446400  | -1.20594000 |
|     | H  | 0.07985300  | 3.40823600  | -1.16332200 |
|     | C  | -3.60947700 | -0.37634400 | -0.01382100 |
|     | H  | -4.34659600 | 0.42430200  | -0.01755900 |
|     | H  | -3.73979100 | -0.99509900 | -0.90625500 |
|     | H  | -3.74277900 | -0.98959600 | 0.88197000  |
|     | C  | 3.60952200  | -0.37613100 | 0.01382400  |
|     | H  | 3.74287400  | -0.98936500 | -0.88197200 |
|     | H  | 4.34659800  | 0.42455400  | 0.01758900  |
|     | H  | 3.73984700  | -0.99489200 | 0.90625200  |
|     | O  | -2.33485100 | 0.26893600  | -0.01346100 |
|     | O  | 2.33486200  | 0.26908100  | 0.01344500  |
| B22 | <p>Detailed description: A 3D ball-and-stick model of a molecule. Carbon atoms are grey spheres, hydrogen atoms are white spheres, and oxygen atoms are red spheres. Bond lengths are labeled in parentheses next to the atoms. For example, one carbon atom has a bond length of 0.355, another has 0.440, and so on.</p> |             |             |             |
|     | C  | -0.59526200 | -1.16955400 | 0.02223300  |
|     | C  | 0.15719500  | 0.00006100  | -0.00001200 |
|     | C  | -0.59546600 | 1.16954100  | -0.02224800 |
|     | C  | -1.98024400 | 1.21059200  | -0.02415700 |

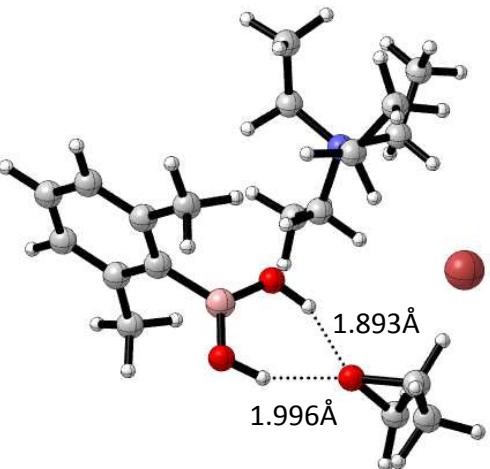
|     |   |             |             |             |  |
|-----|---|-------------|-------------|-------------|--|
|     | C | -2.67091800 | -0.00019100 | 0.00001200  |  |
|     | C | -1.98003200 | -1.21085400 | 0.02416600  |  |
|     | H | -2.49623200 | 2.16169700  | -0.04474800 |  |
|     | H | -3.75388400 | -0.00028600 | 0.00002000  |  |
|     | H | -2.49585400 | -2.16204900 | 0.04477000  |  |
|     | B | 1.74193300  | 0.00016600  | -0.00000800 |  |
|     | O | 2.36722800  | 0.13447400  | 1.20397100  |  |
|     | H | 3.33202700  | 0.13266300  | 1.18160900  |  |
|     | O | 2.36727100  | -0.13432100 | -1.20394900 |  |
|     | H | 3.33206800  | -0.13264000 | -1.18153000 |  |
|     | F | 0.08268700  | -2.35423800 | 0.04826200  |  |
|     | F | 0.08226700  | 2.35434900  | -0.04828600 |  |
| B23 |   |             |             |             |  |
|     | C | -1.18216200 | 0.67119900  | -0.00381300 |  |
|     | C | -0.00001900 | -0.07582600 | -0.00000100 |  |
|     | C | 1.18186000  | 0.67161500  | 0.00381500  |  |
|     | C | 1.20836500  | 2.06174900  | 0.00354900  |  |
|     | C | -0.00051300 | 2.75279800  | 0.00001800  |  |
|     | C | -1.20914900 | 2.06132400  | -0.00352700 |  |
|     | H | 2.15145300  | 2.59197200  | 0.00637700  |  |
|     | H | -0.00070300 | 3.83607900  | 0.00002500  |  |
|     | H | -2.15242200 | 2.59121700  | -0.00635500 |  |
|     | B | 0.00026500  | -1.66294600 | 0.00001200  |  |
|     | O | -0.06013800 | -2.28760200 | 1.21059700  |  |

|     |   |             |             |             |
|-----|---|-------------|-------------|-------------|
|     | H   | -0.06988900 | -3.25221500 | 1.18726100  |
|     | O   | 0.06119400  | -2.28759900 | -1.21055300 |
|     | H   | 0.07159100  | -3.25220100 | -1.18721700 |
|     | Cl  | -2.72894100 | -0.19034600 | -0.01306500 |
|     | Cl  | 2.72893600  | -0.18939800 | 0.01302100  |
|     |   |             |             |             |
| B24 | <p>Detailed description: A 3D ball-and-stick model of a molecule. It consists of 12 atoms: four red spheres (oxygen), eight grey spheres (carbon), and one small white sphere (hydrogen). The atoms are interconnected by grey sticks representing bonds. Bond lengths are labeled in parentheses next to the atoms. For example, one oxygen atom has a bond length of (0.497) and another has (0.889).</p> |             |             |             |
|     | C   | -1.18226600 | 0.75915500  | 0.00006400  |
|     | C   | 0.00000400  | 0.00958200  | 0.00000400  |
|     | C   | 1.18228100  | 0.75914400  | -0.00005000 |
|     | C   | 1.20867300  | 2.14962000  | 0.00039200  |
|     | C   | 0.00001500  | 2.84132000  | 0.00003100  |
|     | C   | -1.20864800 | 2.14963100  | -0.00034900 |
|     | H   | 2.14933300  | 2.68375600  | 0.00080400  |
|     | H   | 0.00002100  | 3.92477800  | 0.00004100  |
|     | H   | -2.14930400 | 2.68377400  | -0.00075200 |
|     | B   | -0.00000700 | -1.57807900 | 0.00004300  |
|     | O   | 0.04496600  | -2.20289900 | 1.21144200  |
|     | H   | 0.05735400  | -3.16742500 | 1.18775500  |
|     | O   | -0.04503100 | -2.20295200 | -1.21134500 |
|     | H   | -0.05748900 | -3.16747500 | -1.18767100 |
|     | Br  | -2.87584500 | -0.16900200 | 0.00502500  |
|     | Br  | 2.87585400  | -0.16902400 | -0.00507400 |

|     |   |  |             |
|-----|---|--|-------------|
|     |   |  |             |
| B25 | C | -1.19423500  | 0.72974800  |
|     | C | 0.00000800   | -0.01407300 |
|     | C | 1.19424700   | 0.72976700  |
|     | C | 1.19904900   | 2.12589700  |
|     | C | -0.00001300  | 2.82567000  |
|     | C | -1.19906000  | 2.12588400  |
|     | H | 2.13754100   | 2.66391700  |
|     | H | -0.00001800  | 3.90822300  |
|     | H | -2.13756300  | 2.66388700  |
|     | B | 0.00001400   | -1.61117000 |
|     | O | 0.38739300   | -2.23024700 |
|     | H | 0.39997400   | -3.19446100 |
|     | O | -0.38740700  | -2.23014200 |
|     | H | -0.40003000  | -3.19435800 |
|     | C | -2.53528800  | 0.03739500  |
|     | C | 2.53529800   | 0.03740900  |
|     | F | -2.98669700  | -0.21284500 |
|     | F | -3.49405100  | 0.77521900  |
|     | F | 2.50788500   | -1.15646800 |
|     | F | 2.98657600   | -0.21291000 |
|     | F | 3.49413100   | 0.77523900  |
|     |   |  | -0.64276500 |

|  |   |             |             |            |
|--|---|-------------|-------------|------------|
|  | F | -2.50783300 | -1.15650600 | 0.67957600 |
|--|---|-------------|-------------|------------|

**8. Cartesian coordinates for the optimized geometries in Fig.S1**

|   |  |             |             |             |
|---|--|-------------|-------------|-------------|
| A |  |             |             |             |
|   | C  | 1.33153800  | 4.02895700  | 0.99911600  |
|   | C  | 1.41391700  | 4.10222700  | -0.46098500 |
|   | H  | 1.02535300  | 4.90633800  | 1.56231500  |
|   | H  | 1.94063000  | 3.28979100  | 1.50978500  |
|   | H  | 2.07747700  | 3.37536600  | -0.92344200 |
|   | O  | 0.27096300  | 3.46066800  | 0.18216200  |
|   | C  | 1.11791000  | 5.35733000  | -1.23188300 |
|   | H  | 2.04888600  | 5.89945200  | -1.42340700 |
|   | H  | 0.66337200  | 5.12184400  | -2.19826500 |
|   | H  | 0.44062500  | 6.01239600  | -0.67881000 |
|   | C  | -3.86664400 | -0.12976500 | -1.24075200 |
|   | C  | -3.38865900 | 0.33619500  | 0.00065000  |
|   | C  | -3.95109100 | -0.16588600 | 1.19136800  |
|   | C  | -4.96303200 | -1.12930100 | 1.12870300  |
|   | C  | -5.42489100 | -1.59449500 | -0.09893200 |
|   | C  | -4.87970300 | -1.09328200 | -1.27718800 |
|   | H  | -5.39494500 | -1.51213300 | 2.04825700  |

|  |    |             |             |             |
|--|----|-------------|-------------|-------------|
|  | H  | -6.21194100 | -2.34024100 | -0.13733400 |
|  | H  | -5.24623400 | -1.44821600 | -2.23551500 |
|  | B  | -2.21500200 | 1.39676400  | 0.05594500  |
|  | O  | -0.92531800 | 0.92784000  | 0.10009200  |
|  | H  | -0.26106100 | 1.64472200  | 0.12903100  |
|  | O  | -2.50956000 | 2.73099800  | 0.05737400  |
|  | H  | -1.71567300 | 3.28938000  | 0.09676000  |
|  | C  | 0.59977400  | -3.54749100 | 0.16411800  |
|  | H  | -0.37714600 | -3.19652000 | 0.49928400  |
|  | H  | 0.99590000  | -4.20274500 | 0.94045900  |
|  | C  | 1.23390900  | -1.41085300 | -1.06419000 |
|  | H  | 1.55416200  | -0.41911600 | -0.73972800 |
|  | H  | 0.15167300  | -1.40191800 | -1.19394300 |
|  | C  | 2.97595200  | -2.61449500 | 0.34829200  |
|  | H  | 3.10027000  | -2.79855000 | 1.41400900  |
|  | H  | 3.48126200  | -1.66986300 | 0.12755100  |
|  | C  | 1.06494700  | -1.42745100 | 1.35744200  |
|  | H  | 0.10764500  | -0.99228200 | 1.07061800  |
|  | H  | 1.80327600  | -0.62064200 | 1.37515900  |
|  | N  | 1.48651100  | -2.31237200 | 0.15880500  |
|  | C  | -3.48616000 | 0.34809900  | 2.53724900  |
|  | H  | -2.39956000 | 0.27313300  | 2.64510700  |
|  | H  | -3.74784100 | 1.40317000  | 2.66602800  |
|  | H  | -3.94468900 | -0.21123900 | 3.35567700  |
|  | C  | -3.30862500 | 0.42262000  | -2.53510100 |
|  | H  | -3.56569700 | 1.48005200  | -2.65347300 |
|  | H  | -2.21670300 | 0.35399100  | -2.56588800 |
|  | H  | -3.70416700 | -0.11515900 | -3.39957200 |
|  | Br | 3.52814100  | 1.05177700  | 0.22635800  |

|     |   |             |             |             |
|-----|---|-------------|-------------|-------------|
|     | C | 1.96913800  | -1.72477600 | -2.35912000 |
|     | H | 1.62495700  | -0.98627600 | -3.08846800 |
|     | H | 3.04369900  | -1.57381500 | -2.25371400 |
|     | H | 1.77313600  | -2.71253000 | -2.77403100 |
|     | C | 0.96425300  | -2.11852500 | 2.70994400  |
|     | H | 0.71616200  | -1.34181500 | 3.43782200  |
|     | H | 0.17466900  | -2.87053600 | 2.76033300  |
|     | H | 1.90139800  | -2.56984900 | 3.04216100  |
|     | C | 0.41212000  | -4.31418400 | -1.14036000 |
|     | H | -0.24163900 | -5.16262200 | -0.92011000 |
|     | H | -0.08667900 | -3.71286000 | -1.90024400 |
|     | H | 1.33800400  | -4.70911700 | -1.55299900 |
|     | C | 3.57659500  | -3.78946000 | -0.41305600 |
|     | H | 4.63760600  | -3.81967400 | -0.15080100 |
|     | H | 3.14740700  | -4.74966700 | -0.11862200 |
|     | H | 3.51476200  | -3.69050500 | -1.49479100 |
| TS1 |   |             |             |             |
|     | C | -2.43061100 | -2.18871500 | 0.76459800  |
|     | C | -1.77722600 | -2.76738100 | -0.41568300 |

|  |   |             |             |             |
|--|---|-------------|-------------|-------------|
|  | H | -3.16420000 | -2.78316400 | 1.28844400  |
|  | H | -1.91561500 | -1.43070900 | 1.32436200  |
|  | H | -1.24756100 | -2.03075800 | -1.03735600 |
|  | O | -0.95449500 | -3.37957700 | 0.54863500  |
|  | C | -2.58121100 | -3.72114300 | -1.27698400 |
|  | H | -3.31562000 | -3.17579300 | -1.87596200 |
|  | H | -1.91318000 | -4.26795800 | -1.94811800 |
|  | H | -3.10384000 | -4.44708400 | -0.64915700 |
|  | C | 3.53090900  | -0.61466800 | -1.25295700 |
|  | C | 3.13809000  | -0.98152700 | 0.05479800  |
|  | C | 3.82661900  | -0.42663400 | 1.15811800  |
|  | C | 4.86621200  | 0.48511100  | 0.94377400  |
|  | C | 5.23364400  | 0.85726400  | -0.34551900 |
|  | C | 4.56828100  | 0.30688000  | -1.43616700 |
|  | H | 5.39767200  | 0.89755400  | 1.79592400  |
|  | H | 6.04231600  | 1.56409500  | -0.49991900 |
|  | H | 4.86308100  | 0.58460500  | -2.44350800 |
|  | B | 1.91730700  | -1.96990400 | 0.27390100  |
|  | O | 0.84526600  | -1.55669400 | 1.01395200  |
|  | H | 0.12319200  | -2.26628000 | 0.98169700  |
|  | O | 1.92851600  | -3.20458100 | -0.32323000 |
|  | H | 1.10062900  | -3.68544600 | -0.15264500 |
|  | C | 0.60791100  | 2.86724000  | 0.24303000  |
|  | H | 1.29658500  | 2.16301400  | 0.71100100  |
|  | H | 0.46870700  | 3.70218000  | 0.93023800  |
|  | C | -0.78687400 | 1.09604300  | -0.93833900 |
|  | H | -1.53491700 | 0.37488900  | -0.60866300 |
|  | H | 0.19076700  | 0.61461500  | -0.92924400 |
|  | C | -1.95075200 | 3.06085400  | 0.17018000  |

|  |    |             |             |             |
|--|----|-------------|-------------|-------------|
|  | H  | -2.09677500 | 3.37573200  | 1.20180000  |
|  | H  | -2.78921700 | 2.41141700  | -0.08867600 |
|  | C  | -0.84629600 | 1.29265800  | 1.48365800  |
|  | H  | -0.14727100 | 0.46414900  | 1.35472300  |
|  | H  | -1.86395200 | 0.89793100  | 1.45935300  |
|  | N  | -0.73088100 | 2.13795800  | 0.19190000  |
|  | C  | 3.50225600  | -0.84470900 | 2.57737900  |
|  | H  | 2.43005900  | -0.81116700 | 2.77541800  |
|  | H  | 3.82527800  | -1.87540200 | 2.76046200  |
|  | H  | 4.01637300  | -0.20812600 | 3.30112000  |
|  | C  | 2.86424900  | -1.21166400 | -2.47529100 |
|  | H  | 3.08768100  | -2.27750000 | -2.56128500 |
|  | H  | 1.77365900  | -1.13114100 | -2.43276000 |
|  | H  | 3.20356000  | -0.71337400 | -3.38631200 |
|  | Br | -4.08101600 | -0.35072900 | 0.11268000  |
|  | C  | -1.18299700 | 1.56033700  | -2.33277700 |
|  | H  | -1.13337000 | 0.67614700  | -2.97380600 |
|  | H  | -2.21628300 | 1.90656800  | -2.36583800 |
|  | H  | -0.52858900 | 2.31557900  | -2.76376900 |
|  | C  | -0.57562000 | 2.01560500  | 2.79617200  |
|  | H  | -0.76055300 | 1.29145100  | 3.59350600  |
|  | H  | 0.45776700  | 2.34887200  | 2.89983700  |
|  | H  | -1.24051000 | 2.86228900  | 2.97859100  |
|  | C  | 1.22912400  | 3.34430700  | -1.06448000 |
|  | H  | 2.16296300  | 3.84824500  | -0.80190100 |
|  | H  | 1.49316700  | 2.51506600  | -1.72016400 |
|  | H  | 0.61206200  | 4.05391400  | -1.61210800 |
|  | C  | -1.90156200 | 4.30520000  | -0.70808900 |
|  | H  | -2.86105400 | 4.81442700  | -0.58431400 |

|   |   |             |             |             |
|---|---|-------------|-------------|-------------|
|   | H | -1.12498800 | 5.00607700  | -0.39698300 |
|   | H | -1.78198000 | 4.09086500  | -1.76796700 |
|   |   |             |             |             |
| B | C | -3.54273900 | -1.07547400 | 0.84235100  |
|   | C | -2.68432300 | -2.10992000 | 0.10240300  |
|   | H | -4.18889200 | -1.53660200 | 1.58679000  |
|   | H | -2.91749600 | -0.32150900 | 1.31118900  |
|   | H | -2.24600000 | -1.63011900 | -0.78387100 |
|   | O | -1.66620400 | -2.49339600 | 1.00233600  |
|   | C | -3.47860400 | -3.33681100 | -0.32658800 |
|   | H | -4.31136500 | -3.06519200 | -0.98001500 |
|   | H | -2.82734000 | -4.03184000 | -0.86023600 |
|   | H | -3.87407700 | -3.85063400 | 0.55456100  |
|   | C | 3.37814500  | -1.45506800 | -1.34493600 |
|   | C | 2.90226200  | -1.44125300 | -0.01519000 |
|   | C | 3.75949200  | -0.97356900 | 1.00276200  |
|   | C | 5.03794300  | -0.49660000 | 0.68588700  |
|   | C | 5.48762800  | -0.49139000 | -0.63112000 |
|   | C | 4.65938800  | -0.97772200 | -1.64021300 |
|   | H | 5.68949300  | -0.14085500 | 1.47929200  |

|  |    |             |             |             |
|--|----|-------------|-------------|-------------|
|  | H  | 6.48083500  | -0.12413200 | -0.86856500 |
|  | H  | 5.01355700  | -0.99269200 | -2.66701100 |
|  | B  | 1.39619800  | -1.90144800 | 0.31807200  |
|  | O  | 0.42461700  | -1.02543500 | 0.55996700  |
|  | H  | -0.87932000 | -1.85864800 | 0.88721700  |
|  | O  | 1.21254400  | -3.28836100 | 0.30937200  |
|  | H  | 0.29339200  | -3.51222400 | 0.51237900  |
|  | C  | 1.53814400  | 1.99832500  | 0.13103200  |
|  | H  | 1.62731800  | 0.98673600  | 0.52778500  |
|  | H  | 2.07016800  | 2.69291100  | 0.78150500  |
|  | C  | -0.82303100 | 1.57695600  | -0.71994700 |
|  | H  | -1.80490800 | 1.50740900  | -0.24976100 |
|  | H  | -0.39982000 | 0.56999000  | -0.74179400 |
|  | C  | -0.26421700 | 3.82033700  | 0.33110000  |
|  | H  | -0.04937900 | 4.14912100  | 1.34619800  |
|  | H  | -1.34393000 | 3.89507300  | 0.18915800  |
|  | C  | -0.38001300 | 1.73705100  | 1.66044400  |
|  | H  | -0.32185800 | 0.65552600  | 1.51001200  |
|  | H  | -1.41870300 | 2.04705400  | 1.79091200  |
|  | N  | 0.04817900  | 2.33151000  | 0.29838000  |
|  | C  | 3.33522200  | -1.03810600 | 2.45550200  |
|  | H  | 2.27345500  | -0.81069500 | 2.57545500  |
|  | H  | 3.48664100  | -2.04701600 | 2.85488500  |
|  | H  | 3.91788500  | -0.35050500 | 3.07541700  |
|  | C  | 2.50981500  | -1.99748000 | -2.46033200 |
|  | H  | 2.24880900  | -3.04247900 | -2.27405100 |
|  | H  | 1.56365800  | -1.45018400 | -2.53781800 |
|  | H  | 3.01633700  | -1.93360500 | -3.42654400 |
|  | Br | -4.76356500 | -0.04196700 | -0.36165500 |

|  |   |             |            |             |
|--|---|-------------|------------|-------------|
|  | C | -1.00603100 | 2.18381000 | -2.10453700 |
|  | H | -1.64935200 | 1.49429900 | -2.65749500 |
|  | H | -1.52463100 | 3.14427500 | -2.08017700 |
|  | H | -0.08181000 | 2.29328800 | -2.66786400 |
|  | C | 0.45309700  | 2.13549000 | 2.87093700  |
|  | H | -0.02549500 | 1.68173600 | 3.74271400  |
|  | H | 1.46813700  | 1.74224700 | 2.82602300  |
|  | H | 0.49561500  | 3.21172700 | 3.05484600  |
|  | C | 2.13434100  | 2.00155000 | -1.26941000 |
|  | H | 3.18836100  | 1.73895400 | -1.15032200 |
|  | H | 1.69791500  | 1.22494100 | -1.89564800 |
|  | H | 2.08026300  | 2.95907000 | -1.78537500 |
|  | C | 0.47357500  | 4.74081700 | -0.63445200 |
|  | H | 0.10138600  | 5.75397200 | -0.45886500 |
|  | H | 1.54773200  | 4.75476500 | -0.44758600 |
|  | H | 0.30171600  | 4.50323700 | -1.68202400 |