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General information

All synthetic work was carried out using standard Schlenk techniques. Solvents were dried with an M.Braun Solvent Purification System directly prior to use. The following chemicals were purchased and used as delivered: hexamethylbenzene (99%, abcr), 2,6-di-tert-butylphenol (99%, Sigma Aldrich), 3,5-di-tert-butylcatechol (99%, Acros Organics), benzylamine (99%, Sigma Aldrich), o-phenylenediamine (≥98%, Fluka), 4-methoxytriphenylamine (97%, Sigma Aldrich), triphenylamine (98%, Sigma Aldrich), 4,4′-dibromotriphenylamine (98%, Alfa Aesar), 4-nitrotriphenylamine (98%, abcr). The synthesis of 3,3′,4,4′-tetramethoxy-o-terphenyl,[1] 1(BF₄)₂,[2] and 1(PF₆)₂[3] followed the literature procedures. Elemental analyses were carried out at the Microanalytical Laboratory of the University of Heidelberg. NMR spectra were recorded on a Bruker DPX 200, Bruker DRX 200, Bruker Avance II 400 or Bruker AVANCE III 600 system. Solvent resonances were taken as references for all ¹H NMR spectra. UV-Vis spectra were recorded with a Cary 5000 spectrophotometer and cyclic voltammetry (CV) measurements with an EG&G Princeton Applied Research Potentiostat / Galvanostat 273A or a Methrom Autolab potentiostat PGSTAT 204. A FT-IR Biorad Merlin Excalibur FT300 spectrometer was used for IR measurements. MS-ESI measurements relied on a Bruker microTOF II ESI mass spectrometer.

[1] Linyi Zhai, Ruchi Shukla, Shirya H. Wadumethrigae, Rajendra Rathore, J. Org. Chem. 2010, 75, 4748–4760.
[2] U. Wild, O. Hübner, L. Greb, M. Enders, E. Kaifer, H.-J. Himmel, Eur. J. Org. Chem. 2018, 5910–5915.
[3] U. Wild, S. Federle, A. Wagner, E. Kaifer, H.-J. Himmel, Chem. Eur. J. 2016, 22, 11971–11976.
1) **Experimental details for oxidative coupling of 2,6-di-tert-butylphenol to 3,3',5,5'-tetra-tert-butylidiphenoquinone**

![Reaction Scheme](image)

| entry | A          | B          | C         | D          |
|-------|------------|------------|-----------|------------|
| 1(BF<sub>4</sub>)<sub>2</sub> [mg/µmol] | 4.466/6.34 | -          | 5.244/7.44 | -          |
| 1(PF<sub>6</sub>)<sub>2</sub> [mg/µmol] | -          | 5.206/6.34 | -          | 5.488/6.69 |
| 2,6-di-tert-butylphenol [mg/µmol] | 1.270/6.16 | 1.318/6.39 | 1.514/7.34 | 1.310/6.34 |
| HMB [mg/µmol] | 1.022/6.30 | 0.800/4.93 | 1.360/8.38 | 1.552/9.56 |
| Na<sub>2</sub>SO<sub>4</sub> [mg] | -          | 3.504      | -          | -          |
| CH<sub>3</sub>CN [mL] | 0.45       | 0.45       | 0.45       | 0.45       |
| reaction time (temperature) | 24 h (60 °C) | 24 h (60 °C) | 28 h (60 °C) | 28 h (60 °C) |
| conversion phenol to 3,3',5,5'-tetra-tert-butylidiphenoquinone (rel. to 1<sup>2+</sup>/({1+2H})<sup>2+</sup>) [%]* | 82 | 86 | 57 | 54 |
| ratio (substrate/GFA) | 1/1 | 1/1 | 1/1 | 1/1.1 |

| entry | E          | F          |
|-------|------------|------------|
| (1+2H)(BF<sub>4</sub>)<sub>4</sub> [mg/µmol] | 3.992/4.54 | 5.298/6.02 |
| 2,6-di-tert-butylphenol [mg/µmol] | 1.118/5.42 | 1.226/5.94 |
| HMB [mg/µmol] | 0.946/5.83 | 0.938/5.78 |
| CH<sub>3</sub>CN [mL] | 0.45       | 0.45       |
| reaction time (temperature) | 25 h (60°C) | 24 h (60°C) |
| conversion phenol to 3,3',5,5'-tetra-tert-butylidiphenoquinone (rel. to 1<sup>2+</sup>/({1+2H})<sup>2+</sup>) [%]* | 12 | 11 |
| ratio (substrate/GFA) | 1/0.8 | 1/1 |

* The signals of 3,3',5,5'-tetra-tert-butylidiphenoquinone could not be used for peak integration, as it precipitates in crystalline form from the reaction mixture.
General protocol (NMR experiments)

In an NMR tube, the reactants $1(BF_4)_2 / 1(PF_6)_2$ or $(1+2H)(BF_4)_4$, 2,6-di-tert-butylphenol were dissolved (with HMB) under an Ar atmosphere in 0.45 mL CD$_3$CN. The reaction mixture was heated to (60 °C). The conversion was followed by NMR measurements (at room temperature). The overall reaction time refers to the time at (60 °C).

$^1$H NMR spectra (199.87 MHz, 298 K, CD$_3$CN) for entry A: first measurement
$^1$H NMR spectra (199.87 MHz, 298 K, CD$_3$CN) for entry A: last measurement

$^1$H NMR spectra (199.87 MHz, 298 K, CD$_3$CN) for entry C: last measurement
$^1$H NMR spectra (199.87 MHz, 298 K, CD$_3$CN) for entry E: first measurement

$^1$H NMR spectra (199.87 MHz, 298 K, CD$_3$CN) for entry E: last measurement
2) **Experimental details for oxidation of 3,5-di-tert-butylcatechol to di-tert-butyl-o-benzoquinone**

![Reaction Scheme](attachment:image.png)

| entry | A (373-2) | B (334-2) |
|-------|-----------|-----------|
| 1(BF<sub>4</sub>)<sub>2</sub> [mg/µmol] | - | 5.286/7.50 |
| (1+2H)(BF<sub>4</sub>)<sub>4</sub> [mg/µmol] | 5.882/6.68 | - |
| 3,5 di-tert-butylcatechol [mg/µmol] | 1.460/6.58 | 1.634/7.35 |
| HMB [mg/µmol] | 0.982/6.05 | 1.188/7.32 |
| CD<sub>3</sub>CN [mL] | 0.45 | 0.45 |
| reaction time (temperature) | 1.4 h (r.t.) | 6 min (r.t.) |
| conversion (rel. to 3,5 di-tert-butylcatechol) [%] | >99 | 87 |
| conversion (rel. to [1+nH<sup>+</sup>]/[1<sup>2+</sup>]) [%] | 95 | 83 |
| ratio (substrate/GFA) | 1/1 | 1/1 |

**General protocol (NMR experiments)**

In an NMR tube, the reactants 1(BF<sub>4</sub>)<sub>2</sub> or (1+2H)(BF<sub>4</sub>)<sub>4</sub> and 3,5 di-tert-butylcatechol were dissolved (with HMB) under an Ar atmosphere in 0.45 mL CD<sub>3</sub>CN.
$^1$H NMR spectra (200.13 MHz, 298 K, CD$_3$CN) for entry A: first measurement

$^1$H NMR spectra (200.13 MHz, 298 K, CD$_3$CN) for entry A: last measurement

$^1$H NMR of di-tert-butyl-o-quinone: (200.13 MHz, 298 K, CD$_3$CN): $\delta = 1.23$ (d, 7.0 Hz, 18 H), 6.15 (d, $J = 2.3$ Hz, 1 H), 7.01 (d, $J = 2.3$ Hz, 1 H) ppm.
\(^1\text{H} \) NMR spectra (199.87 MHz, 298 K, CD\(_3\)CN) for entry B: last measurement

No significant further product formation for prolonged reaction times.
3) **Experimental details for oxidative coupling of benzylamine to\n**
\n\textit{N-}(phenylmethylene)-benzenemethanamine

![Chemical structure]

**Table:**

| entry | A | B | C | D |
|---|---|---|---|---|
| 1(BF$_4$)$_2$ [mg/µmol] | - | - | 5.346/7.59 | 4.606/6.54 |
| (1+2H)(BF$_4$)$_4$ [mg/µmol] | 5.586/6.35 | 4.87/5.53 | - | - |
| benzylamine (10% in CH$_3$CN) [µL/mmol] | 14/12.80 | 12/10.97 | 17/15.54 | 15/13.71 |
| NH$_4$PF$_6$ [mg] | - | - | 2.7/16.6 | 2.3/14.1 |
| HMB [mg/µmol] | 0.882/5.44 | 0.874/5.39 | 0.920/5.67 | 1.014/6.25 |
| CH$_3$CN [mL] | 0.45 | 0.45 | 0.45 | 0.47 |
| reaction time (temperature) | 24 h (60 °C) | 25 h (60 °C) | 25.5 h (60 °C) | 25 h (60 °C) |
| conversion (rel. to 1$^{2+}/(1+2H)^{2+}$) [%] | 79 | 78 | 84 | 79 |
| ratio (substrate/GFA) | 1/0.5 | 1/0.5 | 1/0.49 | 1/0.48 |

| entry | E | F |
|---|---|---|
| 1(BF$_4$)$_2$ [mg/µmol] | 5.396/7.66 | - |
| 1(PF$_6$)$_2$ [mg/µmol] | - | 5.226/6.37 |
| benzylamine (10% in CH$_3$CN) [µL/mmol] | 15/13.71 | 14/12.80 |
| CH$_3$CN [mL] | 0.45 | 0.45 |
| HMB [mg/µmol] | 0.686/4.23 | 0.768/4.73 |
| reaction time (temperature) | 24 h (60 °C) | 24 h (60 °C) |
| conversion (rel. to 1$^{2+}/(1+2H)^{2+}$) [%] | < 5 | < 10 |
| ratio (substrate/GFA) | 1/0.56 | 1/0.5 |
General protocol (NMR experiments)

In an NMR tube, the reactants $1(BF_4)_2$ or $1(PF_6)_2$, and in some experiments also NH$_4$PF$_6$ were dissolved (with HMB) in an Ar atmosphere in 0.45 mL CD$_3$CN. Then a benzylamine solution (10% in CH$_3$CN) was added dropwise via microliter injection and the reaction mixture heated to 60 °C. The conversion was followed by NMR measurements (at room temperature). The overall reaction time refers to the time at 60 °C.

$^1$H NMR spectra (200.13 MHz, 298 K, CD$_3$CN) for entry B: first measurement

[Diagram of NMR spectrum showing signals for $1^{2+}$ and protonated form of benzylamine, labeled HMB and CD$_3$CN.]
$^1$H NMR spectra (200.13 MHz, 298 K, CD$_3$CN) for entry B: last measurement

$^1$H NMR of $N$-(phenylmethylene)-benzenemethanamine: (200.13 MHz, 298 K, CD$_3$CN): $\delta = 4.77$ (d, $J = 1.0$ Hz, 2 H), 7.44 - 7.34 (m, 8 H), 7.78 (dd, $J = 6.9; 2.9$ Hz, 2 H), 8.47 (s, 1 H) ppm.
$^1$H NMR spectra (200.13 MHz, 298 K, CD$_3$CN) for entry C: first measurement

$^1$H NMR spectra (200.13 MHz, 298 K, CD$_3$CN) for entry C: last measurement

- $^1$H$^{2+}$
- benzylamine / NH$_4$PF$_6$
- (1+2H)$^{2+}$
- $N$-(phenylmethylene)-benzenemethanamine
- benzylamine
- * traces of some species of 1

Chemical shift (ppm)

13
$^1$H NMR spectra (200.13 MHz, 298 K, CD$_3$CN) for entry F: first measurement

$^1$H NMR spectra (199.87 MHz, 298 K, CD$_3$CN) for entry F: last measurement
4) **Experimental details for oxidative coupling of o-phenylene-diamine to 2,3-diaminophenazine**

![Chemical structure](image)

| entry                        | A     | B                 | C                 |
|------------------------------|-------|-------------------|-------------------|
| 1(BF$_4$)$_2$ [mg/µmol]      | -     | -                 | 6.696 mg/9.51     |
| (1+2H)(BF$_4$)$_4$ [mg/µmol]| 6.059/6.89 | 5.036/7.15      | -                 |
| o-phenylene-diamine          | 0.506/4.68 | 0.414/3.83       | 0.666/6.16        |
| HMB [mg/µmol]                | 0.736/4.54 | 1.182/7.28       | 0.764/4.71        |
| CH$_3$CN [mL]                | 0.5   | 0.45              | 0.45              |
| reaction time (temperature)  | 1 h (60 °C) | 1 h (60 °C)     | 25 h (60 °C)      |
| conversion (rel. to 1$^{+}$/ (1+4H)$^{4+}$) [%] | 91 | 96 | <5 |
| ratio substrate/GFA          | 1/1.5 | 1/1.9             | 1/1.5             |

**General protocol (NMR experiments)**

In an NMR tube, the reactants 1(BF$_4$)$_2$ or (1+2H)(BF$_4$)$_4$ and o-phenylene-diamine were dissolved (with HMB) in an Ar atmosphere in 0.45 or 0.5 mL CD$_3$CN. Then the reaction mixture was heated to 60 °C. The conversion was followed by NMR measurements (at room temperature). The overall reaction time refers to the time at 60 °C.
$^{1}H$ NMR spectra (199.87 MHz, 298 K, CD$_3$CN) for entry B: first measurement

$^{1}H$ NMR spectra (199.87 MHz, 298 K, CD$_3$CN) for entry A: last measurement

$^{1}H$ NMR of 2,3-diaminophenazine: (199.87 MHz, 298 K, CD$_3$CN): $\delta = 5.29$ (bs, 4 H), 7.08 (s, 2 H), 7.68 (dd, $J = 6.6$; 3.4 Hz, 2 H), 7.99 (dd, $J = 6.5$; 3.4 Hz, 2 H) ppm.
Reaction was also monitored by UV-Vis spectroscopy in CH$_3$CN.
Reactivity with lower concentrations of the reactants (therefore slower) at 60 °C.

\[A(\lambda)\]

$^1$H NMR spectra (199.87 MHz, 298 K, CD$_3$CN) for entry C: first measurement.
\(^1\)H NMR spectra (199.87 MHz, 298 K, CD\(_2\)CN) for entry C: last measurement

Chemical shift (ppm)
5) **Experimental details for oxidative coupling of 4-methoxytriphenylamine to N,N'-bis(4-methoxyphenyl)-N,N'-diphenylbenzidine**

![Chemical Structure]

| entry                                      | A               | B               |
|--------------------------------------------|-----------------|-----------------|
| 1(BF₄)₂ [mg/µmol]                          | 5.992/8.51      | -               |
| 1(PF₆)₂ [mg/µmol]                          | -               | 6.492/7.91      |
| 4-methoxytriphenylamine [mg/mmol]          | 2.350/8.53      | 2.196/7.98      |
| HBF₄·Et₂O (5% in CH₃CN) [mL/µmol]          | 0.5/182.3       | 0.5/182.3       |
| HMB [mg/µmol]                              | 1.850/11.40     | 1.354/8.34      |
| reaction time (temperature)                | 5 min (ice cooling) 1.9 h (r.t.) | 5 min (ice cooling) 1.3 h (r.t.) |
| conversion (rel. to 1²⁺/(1+2H)²⁺) [%]     | 90              | 86              |
| ratio (substrate/GFA)                      | 1/1             | 1/0.99          |

**General protocol**

In a Schlenk flask, 0.5 mL of a HBF₄·Et₂O solution (5% in CH₃CN) was added under ice cooling in an Ar atmosphere to the reactants 1(BF₄)₂ / 1(PF₆)₂ and 4-methoxytriphenylamine. The reaction was stirred for 5 min under ice cooling and then allowed to warm up to room temperature. The reaction was stopped by the addition of an aqueous saturated NaHCO₃ solution. The small amount of CH₃CN was removed under high-vacuum. Then an aqueous diluted solution of NaOH (8%) was added (pH > 9), converting all formed (1+4H)⁴⁺ to (1+2H)²⁺ (for subsequent transfer into the organic phase). A clear solution was obtained that was extracted several times with CH₂Cl₂. The combined organic phases were dried over Na₂SO₄, filtrated and condensed.
$^1$H NMR spectra (399.87 MHz, 295.1 K, CD$_2$Cl$_2$) for entry A

$^1$H NMR of N,N'-bis(4-methoxyphenyl)-N,N'-diphenylbenzidine: (399.89 MHz, 295.1 K, CD$_2$Cl$_2$):
$\delta$ = 3.78 (s, 6 H), 6.85 (d, J = 9.0 Hz, 4 H), 6.95 (t, J = 7.3 Hz, 2 H), 7.01 - 7.05 (m, 8 H), 7.07 (d, J = 9.0 Hz, 4 H), 7.22 (dd, J = 8.5; 7.4 Hz, 4 H), 7.41 (d, J = 8.7 Hz, 4 H) ppm.

The reaction was also monitored by UV-Vis spectroscopy in CH$_2$Cl$_2$ for a ratio substrate/GFA of 1:1
Reaction was also monitored by UV-Vis spectroscopy in CH₂Cl₂ for a ratio substrate/GFA of 1:0.65

SCE potentials vs. Fc/Fc⁺, measured with a scan rate of 100 mV·s⁻¹ and nBu₄N(PF₆) as supporting electrolyte in CH₃CN solution
6) **Experimental details for oxidative coupling of triphenylamine to \(N,N,N',N'\)-tetraphenylbenzidine**

![Chemical structures](image)

| entry | A | B |
|-------|---|---|
| 1\((\text{BF}_4)_2\) [mg/µmol] | 6.492/9.22 | - |
| 1\((\text{PF}_6)_2\) [mg/µmol] | - | 8.496/10.35 |
| triphenylamine [mg/mmol] | 2.254/9.19 | 2.518/10.26 |
| HBF\(_4\)·Et\(_2\)O (5% in CH\(_3\)CN) [mL/µmol] | 0.5/182.3 | 0.5/182.3 |
| HMB [mg/µmol] | 1.150/7.09 | 2.072/12.77 |
| reaction time (temperature) | 5 min (ice cooling) 25 min (r.t.) | 10 min (ice cooling) 15 min (r.t.) |
| conversion (rel. to \(1^{2+}/(1+2\text{H})^{2+}\)) [%] | >99 | 97 |
| ratio (substrate/GFA) | 1/1 | 1/1 |

| entry | C | D | E |
|-------|---|---|---|
| 1\((\text{BF}_4)_2\) [mg/µmol] | - | - | 5.720/8.12 |
| 1\((\text{PF}_6)_2\) [mg/µmol] | 8.032/9.79 | 8.828/10.76 | - |
| triphenylamine [mg/mmol] | 1.386/5.65 | 2.954/12.04 | 3.088/12.59 |
| HBF\(_4\)·Et\(_2\)O (5% in CH\(_3\)CN) [mL/µmol] | 0.5/182.3 | 0.6/218.7 | 0.5/182.3 |
| HMB [mg/µmol] | 1.342/8.27 | 1.072/6.61 | 1.012/6.24 |
| reaction time (temperature) | 5 min (ice cooling) 10 min (r.t.) | 10 min (ice cooling) 10 min (r.t.) | 5 min (ice cooling) 40 min (r.t.) |
| conversion (rel. to \(1^{2+}/(1+2\text{H})^{2+}\)) [%] | >99 | 88 | 62 |
| ratio (substrate/GFA) | 1/1.73 | 1/0.89 | 1/0.64 |
General protocol

In a Schlenk flask, 0.5 mL of a HBF₄·Et₂O solution (5% in CH₃CN) was added under ice cooling in an Ar atmosphere to the reactants 1(BF₄)₂ / 1(PF₆)₂ and triphenylamine. The reaction was stirred for several minutes under ice cooling and then allowed to warm up to room temperature. The reaction was stopped by the addition of an aqueous saturated NaHCO₃ solution. The small amount of CH₃CN was removed under high-vacuum. Then an aqueous diluted solution of NaOH (8%) was added (pH > 9), converting all formed (1+4H)⁴⁺ to (1+2H)²⁺ (for subsequent transfer into the organic phase). A clear solution was obtained that was extracted several times with CH₂Cl₂. The combined organic phases were dried over Na₂SO₄, filtrated and condensed.

Separation of 1(BF₄)₂ / [(1+2H)(BF₄)₂]

The residue was collected in diethylether and filtrated, allowing the isolation of the coupling product in the filtrate. The residue in the filter, consisting of 1(BF₄)₂/[(1+2H)(BF₄)₂], was dissolved in CH₃CN for recycling of the guanidine PCET reagent.

¹H NMR spectra (399.89 MHz, 295.1 K, CD₂Cl₂) for entry A

¹H NMR of N,N,N',N'-tetraphenylbenzidine: (399.89 MHz, 295.1 K, CD₂Cl₂): δ = 7.00 (t, J = 7.3 Hz, 4 H), 7.05 - 7.08 (m, 12 H), 7.23 (dd, J = 8.5; 7.4 Hz, 8 H), 7.43 (d, J = 8.7 Hz, 4 H) ppm.
Reaction was also monitored by UV-Vis spectroscopy in CH₂Cl₂ for a ratio substrate/GFA of 1:1

Reaction was also monitored by UV-Vis spectroscopy in CH₂Cl₂ for a ratio substrate/GFA of 1:0.64
Triphenylamine reactions with small quantities of HBF₄

| entry | A: -NMR experiment | B | C | D |
|-------|--------------------|---|---|---|
| 1(BF₄)₂ [mg/µmol] | 7.098/10.08 | 8.520/12.10 | - | 9.584/13.61 |
| 1(PF₆)₂ [mg/µmol] | | | 8.320/10.14 | |
| triphenylamine [mg/mmol] | 4.856/19.79 | 6.052/24.67 | 5.046/20.57 | 6.882/28.05 |
| HBF₄·Et₂O (5% in CH₃CN) [mL/µmol] | a0.05/18.3 b0.27/98.4 | 0.22/80.2 | 0.18/65.6 | 0.25/91.1 |
| CH₃CN/CD₃CN (NMR experiment) [mL] | 0.45 | 1 | 1 | 1 |
| HMB [mg/µmol] | 0.964/5.94 | 2.090/12.88 | 3.024/18.63 | 1.988/12.25 |
| reaction time (temperature) | not determined (instantly) | 1 h (ice cooling) | 5 min (ice cooling) | 2.5 h (r.t.) |
| ratio (substrate/GFA) | 1/0.51 | 1/0.49 | 1/0.49 | 1/0.49 |

*a* first addition; *b* second addition

**Reaction in an NMR tube (entry A)**

In an NMR tube, the reactants 1(BF₄)₂ and triphenylamine (and HMB) were dissolved in an Ar atmosphere in 0.45 mL CD₃CN. An NMR spectrum was recorded, showing that no reaction took place. Then 0.05 mL of a HBF₄·Et₂O solution (5% in CD₃CN) were dropwise added with a syringe and a NMR spectrum taken from the reaction mixture. After a second (dropwise) addition of 0.27 mL of the HBF₄·Et₂O solution (5% in CD₃CN) another NMR spectrum was recorded.

**Reactions in Schlenk flasks (entries B - D)**

In a Schlenk flask, a HBF₄·Et₂O solution (5% in CH₃CN) was added with a syringe under ice cooling in an Ar atmosphere to a solution of the reactants 1(BF₄)₂ / 1(PF₆)₂ and triphenylamine in 1 mL CH₃CN. The reaction was stirred for several minutes under ice cooling and then allowed to warm up to room temperature for further reaction.

**Work-up (entries B - D)**

The reaction was stopped by the addition of an aqueous saturated NaHCO₃ solution. The small amount of CH₃CN was removed under high-vacuum. For entry B, an aqueous diluted solution of NaOH (8%) was added (pH > 9), converting all formed (1+4H)⁴⁺ to (1+2H)²⁺ (for subsequent transfer into the organic phase). In the case of entries C and D, a larger amount of NaHCO₃ solution was used in place for the NaOH solution. A colourless and clear solution was obtained that was extracted several times with CH₂Cl₂. The combined organic phases were dried over Na₂SO₄, filtrated and condensed.
$^1$H NMR experiment entry A (199.87 MHz, 298 K, CD$_3$CN): reaction of 1(BF$_4$)$_2$ and triphenylamine without addition of the HBF$_4$·Et$_2$O solution (5% in CD$_3$CN)

$^1$H NMR experiment entry A (199.87 MHz, 298 K, CD$_3$CN): reaction of 1(BF$_4$)$_2$ and triphenylamine after first addition of the HBF$_4$·Et$_2$O solution (5% in CD$_3$CN)
$^1$H NMR experiment entry A (199.87 MHz, 298 K, CD$_3$CN): reaction of 1(BF$_4$)$_2$ and triphenylamine after second addition of the HBF$_4$·Et$_2$O solution (5% in CD$_3$CN)

$^1$H NMR spectra (399.89 MHz, 295.6 K, CD$_2$Cl$_2$) for entry B
\(^1\)H NMR spectra (399.89 MHz, 294.9 K, CD\(_2\)Cl\(_2\)) for entry C

\[(1+2H)^{2+}\]

\(1^{2+}\)

mixture of N,N,N',N'-tetraphenybenzidine, triphenylamine and other coupling products

\[^1\)H NMR spectra (399.89 MHz, 295.6 K, CD\(_2\)Cl\(_2\)) for entry D

\[(1+2H)^{2+}\]

\(1^{2+}\)

mixture of N,N,N',N'-tetraphenybenzidine, triphenylamine and other coupling products
Reaction was monitored by UV-Vis spectroscopy in CH$_2$Cl$_2$ for entry B

SCE potentials vs. Fc/Fc$^+$, measured with a scan rate of 100 mV·s$^{-1}$ and nBu$_4$N(PF$_6$) as supporting electrolyte in CH$_3$CN
triphenylamine

\[ I / \mu A \]

\[ E / V \]

0.6
0.46
0.33
7) Experimental Details for oxidative coupling of 4,4'-dibromotriphenylamine to \(N,N,N',N'\)-tetrakis(4-bromophenyl)-benzidine

![Chemical structure]

| entry | A | B | C |
|-------|---|---|---|
| 1(BF₄)₂ [mg/µmol] | 5.376/7.63 | - | - |
| 1(PF₆)₂ [mg/µmol] | - | 6.374/7.77 | 5.800/7.07 |
| 4,4'-dibromotriphenylamine [mg/mmol] | 3.078/7.64 | 3.132/7.77 | 4.47/11.09 |
| HBF₄·Et₂O (5% in CH₃CN)[mL/µmol] | 0.5/182.3 | 0.5/182.3 | 0.11/40.1 |
| HMB [mg/µmol] | 1.974/12.16 | 1.562/9.63 | 1.696/10.45 |
| CH₃CN [mL] | - | - | 0.6 |
| reaction time (temperature) | 10 min (ice cooling) 1.4 h (r.t.) | 5 min (ice cooling) 1.2 h (r.t.) | 23 h (r.t.) |
| conversion (rel. to \(1^{2+}/(1+2H)^{2+}\)%) | 95 | 92 | 89 |
| ratio (substrate/GFA) | 1/1 | 1/1 | 1/0.64 |

**General protocol**

**Entries A and B:**

In a Schlenk flask, 0.5 mL of a HBF₄·Et₂O solution (5% in CH₃CN) was added with a syringe under ice cooling in an Ar atmosphere to a solution of 1(BF₄)₂ / 1(PF₆)₂ and 4,4'-dibromotriphenylamine in 1 mL CH₃CN. The reaction was stirred for several minutes under ice cooling and then allowed to warm up to room temperature for further reaction.
**Entry C:**

In a Schlenk flask, 0.11 mL (40.1 µmol) of a HBF$_4$·Et$_2$O solution (5% in CH$_3$CN) was added with a syringe in an Ar atmosphere to a solution of 1(PF$_6$)$_2$ and 4,4’-dibromotriphenylamine in 0.6 mL CH$_3$CN. The reaction was stirred for 23 h at room temperature.

**Work-up (for all experiments):**

The reaction was stopped by the addition of an aqueous saturated NaHCO$_3$ solution. The small amount of CH$_3$CN was removed under high-vacuum. An aqueous diluted solution of NaOH (8%) was added (pH > 9), converting all formed (1+4H)$^{4+}$ to (1+2H)$^{2+}$ (for subsequent transfer into the organic phase). A clear solution was obtained that was extracted several times with CH$_2$Cl$_2$. The combined organic phases were dried over Na$_2$SO$_4$, filtrated and condensed.

**$^1$H NMR spectra (600.13 MHz, 295.2 K, CD$_2$Cl$_2$) for entry A**

![NMR spectrum](image)

$^1$H NMR of N,N,N',N'-tetraakis(4-bromophenyl)-benzidine (600.13 MHz, 295.2 K, CD$_2$Cl$_2$): $\delta = 6.97$ (d, $J = 8.8$ Hz, 8 H), 7.09 (d, $J = 8.6$ Hz, 4 H), 7.36 (d, $J = 8.8$ Hz, 8 H), 7.48 (d, $J = 8.6$ Hz, 4 H ppm)
Reaction was also monitored by UV-Vis spectroscopy in CH$_2$Cl$_2$: entry A

$^1$H NMR spectra (600.13 MHz, 295.2 K, CD$_2$Cl$_2$) for entry C
SCE potentials vs. Fc/Fc⁺, measured with a scan rate of 100 mV·s⁻¹ and nBu₄N(PF₆) as supporting electrolyte in CH₃CN

SCE potentials vs. Fc/Fc⁺, measured with a scan rate of 50 mV·s⁻¹ and nBu₄N(PF₆) as supporting electrolyte in CH₃CN
8) **Experimental Details for oxidative coupling of 4-nitrotriphenylamine to $N,N'$-bis(4-nitrophenyl)-$N,N'$-diphenylbenzidine**

In a Schlenk flask, 0.5 mL of a HBF$_4$·Et$_2$O solution (5% in CH$_3$CN) was added under ice cooling in an Ar atmosphere to the reactants 1(BF$_4$)$_2$ / 1(PF$_6$)$_2$ and 4-nitrotriphenylamine. The reaction was stirred for several minutes under ice cooling and then allowed to warm up to room temperature for further reaction. The reaction was stopped by the addition of an aqueous saturated NaHCO$_3$ solution. The small amount of CH$_3$CN was removed under high-vacuum. Then an aqueous diluted solution of NaOH (8%) was added (pH > 9), converting all formed (1+4H)$^{4+}$ to (1+2H)$^{2+}$ (for subsequent transfer into the organic phase). A clear solution was obtained that was extracted several times with CH$_2$Cl$_2$. The combined organic phases were dried over Na$_2$SO$_4$, filtrated and condensed.

| entry | A | B | C |
|-------|---|---|---|
| 1(BF$_4$)$_2$ [mg/µmol] | 5.60/7.95 | 9.464/13.44 | - |
| 1(PF$_6$)$_2$ [mg/µmol] | - | - | 10.68/13.01 |
| 4-nitrotriphenylamine [mg/mmol] | 2.244/7.73 | 2.622/9.03 | 2.51/8.65 |
| HBF$_4$·Et$_2$O (5% in CH$_3$CN)[mL/µmol] | 0.5/182.3 | 0.5/182.3 | 0.5/182.3 |
| HMB [mg/µmol] | 1.974/12.16 | 1.136/7.00 | 1.696/10.45 |
| reaction time (temperature) | 20 min (ice cooling) 2.25 h (r.t.) | 10 min (ice cooling) 1 h (r.t.) | 10 min (ice cooling) 1 h (r.t.) |
| conversion (rel. to $1^{2+}$/(1+2H)$^{2+}$)[%] | 95 | 95 | 98 |
| ratio (substrate/GFA) | 1/1.03 | 1/1.49 | 1/1.5 |
\(^1\)H NMR spectra (399.89 MHz, 295.1 K, CD\(_2\)Cl\(_2\)) for entry A

\(N,N'\)-bis(4-nitrophenyl)-N,N'-diphenylbenzidine

\(1^{2+}\)

\((1+2H)^{2+}\)

Reaction was also monitored by UV-Vis spectroscopy in CH\(_2\)Cl\(_2\): entry A
SCE potentials vs. Fc/Fc⁺, measured with a scan rate of 100 mV·s⁻¹ and nBu₄N(PF₆) as supporting electrolyte in CH₃CN.
9) **UV-Vis data [Å in nm (solvent)]**

|          | -OMe | -H     | 2-Br | -NO₂ |
|----------|------|--------|------|------|
| TPA      | -    | 370ᵃ  | -    | -    |
| TPA⁺⁺    | 695ᵇ (ACN) | 679ᵇ (ACN) | -    | 656ᵇ (ACN) |
| TPB⁺⁺    | 1574; 492ᵈ (DCM) | 1385; 481ᵈ (DCM) | 1490; 489ᶜ (DCM) | - |
| TPB²⁺    | 878ᵈ (DCM)     | 742ᵈ (DCM)     | 807ᶜ (DCM)     | - |

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**Conclusions from the experiments**

With a substrate/GFA ratio of 1:1 the reactions proceeded almost quantitatively, without side products under the applied conditions. In the case of a substrate: GFA ratio of 1:0.65 the reactions were slower and substrate was still present when the reaction time was doublet.

The NMR spectra taken for the experiments with only small amounts of HBF₄ either show still the presence of unreacted substrate (for small reaction times) or the products of additional coupling (for longer reaction times). The reaction with 4,4'-dibromtriphenylamine was an exception, since formation of additional coupling products is prohibited by the bromo substituents. In this case the reaction time can be increased without the observation of further products. However, the reaction was much slower and not quantitative.
Experimental Details for oxidative coupling of 3,3′′,4,4′′-tetramethoxy-o-terphenyl to 2,3,10,11-tetramethoxy-triphenylene

| entry | A | B | C |
|-------|---|---|---|
| 1(BF₄)₂ [mg/µmol] | 6.224/8.84 | - | 6.256/8.88 |
| 1(PF₆)₂ [mg/µmol] | - | 5.424/6.61 | - |
| 3,3′′,4,4′′-tetramethoxy-o-terphenyl [mg/µmol] | 3.054/8.72 | 2.286/6.52 | 3.026/8.64 |
| HBF₄·Et₂O (5% in CH₃CN) [mL/µmol] | 0.5/182.3 | 0.5/182.3 | 0.15/54.7 |
| HMB [mg/µmol] | 2.160/13.31 | 1.758/10.83 | 1.380/8.50 |
| CH₃CN [mL] | - | - | 1 |
| reaction time (temperature) | 5 min (ice cooling) | 10 min (ice cooling) | 5 h (60 °C) |
| conversion (rel. to 1²⁺/(1+2H)²⁺) [%] | 99 | 98 | 97 |
| ratio (substrate/GFA) | 1/1 | 1/1 | 1/1 |

Protocol for entries A & B

In a Schlenk flask, 0.5 mL of a HBF₄·Et₂O solution (5% in CH₃CN) was added with a syringe under ice cooling in an Ar atmosphere to the reactants 1(BF₄)₂ / 1(PF₆)₂ and 3,3′′,4,4′′-tetramethoxy-o-terphenyl. The reaction was stirred for several minutes under ice cooling and then allowed to warm up to room temperature for further reaction.
Protocol for entry C

In a Schlenk flask, 0.5 mL of a HBF₄·Et₂O solution (5% in CH₃CN) was added with a syringe in an Ar atmosphere to a solution of the reactants 1(BF₄)₂ and 3,3”,4,4”-tetramethoxy-o-terphenyl in 1 mL CH₃CN. The reaction was stirred for 5 h at a temperature of 60 °C.

Work-up entries A - C

The reaction was stopped by the addition of an aqueous saturated NaHCO₃ solution. The small amount of CH₃CN was removed under high-vacuum. An aqueous diluted solution of NaOH (8%) was added (pH > 9), converting all formed (1+4H)⁺⁺ to (1+2H)⁺⁺ (for subsequent transfer into the organic phase). A clear solution was obtained that was extracted several times with CH₂Cl₂. The combined organic phases were dried over Na₂SO₄, filtrated and condensed.

¹H NMR spectra (399.89 MHz, 295.5 K, CD₂Cl₂) for entry A

¹H NMR of 2,3,10,11-tetramethoxytriphenylene: (399.89 MHz, 295.5 K, CD₂Cl₂): δ = 4.07 (d, J = 4.4 Hz, 12 H), 7.60 (dd, J = 6.3; 3.3 Hz, 2 H), 7.82 (s, 2 H), 8.00 (s, 2 H), 8.52 (dd, J = 6.3; 3.4 Hz, 2 H) ppm.
Protocol for additional NMR experiments

5.256 mg (7.46 µmol) of 1(BF₄)₂, 0.810 mg (4.99 µmol) HMB and 2.474 mg (7.06 µmol) of 3,3″,4,4″-tetramethoxy-o-terphenyl were dissolved in an NMR tube under an Ar atmosphere in 0.45 mL CD₃CN. Then 0.05 mL (18.23 µmol) of a HBF₄·Et₂O solution (5% in CD₃CN) were added with a syringe. The reaction mixture was heated to a temperature of 60 °C.

¹H NMR experiment (199.87 MHz, 298 K, CD₃CN): reaction of 1(BF₄)₂ and 3,3″,4,4″-tetramethoxy-o-terphenyl without addition of HBF₄·Et₂O solution (5% in CD₃CN)
$^1$H NMR experiment (199.87 MHz, 298 K, CD$_3$CN): reaction of 1(BF$_4$)$_2$ and 3,3'',4,4''-tetramethoxy-o-terphenyl after the addition of 0.05 mL HBF$_4$·Et$_2$O solution (5% in CD$_3$CN)

$^1$H NMR experiment (199.87 MHz, 298 K, CD$_3$CN): reaction of 1(BF$_4$)$_2$ and 3,3'',4,4''-tetramethoxy-o-terphenyl 1 h after the addition of 0.05 mL HBF$_4$·Et$_2$O solution (5% in CD$_3$CN)
11) Recycling experiments

\[
\text{O}_2, \ 3 \text{ mol\% cat, Et}_3\text{N} \\
\text{CH}_3\text{CN, 60°C, 30 min}
\]

| entry | A          | B          | C          |
|-------|------------|------------|------------|
| (1+4H)(BF\textsubscript{4})\textsubscript{4} [mg/µmol] | 33.03/37.45 | 8.81/9.99  | 4.278/4.85 |
| CuCl\textsubscript{2} [µmol/mol%] | 1.13/3.0    | 0.30/3.0   | 0.15/3.1   |
| [Cu(H\textsubscript{2}O)\textsubscript{6}(BF\textsubscript{4})\textsubscript{2}] [µmol/mol%] | 1.11/3.0    | 0.29/3.0   | 0.14/2.9   |
| NEt\textsubscript{3} [µL/µmol] | 15/107.6    | 4/28.7     | 2/14.4     |
| Na\textsubscript{2}SO\textsubscript{4} [mg] | 2.446       | 1.566      | 1.900      |
| CD\textsubscript{3}CN [mL] | 0.6         | 0.6        | 0.6        |
| reaction time (temperature) | 0.5 h (60 °C) | 0.5 h (60 °C) | 0.5 h (60 °C) |
| c (mmol·l\textsuperscript{-1}) | 62          | 17         | 8          |
| conversion [%] | >99         | >99        | >99        |

First stock solutions of the copper compounds (CuCl\textsubscript{2} and [Cu(H\textsubscript{2}O)\textsubscript{6}(BF\textsubscript{4})\textsubscript{2}]) in CH\textsubscript{3}CN were prepared. Then the desired amount of catalyst was introduced with a syringe into a Schlenk flask. The solvent was removed under vacuum, and the solid catalyst (cat = equimolar mixture of CuCl\textsubscript{2} and [Cu(H\textsubscript{2}O)\textsubscript{6}(BF\textsubscript{4})\textsubscript{2}]) re-dissolved in 0.6 mL CD\textsubscript{3}CN.

In a vial, the catalyst solution and NEt\textsubscript{3} was added under an atmosphere of dioxygen to (1+4H)(BF\textsubscript{4})\textsubscript{4} and Na\textsubscript{2}SO\textsubscript{4}. The vial was locked with a septum and the reaction mixture stirred under 0.2 bar of dioxygen for a period of 30 min at 60 °C. The conversion was followed by NMR spectroscopy. The reaction was stopped by the addition of a saturated NaHCO\textsubscript{3} solution. After solvent removal the residue was collected with H\textsubscript{2}O and CH\textsubscript{2}Cl\textsubscript{2}. The organic phases were separated and the aqueous phase extracted several times with CH\textsubscript{2}Cl\textsubscript{2}. The combined organic phases were dried over Na\textsubscript{2}SO\textsubscript{4}.
$^1$H NMR spectra (199.87 MHz, 298 K, CD$_3$CN) for entry B

$^1$H NMR spectra (199.87 MHz, 298 K, CD$_3$CN) of combined entries A - C after work-up

$^1$H NMR of 1(BF$_4$)$_2$: (199.87 MHz, 298 K, CD$_3$CN): $\delta$ = 2.87 (s, 48 H), 5.16 (s, 2 H) ppm.
Synthesis of (1+4H)(BF$_4$)$_4$

In a Schenk flask, 1.15 mL (419.18 µmol) of a HBF$_4$·Et$_2$O solution (5% in CH$_3$CN) were dropwise added with a syringe to a suspension of 55 mg (103.62 µmol) of 1 in 4 mL CH$_3$CN. The reaction mixture was stirred for 1 h at room temperature. The solvent was removed under vacuum and the colourless residue washed several times with diethylether. Yield: 72 mg (81.63 µmol, 79 %). C$_{26}$H$_{54}$N$_{12}$B$_4$F$_{16}$ (882.01 g mol$^{-1}$): calcd. C 35.41, H 6.17, N 19.06; found C 35.05, H 5.91, N 19.03. $^1$H NMR (399.87 MHz, CD$_3$CN, 295.7 K): $\delta$ = 2.98 (s, 48 H, CH$_3$), 6.72 (s, 2 H, CH), 7.59 (s, 4 H, NH) ppm. $^{11}$B-NMR (128.30 MHz, CD$_3$CN, 295.7 K): $\delta$ = -1.17 ppm. $^{13}$C NMR (100.56 MHz, CD$_3$CN, 295.7 K): $\delta$ = 41.09 (CH$_3$), 118.81 (C$_{arom.}$), 129.96, 159.44 (C$_g$) ppm. MS (ESI, CH$_3$CN): m/z (%) = 619 (100) [(1+2H)(BF$_4$)$_2$]$^+$, 531 (70) [1]$^+$, 707 (52) [(1+3H)(BF$_4$)$_2$]$^+$, 795 (10) [(1+4H)(BF$_4$)$_3$]$^+$, 341 (36). IR (CsI): $\tilde{\nu}$ = 3319 (m), 2961 (m), 1734 (sh), 1636 (s), 1549 (s), 1497 (sh), 1457 (m), 1447 (m), 1422 (s), 1403 (s), 1305 (m), 1262 (w), 1240 (w), 1193 (w), 1169 (m), 1145 (sh), 1076 (sh), 1058 (vs), 1040 (sh), 897 (w), 881 (w), 800 (w), 720 (w), 676 (w), 648 (w), 599 (w), 522 (m), 473 (w) cm$^{-1}$. UV-Vis (CH$_3$CN, c = 5.60·10$^{-5}$ M, d = 1 cm): $\lambda$ (ε in L mol$^{-1}$ cm$^{-1}$) = 316 (sh, 7850), 284 (23630), 256 (sh, 33030), 242 (40430) nm.

$^1$H NMR spectra (399.89 MHz, 295.7 K, CD$_3$CN) of (1+4H)(BF$_4$)$_4$
12) Quantum chemical calculations

Details of the quantum-chemical calculations
Quantum-chemical calculations were carried out on the compounds $1^{2+}$, $(1+2H)^{2+}$, $1(BF_4)_2$, $(1+2H)(BF_4)_2$, C$_6$Cl$_4$(OH)$_2$, C$_6$Cl$_4$O$_2$ (CA), C$_6$H$_4$(OH)$_2$, C$_6$H$_4$O$_2$ (BQ), C$_6$Cl$_2$(CN)$_2$(OH)$_2$, C$_6$Cl$_2$(CN)$_2$O$_2$ (DDQ), $(1+2H)^{4+}$, $(1+4H)^{4+}$, $(1+2H)(BF_4)_4$, $(1+4H)(BF_4)_4$, $(C_6$Cl$_4$O$_2$+2H)$^{2+}$, C$_6$Cl$_4$O$_2$(HF)$_2$(BF$_3$)$_2$ (result of the attempt to calculate the twofold protonated CA with two BF$_4^{−}$ counter-ions), (C$_6$H$_4$O$_2$+2H)$^{2+}$, C$_6$H$_4$O$_2$(HF)$_2$(BF$_3$)$_2$, $(1+H)^{3+}$ (C$_6$Cl$_4$O$_2$+H)$^{+}$, and BF$_4^{−}$. These calculations relied on the TURBOMOLE program.\cite{1,2,3} The B3LYP functional\cite{4,5} was used in combination with the def2-SV(P) or def2-TZVP basis set.\cite{6} The influence of a polarizable environment was considered by the conductor-like screening model (COSMO).\cite{7}

| Compound | $E$ (TZVP) / hartree | $E$ (SV(P)) / hartree | ZPVE (SV(P)) / kJ mol$^{-1}$ | $\mu_{298}$ / kJ mol$^{-1}$ |
|----------|----------------------|----------------------|-------------------------------|---------------------------|
| $1^{2+}$ | -1676.926440 | -1674.983327 | 0.7725901 | 1807.58 |
| $(1+2H)^{2+}$ | -1678.160534 | -1676.213037 | 0.7973611 | 1882.61 |
| $1(BF_4)_2$ | -2526.372388 | -2523.389345 | 0.8071689 | 1867.12 |
| $(1+2H)(BF_4)_2$ | -2527.606309 | -2524.616407 | 0.8314375 | 1933.59 |
| C$_6$Cl$_4$(OH)$_2$ | -2220.868853 | -2219.781158 | 0.0703544 | 85.67 |
| C$_6$Cl$_4$O$_2$ (CA) | -2219.631177 | -2218.563340 | 0.0471586 | 24.58 |
| C$_6$H$_4$(OH)$_2$ | -382.630902 | -382.168603 | 0.1082916 | 205.94 |
| C$_6$H$_4$O$_2$ (BQ) | -381.397659 | -380.955550 | 0.0852803 | 147.24 |
| C$_6$Cl$_3$(CN)$_2$(OH)$_2$ | -1486.204688 | -1485.227188 | 0.0866643 | 125.64 |
| C$_6$Cl$_2$(CN)$_2$O$_2$ (DDQ) | -1484.953539 | -1483.996510 | 0.0631770 | 62.13 |
| $(1+2H)^{3+}$ | -1677.301599 | -1675.348289 | 0.7996077 | 1886.48 |
| $(1+4H)^{4+}$ | -1678.549891 | -1676.591423 | 0.8241836 | 1955.26 |
| $(1+2H)(BF_4)_4$ | -3376.623575 | -3372.606495 | 0.8666310 | 1984.75 |
| $(1+4H)(BF_4)_4$ | -3377.888141 | -3373.865924 | 0.8919710 | 2054.67 |
| $(C_6$Cl$_4$O$_2$+2H)$^{2+}$ | -2220.102422 | -2219.017931 | 0.0699483 | 82.21 |
| C$_6$Cl$_4$O$_2$(HF)$_2$(BF$_3$)$_2$ | -3069.758291 | -3067.620892 | 0.0984588 | 92.34 |
| $(C_6$H$_4$O$_2$+2H)$^{2+}$ | -381.863637 | -381.404077 | 0.1086933 | 206.16 |
| C$_6$H$_4$O$_2$(HF)$_2$(BF$_3$)$_2$ | -1231.535578 | -1230.028537 | 0.1371169 | 221.67 |
| $(1+H)^{5+}$ | -1677.166120 | -1675.218750 | 0.7867587 | 1851.15 |
| $(C_6$Cl$_4$O$_2$+H)$^{+}$ | -2219.945117 | -2218.871082 | 0.0589688 | 52.32 |
| BF$_4^{−}$ | -424.575347 | -424.036813 | 0.0146443 | -27.92 |
Reaction energies, enthalpies (at 0 K) and Gibbs free energies (at 298 K)

\[ \text{C}_6\text{Cl}_4\text{(OH)}_2 + 1^{2+} \rightarrow \text{C}_6\text{Cl}_4\text{O}_2 + (1+2\text{H})^{2+} \]

\[ \Delta E_{\text{el}}(\text{B3LYP/TZVP}) = 9.4045 \text{ kJ/mol} = 0.0975 \text{ eV} \]
\[ \Delta E_{\text{el}}(\text{B3LYP/SV(P)}) = -31.2224 \text{ kJ/mol} = -0.3236 \text{ eV} \]
\[ \Delta H(0 \text{ K}) (\text{B3LYP/TZVP/SV(P)}) = 13.5402 \text{ kJ/mol} = 0.1404 \text{ eV} \]
\[ \Delta G_{298}(\text{B3LYP/TZVP/SV(P)}) = 23.34 \text{ kJ/mol} = 0.2420 \text{ eV} \]

\[ \Delta E_{\text{vib}}(0 \text{ K}) (\text{B3LYP/SV(P)}) = 4.1357 \text{ kJ/mol} = 0.0429 \text{ eV} \]
\[ \Delta G_{298}(\text{B3LYP/SV(P)}) = 13.94 \text{ kJ/mol} = 0.1445 \text{ eV} \]

\[ \text{C}_6\text{Cl}_4\text{(OH)}_2 + 1(\text{BF}_4)^2_2 \rightarrow \text{C}_6\text{Cl}_4\text{O}_2 + (1+2\text{H})(\text{BF}_4)^2_2 \]

\[ \Delta E_{\text{el}}(\text{B3LYP/TZVP}) = 9.8588 \text{ kJ/mol} = 0.1022 \text{ eV} \]
\[ \Delta E_{\text{el}}(\text{B3LYP/SV(P)}) = -24.2701 \text{ kJ/mol} = -0.2515 \text{ eV} \]
\[ \Delta H(0 \text{ K}) (\text{B3LYP/TZVP/SV(P)}) = 12.6754 \text{ kJ/mol} = 0.1314 \text{ eV} \]
\[ \Delta G_{298}(\text{B3LYP/TZVP/SV(P)}) = 5.24 \text{ kJ/mol} = 0.1580 \text{ eV} \]

\[ \Delta E_{\text{vib}}(0 \text{ K}) (\text{B3LYP/SV(P)}) = 2.8166 \text{ kJ/mol} = 0.0292 \text{ eV} \]
\[ \Delta G_{298}(\text{B3LYP/SV(P)}) = 5.38 \text{ kJ/mol} = 0.0558 \text{ eV} \]

\[ \text{C}_6\text{H}_4\text{(OH)}_2 + 1(\text{BF}_4)^2_2 \rightarrow \text{C}_6\text{H}_4\text{O}_2 + (1+2\text{H})(\text{BF}_4)^2_2 \]

\[ \Delta E_{\text{el}}(\text{B3LYP/TZVP}) = -1.7801 \text{ kJ/mol} = -0.0184 \text{ eV} \]
\[ \Delta E_{\text{el}}(\text{B3LYP/SV(P)}) = -36.7806 \text{ kJ/mol} = -0.3812 \text{ eV} \]
\[ \Delta H(0 \text{ K}) (\text{B3LYP/TZVP/SV(P)}) = 1.5209 \text{ kJ/mol} = 0.0158 \text{ eV} \]
\[ \Delta G_{298}(\text{B3LYP/TZVP/SV(P)}) = 5.99 \text{ kJ/mol} = 0.0621 \text{ eV} \]

\[ \Delta E_{\text{vib}}(0 \text{ K}) (\text{B3LYP/SV(P)}) = 3.3010 \text{ kJ/mol} = 0.0342 \text{ eV} \]
\[ \Delta G_{298}(\text{B3LYP/SV(P)}) = 7.77 \text{ kJ/mol} = 0.0805 \text{ eV} \]

\[ \text{C}_6\text{Cl}_2\text{(CN)}_2\text{(OH)}_2 + 1(\text{BF}_4)^2_2 \rightarrow \text{C}_6\text{Cl}_2\text{(CN)}_2\text{O}_2 + (1+2\text{H})(\text{BF}_4)^2_2 \]

\[ \Delta E_{\text{el}}(\text{B3LYP/TZVP}) = 45.2321 \text{ kJ/mol} = 0.4688 \text{ eV} \]
\[ \Delta E_{\text{el}}(\text{B3LYP/SV(P)}) = 9.4938 \text{ kJ/mol} = 0.0984 \text{ eV} \]
\[ \Delta H(0 \text{ K}) (\text{B3LYP/TZVP/SV(P)}) = 47.2334 \text{ kJ/mol} = 0.4901 \text{ eV} \]
\[ \Delta G_{298}(\text{B3LYP/TZVP/SV(P)}) = 48.19 \text{ kJ/mol} = 0.4995 \text{ eV} \]

\[ \Delta E_{\text{vib}}(0 \text{ K}) (\text{B3LYP/SV(P)}) = 2.0513 \text{ kJ/mol} = 0.0213 \text{ eV} \]
\[ \Delta G_{298}(\text{B3LYP/SV(P)}) = 2.96 \text{ kJ/mol} = 0.0307 \text{ eV} \]
\[ \text{C}_6\text{Cl}_4(\text{OH})_2 + (1+2\text{H})^{4+} \rightarrow \text{C}_6\text{Cl}_4\text{O}_2 + (1+4\text{H})^{4+} \]

\[ \Delta E_{\text{el}} \text{(B3LYP/TZVP)} = -27.8723 \text{ kJ/mol} = -0.2889 \text{ eV} \]
\[ \Delta E_{\text{el}} \text{(B3LYP/SV(P))} = -66.4671 \text{ kJ/mol} = -0.6889 \text{ eV} \]
\[ \Delta H \text{ (0 K) (B3LYP/TZVP/SV(P))} = -24.2488 \text{ kJ/mol} = -0.2513 \text{ eV} \]
\[ \Delta G_{298} \text{(B3LYP/TZVP/SV(P))} = -20.18 \text{ kJ/mol} = -0.2092 \text{ eV} \]

\[ \Delta E_{\text{el}} \text{(B3LYP/TZVP)} = -70.5997 \text{ kJ/mol} = -0.7317 \text{ eV} \]
\[ \Delta E_{\text{el}} \text{(B3LYP/SV(P))} = -109.2497 \text{ kJ/mol} = -1.1323 \text{ eV} \]
\[ \Delta H \text{ (0 K) (B3LYP/TZVP/SV(P))} = -64.9701 \text{ kJ/mol} = -0.6734 \text{ eV} \]
\[ \Delta G_{298} \text{(B3LYP/TZVP/SV(P))} = -61.77 \text{ kJ/mol} = -0.6402 \text{ eV} \]

\[ \Delta E_{\text{el}} \text{(B3LYP/TZVP)} = -194.9696 \text{ kJ/mol} = -2.0207 \text{ eV} \]
\[ \Delta E_{\text{el}} \text{(B3LYP/SV(P))} = -189.8735 \text{ kJ/mol} = -1.9679 \text{ eV} \]
\[ \Delta H \text{ (0 K) (B3LYP/TZVP/SV(P))} = -201.1616 \text{ kJ/mol} = -2.0849 \text{ eV} \]
\[ \Delta G_{298} \text{(B3LYP/TZVP/SV(P))} = -210.80 \text{ kJ/mol} = -2.1848 \text{ eV} \]

\[ \Delta E_{\text{el}} \text{(B3LYP/TZVP)} = -252.2738 \text{ kJ/mol} = -2.6146 \text{ eV} \]
\[ \Delta E_{\text{el}} \text{(B3LYP/SV(P))} = -235.3209 \text{ kJ/mol} = -2.4389 \text{ eV} \]
\[ \Delta H \text{ (0 K) (B3LYP/TZVP/SV(P))} = -263.3741 \text{ kJ/mol} = -2.7296 \text{ eV} \]
\[ \Delta G_{298} \text{(B3LYP/TZVP/SV(P))} = -273.54 \text{ kJ/mol} = -2.8350 \text{ eV} \]
\[ \text{C}_6\text{Cl}_4\text{O}_2 + (1+2\text{H})(\text{BF}_4)_2 \rightarrow \text{C}_6\text{Cl}_4\text{O}_2(\text{HF})_2(\text{BF}_3)_2 + \text{1}(\text{BF}_4)_2 \]

\[ \Delta E_{\text{el}}(\text{B3LYP/TZVP}) = 325.7536 \text{ kJ/mol} = 3.3762 \text{ eV} \]
\[ \Delta E_{\text{el}}(\text{B3LYP/SV(P)}) = 419.0245 \text{ kJ/mol} = 4.3429 \text{ eV} \]
\[ \Delta H (0 \text{ K}) (\text{B3LYP/TZVP/SV(P)}) = 304.3245 \text{ kJ/mol} = 3.1541 \text{ eV} \]
\[ \Delta G_{298}(\text{B3LYP/TZVP/SV(P)}) = 275.88 \text{ kJ/mol} = 2.8593 \text{ eV} \]

\[ \Delta E_{\text{el}}(0 \text{ K}) (\text{B3LYP/SV(P)}) = -21.4291 \text{ kJ/mol} = -0.2221 \text{ eV} \]
\[ \Delta \Delta G_{298}(\text{B3LYP/SV(P)}) = -49.87 \text{ kJ/mol} = -0.5169 \text{ eV} \]

\[ \text{C}_6\text{H}_4\text{O}_2 + (1+2\text{H})^{4+} \rightarrow (\text{C}_6\text{H}_4\text{O}_2^{2+})^2 + \text{1}^{2+} \]

\[ \Delta E_{\text{el}}(\text{B3LYP/TZVP}) = -238.4453 \text{ kJ/mol} = -2.4713 \text{ eV} \]
\[ \Delta E_{\text{el}}(\text{B3LYP/SV(P)}) = -219.3999 \text{ kJ/mol} = -2.2739 \text{ eV} \]
\[ \Delta H (0 \text{ K}) (\text{B3LYP/TZVP/SV(P)}) = -247.9092 \text{ kJ/mol} = -2.5694 \text{ eV} \]
\[ \Delta G_{298}(\text{B3LYP/TZVP/SV(P)}) = -258.43 \text{ kJ/mol} = -2.6784 \text{ eV} \]

\[ \Delta E_{\text{el}}(0 \text{ K}) (\text{B3LYP/SV(P)}) = -9.4639 \text{ kJ/mol} = -0.0981 \text{ eV} \]
\[ \Delta \Delta G_{298}(\text{B3LYP/SV(P)}) = -19.98 \text{ kJ/mol} = -0.2071 \text{ eV} \]

\[ \text{C}_6\text{H}_4\text{O}_2 + (1+2\text{H})(\text{BF}_4)_2 \rightarrow \text{C}_6\text{H}_4\text{O}_2(\text{HF})_2(\text{BF}_3)_2 + \text{1}(\text{BF}_4)_2 \]

\[ \Delta E_{\text{el}}(\text{B3LYP/TZVP}) = 297.3851 \text{ kJ/mol} = 3.0822 \text{ eV} \]
\[ \Delta E_{\text{el}}(\text{B3LYP/SV(P)}) = 378.4999 \text{ kJ/mol} = 3.9229 \text{ eV} \]
\[ \Delta H (0 \text{ K}) (\text{B3LYP/TZVP/SV(P)}) = 277.4789 \text{ kJ/mol} = 2.8747 \text{ eV} \]
\[ \Delta G_{298}(\text{B3LYP/TZVP/SV(P)}) = 254.30 \text{ kJ/mol} = 2.6345 \text{ eV} \]

\[ \Delta E_{\text{el}}(0 \text{ K}) (\text{B3LYP/SV(P)}) = -20.0207 \text{ kJ/mol} = -0.2075 \text{ eV} \]
\[ \Delta \Delta G_{298}(\text{B3LYP/SV(P)}) = -43.20 \text{ kJ/mol} = -0.4477 \text{ eV} \]

\[ \text{C}_6\text{H}_4(\text{OH})_2 + (1+2\text{H})(\text{BF}_4)_2 \rightarrow \text{C}_6\text{H}_4\text{O}_2 + \text{ttmgbH}_4(\text{BF}_4)_4 \]

\[ \Delta E_{\text{el}}(\text{B3LYP/TZVP}) = -82.2385 \text{ kJ/mol} = -0.8523 \text{ eV} \]
\[ \Delta E_{\text{el}}(\text{B3LYP/SV(P)}) = -121.7602 \text{ kJ/mol} = -1.2620 \text{ eV} \]
\[ \Delta H (0 \text{ K}) (\text{B3LYP/TZVP/SV(P)}) = -76.1245 \text{ kJ/mol} = -0.7889 \text{ eV} \]
\[ \Delta G_{298}(\text{B3LYP/TZVP/SV(P)}) = -71.02 \text{ kJ/mol} = -0.7360 \text{ eV} \]

\[ \Delta E_{\text{el}}(0 \text{ K}) (\text{B3LYP/SV(P)}) = 6.1140 \text{ kJ/mol} = 0.0634 \text{ eV} \]
\[ \Delta \Delta G_{298}(\text{B3LYP/SV(P)}) = 11.22 \text{ kJ/mol} = 0.1163 \text{ eV} \]

\[ \text{C}_6\text{Cl}_2(\text{CN})_2(\text{OH})_2 + (1+2\text{H})(\text{BF}_4)_2 \rightarrow \text{C}_6\text{Cl}_2(\text{CN})_2\text{O}_2 + \text{ttmgbH}_4(\text{BF}_4)_4 \]

\[ \Delta E_{\text{el}}(\text{B3LYP/TZVP}) = -35.2263 \text{ kJ/mol} = -0.3651 \text{ eV} \]
ΔE_{el}(B3LYP/SV(P)) = -75.4857 kJ/mol = -0.7824 eV
ΔH (0 K) (B3LYP/TZVP/SV(P)) = -30.3620 kJ/mol = -0.3147 eV
ΔG_{298}(B3LYP/TZVP/SV(P)) = -28.82 kJ/mol = -0.2987 eV

ΔE_{vib} (0 K) (B3LYP/SV(P)) = 4.8643 kJ/mol = 0.0504 eV
ΔΔG_{298}(B3LYP/SV(P)) = 6.41 kJ/mol = 0.0664 eV
Calculations with COSMO for varying relative permittivities $\varepsilon_r$

Calculations for the reaction $\text{C}_6\text{H}_4(\text{OH})_2 + 1^{2+} \rightarrow \text{C}_6\text{H}_4\text{O}_2 + (1+2\text{H})^{2+}$

$E(\text{B3LYP/TZVP}) / \text{hartree}$ for the structures optimized at $\varepsilon_r = 1$

| $\varepsilon_r$ | $1^{2+}$ | $(1+2\text{H})^{2+}$ | $\text{C}_6\text{H}_4(\text{OH})_2$ | $\text{C}_6\text{H}_4\text{O}_2$ |
|-----------------|---------|-----------------|----------------|----------------|
| 1               | -1676.926440 | -1678.160534 | -382.630902 | -381.397659 |
| 40              | -1677.107337 | -1678.342689 | -382.646936 | -381.410799 |

$\Delta E_{el}(\text{B3LYP/TZVP}, \varepsilon_r = 1) = -2.2343 \text{ kJ/mol} = -0.0232 \text{ eV}$

$\Delta E_{el}(\text{B3LYP/TZVP}, \varepsilon_r = 40) = 2.0610 \text{ kJ/mol} = 0.0214 \text{ eV}$

Calculations for the reaction $\text{C}_6\text{H}_4(\text{OH})_2 + 1(\text{BF}_4)_2 \rightarrow \text{C}_6\text{H}_4\text{O}_2 + (1+2\text{H})(\text{BF}_4)_2$

$E(\text{B3LYP/TZVP}) / \text{hartree}$ for the structures optimized at $\varepsilon_r = 1$

| $\varepsilon_r$ | $1(\text{BF}_4)_2$ | $(1+2\text{H})(\text{BF}_4)_2$ | $\text{C}_6\text{H}_4(\text{OH})_2$ | $\text{C}_6\text{H}_4\text{O}_2$ |
|-----------------|--------------------|-----------------|----------------|----------------|
| 1               | -2526.372388 | -2527.606309 | -382.630902 | -381.397659 |
| 40              | -2526.439210 | -2527.670528 | -382.646936 | -381.410799 |

$\Delta E_{el}(\text{B3LYP/TZVP}, \varepsilon_r = 1) = -1.7801 \text{ kJ/mol} = -0.0184 \text{ eV}$

$\Delta E_{el}(\text{B3LYP/TZVP}, \varepsilon_r = 40) = 12.6523 \text{ kJ/mol} = 0.1311 \text{ eV}$

$E(\text{B3LYP/TZVP}) / \text{hartree}$ for the structures optimized at each value of $\varepsilon_r$

| $\varepsilon_r$ | $1(\text{BF}_4)_2$ | $(1+2\text{H})(\text{BF}_4)_2$ | $\text{C}_6\text{H}_4(\text{OH})_2$ | $\text{C}_6\text{H}_4\text{O}_2$ |
|-----------------|--------------------|----------------|----------------|----------------|
| 1               | -2526.372388 | -2527.606309 | -382.630902 | -381.397659 |
| 40              | -2526.451653 | -2527.683936 | -382.647011 | -381.410950 |

$\Delta E_{el}(\text{B3LYP/TZVP}, \varepsilon_r = 1) = -1.7801 \text{ kJ/mol} = -0.0184 \text{ eV}$

$\Delta E_{el}(\text{B3LYP/TZVP}, \varepsilon_r = 40) = 9.9191 \text{ kJ/mol} = 0.1028 \text{ eV}$

Calculations for the reaction $\text{C}_6\text{Cl}_4(\text{OH})_2 + 1^{2+} \rightarrow \text{C}_6\text{Cl}_4\text{O}_2 + (1+2\text{H})^{2+}$

$E(\text{B3LYP/TZVP}) / \text{hartree}$ for the structures optimized at $\varepsilon_r = 1$

| $\varepsilon_r$ | $1^{2+}$ | $(1+2\text{H})^{2+}$ | $\text{C}_6\text{Cl}_4(\text{OH})_2$ | $\text{C}_6\text{Cl}_4\text{O}_2$ |
|-----------------|---------|-----------------|----------------|----------------|
| 1               | -1677.926440 | -1678.160534 | -2220.868853 | -2219.631177 |
| 2               | -1677.001172 | -1678.235832 | -2220.872857 | -2219.635256 |
| 5               | -1677.062719 | -1678.297811 | -2220.876410 | -2219.639026 |
| 10              | -1677.087270 | -1678.322513 | -2220.877900 | -2219.640651 |
| 20              | -1677.100478 | -1678.335795 | -2220.878720 | -2219.641557 |
| 40              | -1677.107337 | -1678.342689 | -2220.879151 | -2219.642037 |
| 60              | -1677.109663 | -1678.345027 | -2220.879298 | -2219.642201 |
| 80              | -1677.110834 | -1678.346203 | -2220.879372 | -2219.642284 |

$\Delta E_{el}(\text{B3LYP/TZVP}, \varepsilon_r = 1) = 9.4045 \text{ kJ/mol} = 0.0975 \text{ eV}$

$\Delta E_{el}(\text{B3LYP/TZVP}, \varepsilon_r = 2) = 7.7216 \text{ kJ/mol} = 0.0800 \text{ eV}$

$\Delta E_{el}(\text{B3LYP/TZVP}, \varepsilon_r = 5) = 6.0176 \text{ kJ/mol} = 0.0624 \text{ eV}$
Calculations for the reaction C\(_6\)Cl\(_4\)(OH)\(_2\) + 1(BF\(_4\))\(_2\) → C\(_6\)Cl\(_4\)O\(_2\) + (1+2H)(BF\(_4\))\(_2\)

\[ E(B3LYP/TZVP) / \text{hartree} \]

| \( \varepsilon_r \) | 1(BF\(_4\))\(_2\) | (1+2H)(BF\(_4\))\(_2\) | C\(_6\)Cl\(_4\)(OH)\(_2\) | C\(_6\)Cl\(_4\)O\(_2\) |
|----------------|----------------|----------------|----------------|----------------|
| 1              | -2526.372388  | -2527.606309  | -2220.868853  | -2219.631177  |
| 2              | -2526.398034  | -2527.630933  | -2220.872857  | -2219.635256  |
| 5              | -2526.421144  | -2527.653144  | -2220.876410  | -2219.639026  |
| 10             | -2526.430937  | -2527.662565  | -2220.877900  | -2219.640651  |
| 20             | -2526.436354  | -2527.667778  | -2220.878720  | -2219.641557  |
| 40             | -2526.439210  | -2527.670528  | -2220.879151  | -2219.642037  |
| 80             | -2526.440677  | -2527.671941  | -2220.879372  | -2219.642284  |

\[ \Delta E_{el} (B3LYP/TZVP, \varepsilon_r = 1) = 9.8587 \text{ kJ/mol} = 0.1022 \text{ eV} \]
\[ \Delta E_{el} (B3LYP/TZVP, \varepsilon_r = 2) = 12.3451 \text{ kJ/mol} = 0.1279 \text{ eV} \]
\[ \Delta E_{el} (B3LYP/TZVP, \varepsilon_r = 5) = 14.1357 \text{ kJ/mol} = 0.1465 \text{ eV} \]
\[ \Delta E_{el} (B3LYP/TZVP, \varepsilon_r = 10) = 14.7579 \text{ kJ/mol} = 0.1530 \text{ eV} \]
\[ \Delta E_{el} (B3LYP/TZVP, \varepsilon_r = 20) = 15.0677 \text{ kJ/mol} = 0.1562 \text{ eV} \]
\[ \Delta E_{el} (B3LYP/TZVP, \varepsilon_r = 40) = 15.2174 \text{ kJ/mol} = 0.1577 \text{ eV} \]
\[ \Delta E_{el} (B3LYP/TZVP, \varepsilon_r = 80) = 15.2909 \text{ kJ/mol} = 0.1585 \text{ eV} \]
Calculations for the reaction $\text{C}_6\text{Cl}_2(\text{CN})_2(\text{OH})_2 + 1^{2+} \rightarrow \text{C}_6\text{Cl}_2(\text{CN})_2\text{O}_2 + (1+2\text{H})^{2+}$

$E(\text{B3LYP/TZVP}) / \text{hartree}$ for the structures optimized at $\varepsilon_r = 1$

| $\varepsilon_r$ | $1^{2+}$ | $(1+2\text{H})^{2+}$ | $\text{C}_6\text{Cl}_2(\text{CN})_2(\text{OH})_2$ | $\text{C}_6\text{Cl}_2(\text{CN})_2\text{O}_2$ |
|----------------|----------|----------------------|--------------------------------------|--------------------------------------|
| 1             | -1676.926440 | -1678.160534 | -1486.204688 | -1484.953539 |
| 40            | -1677.107337 | -1678.342689 | -1486.228322 | -1484.973404 |

$\Delta E_{\text{el}}(\text{B3LYP/TZVP}, \varepsilon_r = 1) = 44.7779 \text{ kJ/mol} = 0.4641 \text{ eV}$

$\Delta E_{\text{el}}(\text{B3LYP/TZVP}, \varepsilon_r = 40) = 51.3705 \text{ kJ/mol} = 0.5324 \text{ eV}$

Calculations for the reaction $\text{C}_6\text{Cl}_2(\text{CN})_2(\text{OH})_2 + 1(\text{BF}_4)_2 \rightarrow \text{C}_6\text{Cl}_2(\text{CN})_2\text{O}_2 + (1+2\text{H})(\text{BF}_4)_2$

$E(\text{B3LYP/TZVP}) / \text{hartree}$ for the structures optimized at $\varepsilon_r = 1$

| $\varepsilon_r$ | $1(\text{BF}_4)_2$ | $(1+2\text{H})(\text{BF}_4)_2$ | $\text{C}_6\text{Cl}_2(\text{CN})_2(\text{OH})_2$ | $\text{C}_6\text{Cl}_2(\text{CN})_2\text{O}_2$ |
|----------------|----------------------|--------------------------------------|--------------------------------------|--------------------------------------|
| 1             | -2526.372388 | -2527.606309 | -1486.204688 | -1484.953539 |
| 40            | -2526.439210 | -2527.670528 | -1486.228322 | -1484.973404 |

$\Delta E_{\text{el}}(\text{B3LYP/TZVP}, \varepsilon_r = 1) = 45.2321 \text{ kJ/mol} = 0.4688 \text{ eV}$

$\Delta E_{\text{el}}(\text{B3LYP/TZVP}, \varepsilon_r = 40) = 61.9618 \text{ kJ/mol} = 0.6422 \text{ eV}$

$E(\text{B3LYP/TZVP}) / \text{hartree}$ for the structures optimized at each value of $\varepsilon_r$

| $\varepsilon_r$ | $1(\text{BF}_4)_2$ | $(1+2\text{H})(\text{BF}_4)_2$ | $\text{C}_6\text{Cl}_2(\text{CN})_2(\text{OH})_2$ | $\text{C}_6\text{Cl}_2(\text{CN})_2\text{O}_2$ |
|----------------|----------------------|--------------------------------------|--------------------------------------|--------------------------------------|
| 1             | -2526.372388 | -2527.606309 | -1486.204688 | -1484.953539 |
| 40            | -2526.451653 | -2527.683936 | -1486.228543 | -1484.973475 |

$\Delta E_{\text{el}}(\text{B3LYP/TZVP}, \varepsilon_r = 1) = 45.2321 \text{ kJ/mol} = 0.4688 \text{ eV}$

$\Delta E_{\text{el}}(\text{B3LYP/TZVP}, \varepsilon_r = 40) = 59.8220 \text{ kJ/mol} = 0.6200 \text{ eV}$

Calculations for the reaction $\text{C}_6\text{H}_4(\text{OH})_2 + (1+2\text{H})^{4+} \rightarrow \text{C}_6\text{H}_4\text{O}_2 + (1+4\text{H})^{4+}$

$E(\text{B3LYP/TZVP}) / \text{hartree}$ for the structures optimized at $\varepsilon_r = 1$

| $\varepsilon_r$ | $(1+2\text{H})^{4+}$ | $(1+4\text{H})^{4+}$ | $\text{C}_6\text{H}_4(\text{OH})_2$ | $\text{C}_6\text{H}_4\text{O}_2$ |
|----------------|----------------------|----------------------|--------------------------------------|--------------------------------------|
| 1             | -1677.301599 | -1678.549891 | -382.630902 | -381.397659 |
| 40            | -1677.992607 | -1679.245223 | -382.646936 | -381.410799 |

$\Delta E_{\text{el}}(\text{B3LYP/TZVP}, \varepsilon_r = 1) = -39.5111 \text{ kJ/mol} = -0.4095 \text{ eV}$

$\Delta E_{\text{el}}(\text{B3LYP/TZVP}, \varepsilon_r = 40) = -43.2656 \text{ kJ/mol} = -0.4484 \text{ eV}$

Calculations for the reaction $\text{C}_6\text{H}_4(\text{OH})_2 + 1(\text{BF}_4)_4 \rightarrow \text{C}_6\text{H}_4\text{O}_2 + (1+4\text{H})(\text{BF}_4)_4$

$E(\text{B3LYP/TZVP}) / \text{hartree}$ for the structures optimized at $\varepsilon_r = 1$

| $\varepsilon_r$ | $(1+2\text{H})(\text{BF}_4)_4$ | $(1+4\text{H})(\text{BF}_4)_4$ | $\text{C}_6\text{H}_4(\text{OH})_2$ | $\text{C}_6\text{H}_4\text{O}_2$ |
|----------------|----------------------|----------------------|--------------------------------------|--------------------------------------|
| 1             | -3376.623575 | -3377.888141 | -382.630902 | -381.397659 |
| 40            | -3376.698096 | -3377.962071 | -382.646936 | -381.410799 |
\[ \Delta E_{\text{el}}(\text{B3LYP/TZVP}, \varepsilon_r = 1) = -82.2385 \text{ kJ/mol} = -0.8523 \text{ eV} \]
\[ \Delta E_{\text{el}}(\text{B3LYP/TZVP}, \varepsilon_r = 40) = -73.0887 \text{ kJ/mol} = -0.7575 \text{ eV} \]

\[ E(\text{B3LYP/TZVP}) \text{ / hartree for the structures optimized at each value of } \varepsilon_r \]

| \( \varepsilon_r \) | \((1+2H)(\text{BF}_4)_4\) | \((1+4H)(\text{BF}_4)_4\) | \(\text{C}_6\text{H}_4(\text{OH})_2\) | \(\text{C}_6\text{H}_4\text{O}_2\) |
|-----------------|----------------|----------------|----------------|----------------|
| 1               | -3376.623575   | -3377.888141   | -382.630902    | -381.397659    |
| 40              | -3376.710258   | -3377.971979   | -382.647011    | -381.410950    |

\[ \Delta E_{\text{el}}(\text{B3LYP/TZVP}, \varepsilon_r = 1) = -82.2385 \text{ kJ/mol} = -0.8523 \text{ eV} \]
\[ \Delta E_{\text{el}}(\text{B3LYP/TZVP}, \varepsilon_r = 40) = -67.3703 \text{ kJ/mol} = -0.6982 \text{ eV} \]

Calculations for the reaction \( \text{C}_6\text{Cl}_4(\text{OH})_2 + (1+2H)^{4+} \rightarrow \text{C}_6\text{Cl}_4\text{O}_2 + (1+4H)^{4+} \)

\[ E(\text{B3LYP/TZVP}) \text{ / hartree for the structures optimized at } \varepsilon_r = 1 \]

| \( \varepsilon_r \) | \((1+2H)^{4+}\) | \((1+4H)^{4+}\) | \(\text{C}_6\text{Cl}_4(\text{OH})_2\) | \(\text{C}_6\text{Cl}_4\text{O}_2\) |
|-----------------|----------------|----------------|----------------|----------------|
| 1               | -1677.301599   | -1678.549891   | -2220.868853   | -2219.631177   |
| 40              | -1677.992607   | -1679.245223   | -2220.879151   | -2219.642037   |

\[ \Delta E_{\text{el}}(\text{B3LYP/TZVP}, \varepsilon_r = 1) = -27.8723 \text{ kJ/mol} = -0.2889 \text{ eV} \]
\[ \Delta E_{\text{el}}(\text{B3LYP/TZVP}, \varepsilon_r = 40) = -40.7005 \text{ kJ/mol} = -0.4218 \text{ eV} \]

Calculations for the reaction \( \text{C}_6\text{Cl}_4(\text{OH})_2 + (1+2H)(\text{BF}_4)_4 \rightarrow \text{C}_6\text{Cl}_4\text{O}_2 + (1+4H)(\text{BF}_4)_4 \)

\[ E(\text{B3LYP/TZVP}) \text{ / hartree for the structures optimized at } \varepsilon_r = 1 \]

| \( \varepsilon_r \) | \((1+2H)(\text{BF}_4)_4\) | \((1+4H)(\text{BF}_4)_4\) | \(\text{C}_6\text{Cl}_4(\text{OH})_2\) | \(\text{C}_6\text{Cl}_4\text{O}_2\) |
|-----------------|----------------|----------------|----------------|----------------|
| 1               | -3376.623575   | -3377.888141   | -2220.868853   | -2219.631177   |
| 40              | -3376.698096   | -3377.962071   | -2220.879151   | -2219.642037   |

\[ \Delta E_{\text{el}}(\text{B3LYP/TZVP}, \varepsilon_r = 1) = -70.5997 \text{ kJ/mol} = -0.7317 \text{ eV} \]
\[ \Delta E_{\text{el}}(\text{B3LYP/TZVP}, \varepsilon_r = 40) = -70.5235 \text{ kJ/mol} = -0.7309 \text{ eV} \]

\[ E(\text{B3LYP/TZVP}) \text{ / hartree for the structures optimized at each value of } \varepsilon_r \]

| \( \varepsilon_r \) | \((1+2H)(\text{BF}_4)_4\) | \((1+4H)(\text{BF}_4)_4\) | \(\text{C}_6\text{Cl}_4(\text{OH})_2\) | \(\text{C}_6\text{Cl}_4\text{O}_2\) |
|-----------------|----------------|----------------|----------------|----------------|
| 1               | -3376.623575   | -3377.888141   | -2220.868853   | -2219.631177   |
| 40              | -3376.710258   | -3377.971979   | -2220.879308   | -2219.642096   |

\[ \Delta E_{\text{el}}(\text{B3LYP/TZVP}, \varepsilon_r = 1) = -70.5997 \text{ kJ/mol} = -0.7317 \text{ eV} \]
\[ \Delta E_{\text{el}}(\text{B3LYP/TZVP}, \varepsilon_r = 40) = -64.3484 \text{ kJ/mol} = -0.6669 \text{ eV} \]
Calculations for the reaction $\text{C}_6\text{Cl}_4\text{O}_2 + (1+2\text{H})(\text{BF}_4)_4 \rightarrow \text{C}_6\text{Cl}_4\text{O}_2(\text{HF})_2(\text{BF}_3)_2 + 1(\text{BF}_4)_2$

$E(\text{B3LYP/TZVP})$ / hartree for the structures optimized at $\varepsilon_r = 1$

| $\varepsilon_r$ | $(1+2\text{H})(\text{BF}_4)_4$ | $1(\text{BF}_4)_2$ | $\text{C}_6\text{Cl}_4\text{O}_2$ | $\text{C}_6\text{Cl}_4\text{O}_2(\text{HF})_2(\text{BF}_3)_2$ |
|-----------------|-------------------------------|-------------------|-----------------|-----------------|
| 1               | -3376.623575                 | -2526.372388     | -2219.631177    | -3069.758291    |
| 40              | -3376.698096                 | -2526.439210     | -2219.642037    | -3069.776298    |

$\Delta E_{el} (\text{B3LYP/TZVP}, \varepsilon_r = 1) = 325.7536 \text{kJ/mol} = 3.3762 \text{eV}$

$\Delta E_{el} (\text{B3LYP/TZVP}, \varepsilon_r = 40) = 327.2029 \text{kJ/mol} = 3.3912 \text{eV}$

$E(\text{B3LYP/TZVP})$ / hartree for the structures optimized at each value of $\varepsilon_r$

| $\varepsilon_r$ | $(1+2\text{H})(\text{BF}_4)_4$ | $1(\text{BF}_4)_2$ | $\text{C}_6\text{Cl}_4\text{O}_2$ | $\text{C}_6\text{Cl}_4\text{O}_2(\text{HF})_2(\text{BF}_3)_2$ |
|-----------------|-------------------------------|-------------------|-----------------|-----------------|
| 1               | -3376.623575                 | -2526.372388     | -2219.631177    | -3069.758291    |
| 40              | -3376.710258                 | -2526.451653     | -2219.642096    | -3069.779806    |

$\Delta E_{el} (\text{B3LYP/TZVP}, \varepsilon_r = 1) = 325.7536 \text{kJ/mol} = 3.3762 \text{eV}$

$\Delta E_{el} (\text{B3LYP/TZVP}, \varepsilon_r = 40) = 317.4098 \text{kJ/mol} = 3.2897 \text{eV}$

Calculations for the reaction $\text{C}_6\text{Cl}_2(\text{CN})_2(\text{OH})_2 + (1+2\text{H})^4+ \rightarrow \text{C}_6\text{Cl}_2(\text{CN})_2\text{O}_2 + (1+4\text{H})^{4+}$

$E(\text{B3LYP/TZVP})$ / hartree for the structures optimized at $\varepsilon_r = 1$

| $\varepsilon_r$ | $(1+2\text{H})^4+$ | $(1+4\text{H})^{4+}$ | $\text{C}_6\text{Cl}_2(\text{CN})_2(\text{OH})_2$ | $\text{C}_6\text{Cl}_2(\text{CN})_2\text{O}_2$ |
|-----------------|-------------------|-------------------|-----------------|-----------------|
| 1               | -1677.301599      | -1678.549891      | -1486.204688    | -1484.953539    |
| 40              | -1677.992607      | -1679.245223      | -1486.228322    | -1484.973404    |

$\Delta E_{el} (\text{B3LYP/TZVP}, \varepsilon_r = 1) = 7.5011 \text{kJ/mol} = 0.0777 \text{eV}$

$\Delta E_{el} (\text{B3LYP/TZVP}, \varepsilon_r = 40) = 6.0439 \text{kJ/mol} = 0.0626 \text{eV}$

Calculations for the reaction $\text{C}_6\text{Cl}_2(\text{CN})_2(\text{OH})_2 + (1+2\text{H})(\text{BF}_4)_4 \rightarrow \text{C}_6\text{Cl}_2(\text{CN})_2\text{O}_2 + (1+4\text{H})(\text{BF}_4)_4$

$E(\text{B3LYP/TZVP})$ / hartree for the structures optimized at $\varepsilon_r = 1$

| $\varepsilon_r$ | $(1+2\text{H})(\text{BF}_4)_4$ | $(1+4\text{H})(\text{BF}_4)_4$ | $\text{C}_6\text{Cl}_2(\text{CN})_2(\text{OH})_2$ | $\text{C}_6\text{Cl}_2(\text{CN})_2\text{O}_2$ |
|-----------------|-------------------------------|-------------------------------|-----------------|-----------------|
| 1               | -3376.623575                  | -3377.888141                  | -1486.204688    | -1484.953539    |
| 40              | -3376.698096                  | -3377.962071                  | -1486.228322    | -1484.973404    |

$\Delta E_{el} (\text{B3LYP/TZVP}, \varepsilon_r = 1) = -35.2263 \text{kJ/mol} = -0.3651 \text{eV}$

$\Delta E_{el} (\text{B3LYP/TZVP}, \varepsilon_r = 40) = -23.7792 \text{kJ/mol} = -0.2465 \text{eV}$

$E(\text{B3LYP/TZVP})$ / hartree for the structures optimized at each value of $\varepsilon_r$

| $\varepsilon_r$ | $(1+2\text{H})(\text{BF}_4)_4$ | $(1+4\text{H})(\text{BF}_4)_4$ | $\text{C}_6\text{Cl}_2(\text{CN})_2(\text{OH})_2$ | $\text{C}_6\text{Cl}_2(\text{CN})_2\text{O}_2$ |
|-----------------|-------------------------------|-------------------------------|-----------------|-----------------|
| 1               | -3376.623575                  | -3377.888141                  | -1486.204688    | -1484.953539    |
| 40              | -3376.710258                  | -3377.971979                  | -1486.228543    | -1484.973475    |

$\Delta E_{el} (\text{B3LYP/TZVP}, \varepsilon_r = 1) = -35.2263 \text{kJ/mol} = -0.3651 \text{eV}$

$\Delta E_{el} (\text{B3LYP/TZVP}, \varepsilon_r = 40) = -17.4674 \text{kJ/mol} = -0.1810 \text{eV}$
Calculations for the reaction \((C_6Cl_4O_2+2H)^{2+} + 2 BF_4^- \rightarrow C_6Cl_4O_2(HF)_2(BF_3)_2\)

\[ E(\text{B3LYP/TZVP}) / \text{hartree} \] for the structures optimized at \(\varepsilon_r = 1\)

| \(\varepsilon_r\) | \((C_6Cl_4O_2+2H)^{2+}\) | BF\(_4^-\) | \(C_6Cl_4O_2(HF)_2(BF_3)_2\) |
|---|---|---|---|
| 1  | -2220.102422 | -424.575347 | -3069.758291 |
| 40 | -2220.394034 | -424.669803 | -3069.776298 |

\(\Delta E_{\text{el}}(\text{B3LYP/TZVP}, \varepsilon_r = 1) = -1326.3368 \text{ kJ/mol} = -13.7465 \text{ eV}\)

\(\Delta E_{\text{el}}(\text{B3LYP/TZVP}, \varepsilon_r = 40) = -111.9986 \text{ kJ/mol} = -1.1608 \text{ eV}\)

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Calculations for the reaction \(C_6H_4O_2 + (1+2H)(BF_4)_4 \rightarrow C_6H_4O_2(HF)_2(BF_3)_2 + 1(BF_4)_2\)

\[ E(\text{B3LYP/TZVP}) / \text{hartree} \] for the structures optimized at \(\varepsilon_r = 1\)

| \(\varepsilon_r\) | \((1+2H)(BF_4)_4\) | 1\((BF_4)_2\) | \(C_6H_4O_2\) | \(C_6H_4O_2(HF)_2(BF_3)_2\) |
|---|---|---|---|---|
| 1  | -3376.623575 | -2526.372388 | -381.397659 | -1231.535578 |
| 40 | -3376.698096 | -2526.439210 | -381.410799 | -1231.555635 |

\(\Delta E_{\text{el}}(\text{B3LYP/TZVP}, \varepsilon_r = 1) = 297.3851 \text{ kJ/mol} = 3.0822 \text{ eV}\)

\(\Delta E_{\text{el}}(\text{B3LYP/TZVP}, \varepsilon_r = 40) = 299.4382 \text{ kJ/mol} = 3.1035 \text{ eV}\)

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Calculations for the reaction \((C_6H_4O_2+2H)^{2+} + 2 BF_4^- \rightarrow C_6H_4O_2(HF)_2(BF_3)_2\)

\[ E(\text{B3LYP/TZVP}) / \text{hartree} \] for the structures optimized at each value of \(\varepsilon_r\)

| \(\varepsilon_r\) | \((C_6H_4O_2+2H)^{2+}\) | \(2 BF_4^-\) | \(C_6H_4O_2(HF)_2(BF_3)_2\) |
|---|---|---|---|
| 1  | -3376.623575 | -2526.372388 | -381.397659 | -1231.535578 |
| 40 | -3376.710258 | -2526.451653 | -381.410950 | -1231.573823 |

\(\Delta E_{\text{el}}(\text{B3LYP/TZVP}, \varepsilon_r = 1) = 297.3851 \text{ kJ/mol} = 3.0822 \text{ eV}\)

\(\Delta E_{\text{el}}(\text{B3LYP/TZVP}, \varepsilon_r = 40) = 251.3443 \text{ kJ/mol} = 2.6050 \text{ eV}\)

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Calculations for the reaction \((C_6H_2O_2+2H)^{2+} + 2 BF_4^- \rightarrow C_6H_2O_2(HF)_2(BF_3)_2\)

\[ E(\text{B3LYP/TZVP}) / \text{hartree} \] for the structures optimized at \(\varepsilon_r = 1\)

| \(\varepsilon_r\) | \((C_6H_2O_2+2H)^{2+}\) | \(2 BF_4^-\) | \(C_6H_2O_2(HF)_2(BF_3)_2\) |
|---|---|---|---|
| 1  | -381.863637 | -424.575347 | -1231.535578 |
| 40 | -382.191174 | -424.669803 | -1231.555635 |

\(\Delta E_{\text{el}}(\text{B3LYP/TZVP}, \varepsilon_r = 1) = -1368.5338 \text{ kJ/mol} = -14.1839 \text{ eV}\)

\(\Delta E_{\text{el}}(\text{B3LYP/TZVP}, \varepsilon_r = 40) = -65.2568 \text{ kJ/mol} = -0.6763 \text{ eV}\)
Analysis of the influence of the relative solvent permittivity (dielectric constant) \( \varepsilon_r \) on the reaction energy

The reaction between dihydro-benzoquinones and \( 1^{2+} / 1(BF_4)_2 \) was chosen to study the solvent effect in more detail.

A) Calculations without anions (“single-point” calculations at the optimized structure at \( \varepsilon_r = 1 \))

\[
\begin{array}{ccc}
\text{Cl} & \text{Cl} & \text{OH} \\
\text{Cl} & \text{Cl} & \text{OH} \\
\text{Cl} & \text{Cl} & \text{OH} \\
\end{array}
\quad + \quad 1^{2+} 
\rightarrow 
\begin{array}{ccc}
\text{Cl} & \text{Cl} & \text{Cl} \\
\text{Cl} & \text{Cl} & \text{Cl} \\
\text{Cl} & \text{Cl} & \text{Cl} \\
\end{array}
\quad + \quad (1+2H)^{2+}
\]

| \( \varepsilon_r \) | \( \Delta E / \text{kJ mol}^{-1} \) |
|-------------------|-------------------------------|
| 1                 | 9.4045                        |
| 2                 | 7.7216                        |
| 5                 | 6.0176                        |
| 10                | 5.2668                        |
| 20                | 4.8467                        |
| 40                | 4.6261                        |
| 60                | 4.5500                        |
| 80                | 4.5132                        |

As expected, the effect of solvation on the electronic energy of all compounds (especially the charged ones) is substantial. Nevertheless, the effect on the reaction energy \( \Delta E \) is only small (decrease of \( \Delta E \) from 9.4 kJ mol\(^{-1}\) at \( \varepsilon_r = 1 \) to 4.5 kJ mol\(^{-1}\) at \( \varepsilon_r = 80 \)).
B) Calculations with anions ("single-point" calculations for structures at $\varepsilon_r = 1$)

| $\varepsilon$ | $\Delta E / \text{kJ mol}^{-1}$ |
|---------------|---------------------------------|
| 1             | 9.8587                          |
| 2             | 12.3451                         |
| 5             | 14.1357                         |
| 10            | 14.7579                         |
| 20            | 15.0677                         |
| 40            | 15.2174                         |
| 80            | 15.2909                         |

With inclusion of the anions in of 1(BF$_4$)$_2$ and (1+2H)(BF$_4$)$_2$, the reactions energy $\Delta E$ slightly increases from 9.9 kJ mol$^{-1}$ at $\varepsilon_r = 1$ to 15.3 kJ mol$^{-1}$ at $\varepsilon_r = 80$. 
C) Calculations with anions (optimized structures at each $\varepsilon_r$ value)

| $\varepsilon_r$ | $\Delta E$ / kJ mol$^{-1}$ |
|-----------------|-----------------------------|
| 1               | 9.8587                      |
| 2               | 12.6365                     |
| 5               | 15.7582                     |
| 10              | 14.9627                     |
| 20              | 13.5791                     |
| 40              | 12.9411                     |
| 80              | 12.4449                     |

If the structures are optimized at each $\varepsilon_r$ value (with inclusion of the anions), the $\Delta E$ vs. $\varepsilon_r$ curve (starting with $\Delta E = 9.9$ kJ mol$^{-1}$ at $\varepsilon_r = 1$) passes through a maximum ($\Delta E = 15.8$ kJ mol$^{-1}$ at $\varepsilon_r = 5$), and then slightly decreases to $\Delta E = 12.5$ kJ mol$^{-1}$ at $\varepsilon_r = 80$. The maximum results from the change of the position/orientation of the anions.

**Overall conclusion:** The dependence of the reaction energy $\Delta E$ on the $\varepsilon_r$ value is relatively small. The inclusion of the anions also has only a small effect. Finally, the difference between the $\Delta E$ values from single-point calculations at the optimized structure at $\varepsilon_r = 1$ and the $\Delta E$ values for optimized structures at each $\varepsilon_r$ value is also quite small.
Coordinates for calculated structures at $\varepsilon_r = 1$
B3LYP/def2-TZVP

1\((BF_4)_2\), $\varepsilon_r = 1$

Illustration of the structure (H atoms omitted)

Energy = -2526.372388050 hartree

Coordinates in Å

| Atom | X    | Y    | Z    |
|------|------|------|------|
| F    | -5.7429903 | 0.8957755 | -1.0474906 |
| B    | -6.3372872 | 1.9632514 | -1.7837718 |
| F    | -7.6900456 | 1.7386594 | -1.9470610 |
| F    | -5.6843582 | 2.0509463 | -0.0407220 |
| F    | -6.1023684 | 3.1629867 | -1.0710086 |
| N    | -1.8046572 | 2.0809172 | -0.4258268 |
| C    | -0.9250080 | 1.0841323 | -0.3061112 |
| C    | -2.2465425 | 2.5706110 | -1.5950280 |
| C    | 0.8907717  | 0.4127862 | 1.0474429  |
| C    | -0.0268260 | 0.6461200 | -1.2574432 |
| N    | -2.6107547 | 1.7845934 | -2.6305843 |
| N    | -2.3820875 | 3.9138351 | -1.7117376 |
| N    | -1.6610053 | 0.7708534 | 2.0292996  |
| C    | 0.0267363  | -0.6463650 | 1.2579784 |
| C    | 0.8903734  | -0.4133336 | -1.0470589 |
| H    | -0.0137954 | 1.1066148 | -2.2354018 |
| C    | -2.6620878 | 2.2478379 | -4.0138699 |
| C    | -3.0023178 | 0.3915528 | -2.4576191 |
| C    | -3.5262600 | 4.5480266 | -2.3758285 |
| C    | -1.6405044 | 4.7896017 | -0.8185858 |
| C    | 2.6293982  | 1.6871194 | 2.1837086  |
| C    | 0.9249391  | -1.0843410 | 0.3066461 |
| H    | 0.0137866  | -1.1061820 | 2.2359583  |
| C    | 1.6601608  | -0.7718884 | -2.0291222 |
| H    | -2.2130526 | -0.2800831 | 2.2809978  |
| H    | 3.9177087  | 0.2244749 | -3.0225624 |
| H    | -3.2192317 | 0.1881209 | -1.4158243 |
| H    | -3.2003963 | 5.1865443 | -3.2159928 |
| H    | -4.0357723 | 5.1843215 | -1.6495507 |
| H    | -4.2459307 | 3.8072595 | -2.706734  |
| H    | -2.2036119 | 5.0024740 | 0.0959281  |
(1+2H)(BF₄)₂, εᵣ = 1

Illustration of the structure (C-H atoms omitted)

Energy = -2527.606308625 hartree

Coordinates in Å

|  | X       | Y       | Z       |
|---|---------|---------|---------|
| F | -5.9291476 | 1.1879791 | -0.9327727 |
| B | -5.7448328 | 2.5268806 | -1.3217085 |
| F | -6.8193454 | 3.3155423 | -0.9566299 |
| F | -5.5399756 | 2.5716101 | -2.7275033 |
| F | -4.5514179 | 3.0156388 | -0.6958963 |
| N | -1.5648679 | 2.2078811 | -0.7356396 |
| C | 0.8167482 | 1.0583911 | -0.3895458 |
| C | -0.0556409 | 2.614053 | -1.9262176 |
| C | -0.6624376 | 0.7939279 | 0.9887155 |
| C | -0.1676079 | 0.2749384 | -1.3369730 |
| N | -2.5202239 | 1.7322406 | -2.8173374 |
| N | -2.0307557 | 3.9351703 | -2.194486 |
| N | -1.1391887 | 1.6612175 | 1.9691595 |
| C | 0.1680467 | -0.2741558 | 1.3363474 |
| C | 0.6628739 | -0.7931525 | -0.9893491 |
| H | -0.2927528 | 0.4824004 | -2.3900658 |
| C | -2.5452545 | 1.9941423 | -4.2513844 |
| C | -3.1683231 | 0.4843197 | -2.4113912 |
| C | -3.1181581 | 4.6156761 | -2.9054519 |
| C | -1.1046124 | 4.8274993 | -1.5069396 |
| C | -2.3509159 | 1.7927839 | 2.4216535 |
| C | 0.8170697 | -1.0577106 | 0.3889116 |
| H | 0.2932502 | -0.4815984 | 2.3894339 |
| N | 1.1397234 | -1.6603173 | -1.9698809 |
| H | -2.5508809 | -0.3757657 | -2.6796843 |
(1+2H)(BF₄)₄, εᵣ = 1

Illustration of the structure (C-H atoms omitted)

Energy = -3376.623575238 hartree

Coordinates in Å
F  5.8570700  1.7111454  4.3644926
B  5.3371698  2.9816370  4.2602899
F  4.1158331  3.0595393  5.0456497
F  5.0206599  3.3207307  2.9405328
F  6.2245081  3.9413943  4.8059997
C  2.9415904  8.9604363  6.6217603
C  3.6010814  7.7354131  6.9947232
C  2.5044299  8.0714062  4.3599248
C  3.6847675  6.6972544  6.1286336
C  3.1641788  6.8464731  4.7327985
N  3.4183787  5.8643990  3.9473297
F  1.4935985  8.2147259  1.3485472
B  3.7513789  6.6242648  10.6284482
B  2.3514150  9.1814677  0.7258269
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| F    | 3.0102446 | 7.2553451 | 11.6236827 |
| F    | 2.8910268 | 6.1212258 | 9.6210225  |
| F    | 4.5351405 | 5.5851408 | 1.7319908  |
| F    | 1.5671580 | 10.219033 | 0.2197104  |
| N    | 2.6878324 | 9.9427564 | 7.4070679  |
| C    | 2.4207324 | 9.1095390 | 5.2260293  |
| N    | 3.1590556 | 5.6961658 | 2.6155225  |
| F    | 4.6098394 | 7.5914142 | 10.0072924 |
| C    | 1.2948086 | 10.113447 | 8.7368342  |
| N    | 1.8836681 | 10.340470 | 4.9422192  |
| H    | 4.0260396 | 4.7042041 | 5.7495579  |
| C    | 5.1396568 | 5.1250038 | 7.3810465  |
| N    | 4.0453623 | 6.1162594 | 1.7218178  |
| N    | 2.0776735 | 4.9727107 | 2.2866925  |
| N    | 2.0619799 | 9.6923815 | 9.6330222  |
| H    | 2.0798636 | 11.102742 | 5.6047829  |
| C    | 0.9651572 | 10.681774 | 3.971224   |
| N    | 4.9467738 | 3.9774830 | 8.0184174  |
| N    | 6.2163303 | 5.8906399 | 7.5847815  |
| C    | 5.0864944 | 7.0922360 | 2.0641439  |
| C    | 4.2769587 | 5.4260007 | 0.4493263  |
| C    | 1.3905858 | 5.1001127 | 1.0012487  |
| C    | 1.4178558 | 4.1241773 | 3.2791970  |
| C    | 1.0255627 | 8.7172728 | 9.2915802  |
| C    | 1.8318206 | 10.383157 | 10.9054720 |
| C    | 4.7184376 | 10.706381 | 10.351328  |
| N    | 4.6901040 | 11.681642 | 8.0731423  |
| N    | 1.1578094 | 11.828468 | 3.362315   |
| N    | -0.1116273 | 9.9158869 | 3.7711771  |
| C    | 3.6138228 | 3.3895144 | 8.1802879  |
| C    | 6.0504008 | 3.1357639 | 8.4772408  |
| C    | 6.9142120 | 5.9620287 | 8.8701614  |
| C    | 6.7788791 | 6.7164667 | 6.5196491  |
| C    | 2.4907422 | 12.4165760 | 3.1733535 |
| C    | 0.0540085 | 12.6704189 | 2.8777498 |
| C    | -0.8102032 | 9.8441382 | 2.4861996  |
| C    | -0.6735029 | 9.0902471 | 4.8368005  |
| F    | 1.9920756 | 12.7473594 | 6.3087610 |
| F    | -0.1180484 | 11.8686493 | 6.5471043 |
| B    | 0.7705496 | 12.8267132 | 7.0937350  |
| F    | 0.2527115 | 14.0980902 | 6.9900388  |
| F    | 1.0860159 | 12.4863807 | 8.4133976  |
| H    | 3.9600952 | 7.6441080 | 8.0113216  |
| H    | 2.1452732 | 8.1625693 | 3.3433571  |
| H    | 0.1348444 | 9.2346933 | 8.9258589  |
| H    | 0.7901153 | 8.1558549 | 10.1928605 |
| H    | 1.3816281 | 8.0030020 | 8.5591322  |
| H    | 2.1887138 | 9.7810952 | 11.7411953 |
| H    | 0.7569795 | 10.5357836 | 11.0029357 |
| H    | 2.3016892 | 11.3601710 | 10.8954279 |
| H    | 4.5823676 | 11.5968088 | 10.9689031 |
| H    | 5.7837505 | 10.5804922 | 10.1469917 |
| H    | 4.3837194 | 9.8190877 | 10.8767613 |
| H    | 5.5010188 | 11.1493215 | 7.5668865 |
| H    | 5.1138271 | 12.5397894 | 8.5946563  |
| H    | 3.9662655 | 12.0451393 | 7.3490456  |
| H    | 2.8561517 | 4.1600598 | 8.0947362  |
| H   | 3.5547324  | 2.9711938  | 9.1847103 |
|-----|------------|------------|-----------|
| H   | 3.4587128  | 2.6063137  | 7.4370716 |
| H   | 6.9799503  | 3.4486674  | 8.0128516 |
| H   | 5.8404116  | 2.1150994  | 8.1567527 |
| H   | 6.1409876  | 3.1596473  | 9.5643189 |
| H   | 6.3035956  | 5.5400979  | 9.6611603 |
| H   | 7.0710125  | 7.0141176  | 9.1070831 |
| H   | 7.8829933  | 5.4602948  | 8.8173007 |
| H   | 6.4429643  | 6.3579642  | 5.5515074 |
| H   | 7.8647705  | 6.6229335  | 6.5574270 |
| H   | 6.5136510  | 7.7682313  | 6.6540628 |
| H   | 3.2483589  | 11.6459537 | 3.2586629 |
| H   | 2.5492626  | 12.8345606 | 2.1687416 |
| H   | 2.6464504  | 13.1998855 | 3.9162044 |
| H   | -0.8752621 | 12.3580064 | 3.3429434 |
| H   | 0.2643862  | 13.6913095 | 3.1976133 |
| H   | -0.0373184 | 12.6461500 | 1.7907450 |
| H   | -0.2000749 | 10.2659628 | 1.6947714 |
| H   | -0.9670285 | 8.7919807  | 2.2495953 |
| H   | -1.7790037 | 10.3457911 | 2.5394829 |
| H   | -0.3371041 | 9.4490067  | 5.8046779 |
| H   | -1.7594243 | 9.1836408  | 4.7995800 |
| H   | -0.4082268 | 8.0384795  | 4.7025091 |
| H   | 5.9716683  | 6.5755839  | 2.4302354 |
| H   | 5.1611252  | 7.6541248  | 1.1631609 |
| H   | 4.7234942  | 7.8059830  | 2.7965682 |
| H   | 3.9198482  | 6.0278700  | 0.3864446 |
| H   | 5.3520165  | 5.2745552  | 0.3524198 |
| H   | 3.8081567  | 4.4484757  | 0.4589274 |
| H   | 1.5280086  | 4.2098113  | 0.3836330 |
| H   | 0.3249952  | 5.2193831  | 1.2046595 |
| H   | 1.7249985  | 5.9876892  | 0.4762483 |
| H   | 0.6059423  | 4.6555309  | 3.7850181 |
| H   | 0.9955689  | 3.2656865  | 2.7570905 |
| H   | 2.1414407  | 3.7612738  | 4.0038768 |

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$(1+4\text{H})(\text{BF}_4)_4$, $\varepsilon_r = 1$

Illustration of the structure (C-H atoms omitted)

Energy = -3377.888141278 hartree

Coordinates in Å

| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| F       | 2.8419913 | -5.9706793 | -1.3343576 |
| B       | 2.0967978 | -4.8732892 | -1.6797975 |
| F       | 1.0055502 | -4.7053610 | -0.7510545 |
| F       | 1.5703702 | -4.9409692 | -2.9658626 |
| F       | 2.8990470 | -3.6791527 | -1.5776916 |
| C       | -0.3982685 | 0.8942293 | 1.0078163 |
| C       | 0.3210216 | -0.2530217 | 1.3265420 |
| C       | -0.3210281 | 0.2544107 | -1.3266058 |
| C       | 0.7181415 | -1.1464683 | 0.3382167 |
| C       | 0.3981546 | -0.8964911 | -1.0075891 |
| N       | 0.9064911 | -1.7461754 | -2.0080537 |
| F       | -1.1869046 | 1.2283722 | -4.2573975 |
| B       | -0.0382377 | -1.5916083 | 4.9186356 |
| B       | 0.0374640 | 1.5909896 | -4.9197570 |
| F       | -0.3511230 | -0.5765133 | 5.8369417 |
| F       | -1.0414187 | -1.6616028 | 3.9270258 |
| F       | 0.1295706 | -2.8180522 | 5.5411671 |
| F       | 0.3508410 | 0.5753333 | -5.8372810 |
| F       | 1.0405999 | 1.6621827 | -3.9281985 |
| F       | -0.1309229 | 2.8168719 | -5.5432283 |
| N       | -0.9064137 | 1.7474941 | 2.0080935 |
| C       | -0.7183544 | 1.1477533 | -0.3382388 |
| N       | 1.3495702 | -2.3653170 | 0.6789593 |
| C       | 0.3952529 | -1.9913329 | -3.2463965 |
| F       | 1.1862974 | -1.2290605 | 4.2565818 |
| C       | -0.3952439 | 1.9917239 | 3.2466937 |
| N       | -1.3501788 | 2.3663930 | -0.6791044 |
| H       | 1.0332712 | -3.2110607 | 0.1981337 |
| C       | 2.2962455 | -2.5817448 | 1.6226579 |
| N       | 1.2464103 | -2.0530468 | -4.2661707 |
| N       | -0.9184609 | -2.2198883 | -3.4031956 |
Illustration of the structure

Energy = -381.3976586665 hartree

Coordinates in Å

C      1.4394615 -0.0000004 -0.0002648
C      0.6681633  1.2661677  0.0003196
C     -0.6681607  1.2661685  0.0003945
C     -1.4394562  0.0000005 -0.0001927
C     -0.6681624 -1.2661682  0.0003165
C      0.6681617 -1.2661680  0.0003486
O      2.6573346 -0.0000015 -0.0014168
H      1.2539444  2.1774916  0.0004059
H     -1.2539457  2.1774944  0.0005065
O     -2.6573381  0.0000017 -0.0012447
C₆H₄(OH)₂, εᵣ = 1

Illustration of the structure

Energy = -382.6309021723 hartree

Coordinates in Å

H  -1.2539460 -2.1774949  0.0003697
H   1.2539435 -2.1774914  0.0004575

C       1.3959206  -0.0293616  0.0000988
C         0.7162670  1.1861318  0.0002096
C         -0.6727162  1.2169398  0.0001333
C        -1.3959207   0.0293617  0.0000212
C         -0.7162671 -1.1861319  0.0000233
C          0.6727162 -1.2169396  0.0001504
O            2.7650095 -0.1165930 -0.0002520
H          1.2716448  2.1181840  0.0001779
H         -1.2048008  2.1591512 -0.0000759
O         -2.7650095  0.1165929 -0.0000579
H         -1.2716449 -2.1181843 -0.0001015
H          1.2048009 -2.1591508  0.0002536
H           3.1445676  0.7689073 -0.0004212
H          -3.1445675 -0.7689075 -0.0001595
(C₆H₄O₂+2H)²⁺, τ_f = 1

Illustration of the structure

Energy = -381.8636372977 hartree

Coordinates in Å

|   |   |   |   |
|---|---|---|---|
| C | 1.3820963 | 0.0141577 | -0.0000216 |
| C | 0.6727154 | 1.2897065 | -0.0007568 |
| C | -0.6689336 | 1.2758506 | -0.0008508 |
| C | -1.3821053 | -0.0141578 | -0.0001083 |
| C | -0.6727262 | -1.2897072 | -0.0008363 |
| C | 0.6689235 | -1.2758541 | -0.0007892 |
| O | 2.6441825 | -0.0811072 | 0.0015170 |
| H | 1.2355520 | 2.2184120 | -0.0009927 |
| H | -1.2697255 | 2.1799882 | -0.0010251 |
| O | -2.6441720 | 0.0811098 | 0.0014949 |
| H | -1.2355575 | -2.2184048 | -0.0010616 |
| H | 1.2697239 | -2.1800011 | -0.0009864 |
| H | -3.1695153 | -0.7523415 | 0.0022128 |
| H | 3.1695419 | 0.7523489 | 0.0022039 |
Illustration of the structure

Energy = -1231.535577759 hartree

Coordinates in Å

| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | -0.2291494| 1.3466984 | -0.4100362|
| C    | -1.3100350| 0.5301141 | 0.1772874 |
| C    | -1.0062157| -0.8605273| 0.5735230 |
| H    | -0.4917215| 2.3594610 | -0.6885589|
| O    | -2.4281087| 1.0142585 | 0.3229566 |
| H    | -1.8111819| -1.4390834| 1.0093055 |
| H    | -3.6796506| 0.2392891 | 0.9371004 |
| B    | -4.0559103| -1.1664567| 3.3458688 |
| F    | -4.3968087| -0.2865806| 1.3038983 |
| F    | -3.2247087| -2.0994152| 2.8879938 |
| F    | -5.3236070| -1.4607427| 3.5388666 |
| F    | -3.5409705| -0.0539373| 3.8444319 |
| C    | 0.2208281 | -1.3607874| 0.3992580 |
| C    | 1.3016756 | -0.5442272| -0.1882222|
| C    | 0.9979935 | 0.8465571 | -0.5840098|
| H    | 0.4834629 | -2.3735484| 0.6778857 |
| O    | 2.4196611 | -1.0286087| -0.3342984|
| H    | 1.8031348 | 1.4254384 | -1.0191436|
| H    | 3.6749882 | -0.2541758| -0.9428780|
| B    | 4.0691910 | 1.1940213 | -3.3291159 |
| F    | 4.3962369 | 0.2700843 | -1.3036219 |
| F    | 3.2376772 | 2.1194285 | -2.8564857 |
| F    | 5.3389745 | 1.4885554 | -3.5071909 |
| F    | 3.5542444 | 0.0941843 | -3.8548145 |
C₆Cl₄O₂ (CA), $\varepsilon_r = 1$

Illustration of the structure

Energy = -2219.631177278 hartree

Coordinates in Å

|       |        |        |        |
|-------|--------|--------|--------|
|       | 1.4532675 | 0.0000100 | 0.0000636 |
|       | 0.6725199 | 1.2776468 | -0.0000822 |
|       | -0.6725229 | 1.2776936 | 0.0000595 |
|       | -1.4532293 | 0.0000129 | 0.0000183 |
|       | -0.6725205 | -1.2776768 | -0.0000688 |
|       | 0.6725204 | -1.2776474 | 0.0000437 |
|       | 2.6587402 | 0.0000020 | 0.0002055 |
|       | 1.6065797 | 2.7100788 | -0.0004087 |
|       | -1.6066139 | 2.7098906 | 0.0002611 |
|       | -2.6586980 | 0.0000011 | 0.0000608 |
|       | -1.6066196 | -2.7098927 | -0.0002778 |
|       | 1.6065764 | -2.7100990 | 0.0001250 |
$\text{C}_6\text{Cl}_4(\text{OH})_2$, $\varepsilon_r = 1$

Illustration of the structure

Energy = $-2220.868852789$ hartree

Coordinates in Å

|     | x   | y   | z   |
|-----|-----|-----|-----|
| C   | 1.4096088 | -0.0345987 | -0.0000055 |
| C   | 0.7161868 | 1.1797023 | -0.0000855 |
| C   | -0.6769822 | 1.2243950 | 0.0001093 |
| C   | -1.4096592 | 0.0347294 | -0.0000139 |
| C   | -0.7162713 | -1.1796021 | 0.0000956 |
| C   | 0.6769669 | -1.2243244 | -0.0000142 |
| O   | 2.7582765 | -0.1036511 | 0.0000533 |
| Cl  | 1.6593789 | 2.6397060 | -0.0003209 |
| Cl  | -1.5269482 | 2.7260030 | 0.0004046 |
| O   | -2.7584122 | 0.1036043 | -0.0001917 |
| Cl  | -1.6594146 | -2.6397386 | 0.0002774 |
| Cl  | 1.5268553 | -2.7259428 | -0.0000830 |
| H   | 3.1165766 | 0.7963075 | 0.0000954 |
| H   | -3.1161620 | -0.7965899 | -0.0003210 |
\[(C_6\text{Cl}_4\text{O}_2+2\text{H})^{2+}, \varepsilon_r = 1\]

Illustration of the structure

Energy = -2220.102421622

Coordinates in Å

| Element | X           | Y           | Z           |
|---------|-------------|-------------|-------------|
| C       | 1.3884024   | 0.0158234   | -0.0000251  |
| C       | 0.6954005   | 1.2849843   | -0.0001915  |
| C       | -0.6723145  | 1.2912008   | -0.0000563  |
| C       | -1.3884582  | -0.0158255  | 0.0000136   |
| C       | -0.6722643  | -1.2911965  | -0.0000610  |
| O       | 2.6534332   | -0.0571171  | 0.0002274   |
| Cl      | 1.6415212   | 2.6925623   | -0.0002753  |
| Cl      | -1.5867569  | 2.6858136   | 0.0000220   |
| O       | -2.6534176  | 0.0571269   | 0.0002479   |
| Cl      | -1.6414821  | -2.6925706  | -0.0003699  |
| Cl      | 1.5868087   | -2.6858433  | 0.0000595   |
| H       | -3.1113740  | -0.8191953  | 0.0002935   |
| H       | 3.1114209   | 0.8192311   | 0.0002524   |
Illustration of the structure

Energy = -3069.758290989 hartree

Coordinates in Å

|   |       |       |       |
|---|--------|--------|--------|
| C | -0.4508800 | 1.3707070 | 0.0199408 |
| C | -1.4219516 | 0.2384800 | 0.0690943 |
| C | -0.8811251 | -1.1503709 | 0.0289433 |
| Cl | -1.1290283 | 2.9331709 | 0.0599470 |
| O | -2.6117448 | 0.4604932 | 0.1427122 |
| Cl | -2.0345694 | -2.4044974 | 0.0485655 |
| H | -3.9953954 | -0.3125386 | 0.7713459 |
| B | -4.0778647 | -0.9369416 | 3.5033139 |
| F | -4.7226854 | 0.6513262 | 1.2729966 |
| F | -4.4625704 | -2.1965351 | 3.5450178 |
| F | -4.8630678 | 0.0175772 | 3.9577497 |
| F | -2.8125292 | -0.6537393 | 3.2084959 |
| C | 0.4466068 | -1.3741230 | -0.0239002 |
| C | 1.4177011 | -0.2418756 | -0.0726901 |
| C | 0.8768853 | 1.1469494 | -0.0324594 |
| Cl | 1.1247464 | -2.9365854 | -0.0641190 |
| O | 2.6075048 | -0.4639401 | -0.1458683 |
| Cl | 2.0303166 | 2.4010802 | -0.0514170 |
| H | 3.9930223 | 0.3094004 | -0.7697744 |
| B | 4.0847410 | 0.9432856 | -3.4995693 |
| F | 4.7223092 | 0.6487019 | -1.2681631 |
| F | 4.4728125 | 2.2020314 | -3.5358351 |
| F | 4.8689037 | -0.0116756 | -3.9548816 |
| F | 2.8178621 | 0.6622715 | -3.2094453 |
Illustration of the structure

Energy = -1484.953539242 hartree

Coordinates in Å

| Atom | X    | Y    | Z    |
|------|------|------|------|
| C    | 1.4541230 | 0.0513589 | 0.0002833 |
| C    | 0.6748537 | 1.3238294 | 0.0002496 |
| C    | -0.6748269 | 1.3238354 | 0.0001182 |
| C    | -1.4541073 | 0.0513718 | -0.0002618 |
| C    | -0.6759145 | -1.2334638 | -0.0001499 |
| C    | 0.6759189 | -1.2334697 | -0.0000357 |
| O    | 2.6594395 | 0.0325547 | 0.0005661 |
| Cl   | 1.6057874 | 2.7541341 | -0.0003888 |
| Cl   | -1.6057480 | 2.7541484 | -0.0001119 |
| O    | -2.6594239 | 0.0325782 | -0.0007080 |
| C    | -1.4417411 | -2.4332035 | 0.0000849 |
| C    | 1.4417349 | -2.4332162 | -0.0001618 |
| N    | -2.0605033 | -3.4046022 | 0.0002860 |
| N    | 2.0604884 | -3.4046205 | -0.0002930 |
Illustration of the structure

Energy = -1486.204688409 hartree

Coordinates in Å

| Atom | C   | C   | C   | C   | C   | O   | Cl  | Cl  | O   | C   | C   | H   | H   | N   | N   |
|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
|      | 1.4120512 | 0.0472929 | -0.0001089 |     |     |     |     |     |     |     |     |     |     |     |     |
|      | 0.6958235  | 1.2507080  | 0.0001551  |     |     |     |     |     |     |     |     |     |     |     |     |
|      | -0.6958240 | 1.2507079  | 0.0002077  |     |     |     |     |     |     |     |     |     |     |     |     |
|      | -1.4120513 | 0.0472925  | 0.0000047  |     |     |     |     |     |     |     |     |     |     |     |     |
|      | -0.7050584 | -1.1608556 | -0.000503  |     |     |     |     |     |     |     |     |     |     |     |     |
|      | 0.7050587  | -1.1608553 | -0.000264  |     |     |     |     |     |     |     |     |     |     |     |     |
|      | 2.7553738  | -0.0015616 | -0.0005004 |     |     |     |     |     |     |     |     |     |     |     |     |
|      | 1.5959757  | 2.7302455  | 0.0002095  |     |     |     |     |     |     |     |     |     |     |     |     |
|      | -1.5959766 | 2.7302450  | 0.0003285  |     |     |     |     |     |     |     |     |     |     |     |     |
|      | -2.7553740 | -0.0015626 | -0.0001424 |     |     |     |     |     |     |     |     |     |     |     |     |
|      | -1.4340657 | -2.3857273 | -0.0001508 |     |     |     |     |     |     |     |     |     |     |     |     |
|      | 1.4340666  | -2.3857266 | 0.0002744  |     |     |     |     |     |     |     |     |     |     |     |     |
|      | 3.1176874  | 0.8965946  | -0.0005148 |     |     |     |     |     |     |     |     |     |     |     |     |
|      | -3.1176882 | 0.8965933  | -0.0000591 |     |     |     |     |     |     |     |     |     |     |     |     |
|      | -2.0277600 | -3.3727516 | -0.0003481 |     |     |     |     |     |     |     |     |     |     |     |     |
|      | 2.0277613  | -3.3727507 | 0.0007213  |     |     |     |     |     |     |     |     |     |     |     |     |
Coordinates for calculated structures at $\varepsilon_r = 40$
B3LYP+COSMO/def2-TZVP

1(BF$_4$)$_2$, $\varepsilon_r = 40$

Illustration of the structure (H atoms omitted)

Energy = -2526.451653161 hartee

Coordinates in Å

| Element | X        | Y        | Z        |
|---------|----------|----------|----------|
| F       | -6.5401505 | 1.0585744 | -1.3260030 |
| B       | -7.0057466 | 2.1798562 | -2.0378747 |
| F       | -8.3204313 | 1.9330644 | -2.4879008 |
| F       | -6.1726238 | 2.4161781 | -3.1495089 |
| F       | -7.0040583 | 3.3079290 | -1.1985141 |
| N       | -1.8041512 | 2.0934467 | -0.3495274 |
| C       | -0.9372709 | 1.0801824 | -0.2698289 |
| C       | -2.2794461 | 2.6030621 | -1.4947680 |
| C       | -0.8266295 | 0.4335911 | 1.0910739 |
| C       | -0.1049863 | 0.6198360 | -1.2685335 |
| N       | -2.7501320 | 1.8334803 | -2.5062470 |
| N       | -2.3673498 | 3.9458680 | -1.6072803 |
| C       | -1.5343181 | 0.8164813 | 2.1124351 |
| C       | 0.1045030  | -0.6204282 | 1.2681505 |
| C       | 0.8270999  | -0.4332051 | -1.0911019 |
| H       | -0.1422107 | 1.0716468 | -2.2503354 |
| C       | -2.7522623 | 2.2615799 | -3.9037134 |
| C       | -3.1881745 | 0.4611129 | -2.2984539 |
| C       | -3.4780759 | 4.6224556 | -2.2777370 |
| C       | -1.5345296 | 4.8098038 | -0.7796115 |
| C       | -2.5488509 | 1.7000684 | 2.2253738 |
| C       | 0.9362858  | -1.0811945 | 0.2693338 |
| H       | 0.1414493  | -1.0723885 | 2.2498853 |
| C       | 1.5366560  | -0.8144078 | 2.1118850 |
| H       | -2.4406627 | -0.2540369 | -2.6525531 |
| H       | -4.1171740 | 0.3083807 | -2.8477192 |
| H       | 3.3797283  | 0.2824637 | 1.2457687 |
| H       | -3.1452457 | 5.1598141 | -3.1681921 |
| H       | -3.9050404 | 5.3470729 | -1.5807957 |
| H       | -4.2535918 | 3.9118826 | -2.5469906 |
| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| H    | -2.0671115 | 5.1298356  | 0.1205797  |
| H    | -1.2707567 | 5.6962668  | -1.3583535 |
| H    | -0.6241582 | 4.2942588  | -0.4911796 |
| N    | -2.3086912 | 2.9080435  | 2.7614384  |
| N    | -3.8116821 | 1.2793714  | 2.0171706  |
| N    | 1.8016110  | -2.0960465 | 0.3483276  |
| C    | 2.5529888  | -1.6959322 | -2.2243594 |
| C    | -0.9502241 | 3.4422519  | 2.7665413  |
| C    | -3.2374334 | 3.5779129  | 3.6741687  |
| H    | -1.2707567 | 5.6962668  | -1.3583535 |
| H    | 2.1874273  | 1.6293289  | 2.7614384  |
| C    | 2.2761010  | -2.6073507 | 1.4931380  |
| N    | 2.3161626  | -2.9033691 | -2.7631877 |
| N    | 3.8146318  | -1.2735932 | -2.0123509 |
| H    | 1.0082759  | 4.5299405  | 2.7861815  |
| H    | 0.4062152  | -3.0982384 | -3.6530446 |
| H    | 0.4268517  | -3.1453488 | -1.8742472 |
| H    | 4.0536868  | -2.8984043 | -3.9562991 |
| H    | 2.7001509  | -3.8407548 | -4.5807201 |
| H    | 3.6649698  | -4.771421  | -3.238057 |
| H    | 3.4000173  | 0.7472114  | -2.4058449 |
| H    | 5.1132088  | 0.336325   | -2.217421  |
| H    | 4.0727644  | 0.4461549  | -0.7906551 |
| H    | 5.3497485  | -1.8062600 | -0.7060881 |
| H    | 5.6689966  | 2.2385992  | -2.3964373 |
| H    | 4.5052156  | -3.1740223 | -1.4301893 |
| H    | 3.7611969  | 2.4410296  | 4.2693020  |
| H    | 2.2908702  | 1.4794892  | 4.5025363  |
| H    | 2.1575738  | 3.1739034  | 4.0233271  |
| H    | 2.4382681  | 0.2477323  | 2.6571108  |
| H    | 4.1145821  | -0.3163204 | 2.8505533  |
| H    | 3.3766604  | -0.2864315 | 1.2490074  |
| H    | 3.1411357  | -5.1672519 | 3.1625097  |
| H    | 3.9013307  | -5.3516596 | 1.5749990  |
| H    | 4.2496901  | -3.9182595 | 2.5438701  |
| H    | 2.0633988  | 5.1291367  | -0.1279458 |
| H    | 1.2692812  | -5.7014858 | 1.3501053  |
| H    | 0.6198519  | -4.2977032 | 0.4881226  |
| H    | -3.7661984 | 2.4310375  | -4.269920  |
Illustration of the structure (C-H atoms omitted)

Energy = -2527.683935834 hartree

Coordinates in Å

\[
\begin{align*}
\text{H} & : -2.2955185, 1.4697621, -4.5020729 \\
\text{H} & : -2.1628105, 3.1651115, -4.0260686 \\
\text{F} & : 6.9976336, -3.3027595, 1.1959858 \\
\text{B} & : 6.9986589, -2.1798926, 2.0423099 \\
\text{F} & : 6.5314523, -1.0547100, 1.3378719 \\
\text{F} & : 8.3135486, -1.9345463, 2.4929331 \\
\text{F} & : 6.1667641, -2.4240891, 3.1531158 \\
\text{F} & : 6.9976336, -1.4697621, -4.5020729 \\
\text{B} & : 6.9986589, -3.1651115, -4.0260686 \\
\text{F} & : 6.5314523, -1.0547100, 1.3378719 \\
\text{F} & : 8.3135486, -1.9345463, 2.4929331 \\
\text{F} & : 6.1667641, -2.4240891, 3.1531158 \\
\text{F} & : 6.9976336, -2.1798926, 2.0423099 \\
\text{F} & : 6.5314523, -1.0547100, 1.3378719 \\
\text{F} & : 8.3135486, -1.9345463, 2.4929331 \\
\text{F} & : 6.1667641, -2.4240891, 3.1531158 \\
\end{align*}
\]
| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| N       | 0.9636328 | -1.6129855 | -2.1054209 |
| H       | -2.8063650 | -0.2538265 | -2.3077804 |
| H       | -4.3794926 | 0.5715705 | -2.3961564 |
| H       | -3.4264017 | 0.6527384 | -0.9123432 |
| H       | -2.9241824 | 5.0520966 | -3.6248608 |
| H       | -3.4641061 | 5.5895933 | -2.0250786 |
| H       | -4.0705763 | 4.0652212 | -2.6811438 |
| H       | -1.3425633 | 5.4566908 | -0.5846456 |
| H       | -0.7858327 | 5.6287675 | -2.2546960 |
| H       | -0.1315266 | 4.3304282 | -1.2499625 |
| N       | -2.4828714 | 2.9606128 | 3.1899456 |
| N       | -3.2837134 | 1.0236713 | 2.1651749 |
| N       | -1.4956309 | -2.3072501 | 0.5565575 |
| C       | -2.1997886 | -1.8381555 | 3.2052162 |
| C       | -1.4829190 | 4.0131381 | 3.2767724 |
| C       | -3.3852962 | 2.9152504 | 4.3388581 |
| C       | -3.1577416 | -0.4232289 | 2.0811549 |
| C       | -4.6213086 | 1.5484004 | 1.9177672 |
| C       | -2.1164253 | -2.7203216 | 1.6849663 |
| N       | -2.4766191 | -2.9667767 | -3.1893225 |
| N       | -3.2759808 | -1.0272050 | -2.1679288 |
| H       | -1.9805713 | 4.3995636 | 3.5672292 |
| H       | -0.7077541 | 3.7862302 | 4.0177256 |
| H       | -0.9954656 | 4.1607322 | 2.3161630 |
| H       | -3.9313710 | 1.9779706 | 4.3639595 |
| H       | -2.8083737 | 2.9968090 | 5.2666348 |
| H       | -4.0995023 | 3.7409781 | 4.3050605 |
| H       | -2.2432632 | -0.7513298 | 2.5661552 |
| H       | -4.0039746 | -0.8794841 | 2.6015658 |
| H       | -3.1585059 | -0.7893935 | 1.0498426 |
| H       | -4.9911513 | 1.1744553 | 0.9598440 |
| H       | -5.3278888 | 1.2421929 | 2.6956582 |
| H       | -4.5979067 | 2.6332553 | 1.8698868 |
| N       | -2.7478393 | -1.8512780 | 2.4850843 |
| N       | -2.0956607 | -4.0330924 | 1.9657226 |
| C       | -1.4773321 | -4.0202852 | -3.2732627 |
| C       | -3.3734880 | -2.9190627 | -4.3426779 |
| C       | -3.1483984 | 0.4197988 | -2.0875514 |
| C       | -4.6512640 | -1.5494122 | -1.9236820 |
| C       | -2.8482668 | -2.0479833 | 3.9320375 |
| C       | -3.3641331 | -0.6260324 | 1.9830547 |
| C       | -3.2138555 | -4.7152033 | 1.6143465 |
| C       | -1.0305938 | -4.9112973 | 1.4821066 |
| H       | -1.9748573 | -4.9458371 | 3.5666930 |
| H       | -0.6988753 | -3.7934954 | -4.0107857 |
| H       | -0.9940603 | -4.1695008 | -2.3107800 |
| H       | -3.9213055 | -1.9827940 | -4.3669840 |
| H       | -2.7925493 | -2.9965674 | -5.2660513 |
| H       | -4.0862598 | -3.7462018 | -4.3148130 |
| H       | -2.2320246 | 0.7453064 | -2.5706612 |
| H       | -3.9924427 | 0.8757335 | -2.6118310 |
| H       | -3.1517940 | 0.7891116 | -1.0573062 |
| H       | -4.9873870 | -1.1742182 | -0.9669859 |
| H       | -5.3191340 | -1.2424658 | -2.7036168 |
| H       | -4.5937801 | 2.6342963 | -1.8752666 |
| H       | -3.8682706 | -2.2984010 | 4.2259869 |
| H       | -2.5609399 | -1.1154258 | 4.4209768 |
| H       | -2.1685835 | -2.8311807 | 4.2541433 |
| H       | -2.8007392 | 0.2539146 | 2.2997733 |
| H       | -4.3783626 | -0.5647930 | 2.3771899 |
| H       | -3.4151311 | -0.6496256 | 0.9001378 |
\((1+2\text{H})(\text{BF}_4)_4\), \(\varepsilon_r = 40\)

Illustration of the structure (C-H atoms omitted)

Energy = -3376.710257680 hartree

Coordinates in Å

\[
\begin{array}{lll}
\text{F} & 6.6178211 & 1.8005450 & 4.3483027 \\
\text{B} & 6.0752939 & 3.0921186 & 4.2791082 \\
\text{F} & 4.7630539 & 3.0754275 & 4.8263941 \\
\text{F} & 6.0168009 & 3.5151666 & 2.9435209 \\
\text{F} & 6.8621969 & 3.9846875 & 5.0319964 \\
\text{C} & 2.9168296 & 8.9503084 & 6.6272396 \\
\text{C} & 3.6119460 & 7.7451546 & 6.9906743 \\
\text{C} & 2.4919786 & 8.0592738 & 4.3618314 \\
\text{C} & 3.7561115 & 6.7302317 & 6.1045382 \\
\text{C} & 3.1847350 & 6.8534155 & 4.7261383 \\
\text{N} & 3.3999233 & 5.8469664 & 3.9549918 \\
\end{array}
\]
Illustration of the structure (C-H atoms omitted)

Energy = -3377.971978507 hartree

Coordinates in Å

| Atom | X           | Y           | Z           |
|------|-------------|-------------|-------------|
| F    | 2.977584    | -6.0553513  | -1.2447481  |
| B    | 2.1670984   | -5.0197401  | -1.7022271  |
| F    | 1.0773482   | -4.8306968  | -0.8037982  |
| F    | 1.6683341   | -5.2981309  | -2.9754936  |
| F    | 2.9135088   | -3.8089665  | -1.7407193  |
| C    | 0.3930010   | 0.8869907   | 1.0139167   |
| C    | 0.3199075   | -0.2673576  | 1.3239892   |
| C    | -0.3151838  | 0.2703823   | -1.3255063  |
| C    | 0.7186936   | -1.1513318  | 0.3269471   |
| C    | 0.3976377   | -0.8839423  | -1.0154422  |
| N    | 0.8869570   | -1.7486458  | -2.0168441  |
| F    | -0.9151328  | 1.4720656   | -4.3441810  |
| B    | -0.2566252  | -1.7270579  | 5.1034997   |
| B    | 0.2455034   | 1.7254696   | -5.1116322  |
| F    | -0.4312090  | 0.6881830   | 6.0392395   |
| F    | -1.3662746  | -1.7803026  | 4.2417749   |
| F    | -0.1172933  | 2.9506346   | 5.7789482   |
| F    | 0.4087524   | 0.6902787   | -6.0534461  |
| F    | 1.3612939   | 1.7695353   | -4.2573946  |
| F    | 0.1072806   | 2.9529351   | -5.7803273  |
| N    | -0.8827570  | 1.7515952   | 2.0150134   |
| C    | -0.7143745  | 1.1541631   | -0.3284796  |
| N    | 1.3784355   | -2.3616595  | 0.6471284   |
| C    | 0.3622989   | -1.9896141  | -3.2536305  |
| F    | 0.9081734   | -1.4718453  | 4.3429573   |
| C    | -0.3611215  | 1.9904145   | 3.2535969   |
| N    | -1.3753589  | 2.3639452   | -0.6488598  |
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| H       | 1.0590962 | -3.2072155 | 0.1796028 |
| C       | 2.3305126 | -2.5574969 | 1.6007779 |
| N       | 1.2130081 | -2.1082943 | -4.273820 |
| N       | 1.2146698 | 2.108878  | 4.2699313 |
| N       | 0.9589653 | 2.1484331 | 3.4110072 |
| C       | 2.3307625 | -2.5574969 | 1.6007779 |
| N       | 1.2130081 | -2.1082943 | -4.273820 |
| N       | 1.2146698 | 2.108878  | 4.2699313 |
| N       | 0.9589653 | 2.1484331 | 3.4110072 |
| H       | 0.9589653 | 2.1484331 | 3.4110072 |
| C       | 2.3307625 | -2.5574969 | 1.6007779 |
| N       | 1.2130081 | -2.1082943 | -4.273820 |
| N       | 1.2146698 | 2.108878  | 4.2699313 |
| N       | 0.9589653 | 2.1484331 | 3.4110072 |
| H       | 0.9589653 | 2.1484331 | 3.4110072 |
| C       | 2.3307625 | -2.5574969 | 1.6007779 |
| N       | 1.2130081 | -2.1082943 | -4.273820 |
| N       | 1.2146698 | 2.108878  | 4.2699313 |
| N       | 0.9589653 | 2.1484331 | 3.4110072 |
| H       | 0.9589653 | 2.1484331 | 3.4110072 |
| C       | 2.3307625 | -2.5574969 | 1.6007779 |
| N       | 1.2130081 | -2.1082943 | -4.273820 |
| N       | 1.2146698 | 2.108878  | 4.2699313 |
| N       | 0.9589653 | 2.1484331 | 3.4110072 |
| H       | 0.9589653 | 2.1484331 | 3.4110072 |
| C       | 2.3307625 | -2.5574969 | 1.6007779 |
| N       | 1.2130081 | -2.1082943 | -4.273820 |
| N       | 1.2146698 | 2.108878  | 4.2699313 |
| N       | 0.9589653 | 2.1484331 | 3.4110072 |
| H       | 0.9589653 | 2.1484331 | 3.4110072 |
| C       | 2.3307625 | -2.5574969 | 1.6007779 |
| N       | 1.2130081 | -2.1082943 | -4.273820 |
| N       | 1.2146698 | 2.108878  | 4.2699313 |
| N       | 0.9589653 | 2.1484331 | 3.4110072 |
| H       | 0.9589653 | 2.1484331 | 3.4110072 |
| C       | 2.3307625 | -2.5574969 | 1.6007779 |
| N       | 1.2130081 | -2.1082943 | -4.273820 |
| N       | 1.2146698 | 2.108878  | 4.2699313 |
| N       | 0.9589653 | 2.1484331 | 3.4110072 |
| H       | 0.9589653 | 2.1484331 | 3.4110072 |
| C       | 2.3307625 | -2.5574969 | 1.6007779 |
| N       | 1.2130081 | -2.1082943 | -4.273820 |
| N       | 1.2146698 | 2.108878  | 4.2699313 |
| N       | 0.9589653 | 2.1484331 | 3.4110072 |
| H       | 0.9589653 | 2.1484331 | 3.4110072 |
| C       | 2.3307625 | -2.5574969 | 1.6007779 |
| N       | 1.2130081 | -2.1082943 | -4.273820 |
| N       | 1.2146698 | 2.108878  | 4.2699313 |
| N       | 0.9589653 | 2.1484331 | 3.4110072 |
| H       | 0.9589653 | 2.1484331 | 3.4110072 |
| C       | 2.3307625 | -2.5574969 | 1.6007779 |
| N       | 1.2130081 | -2.1082943 | -4.273820 |
| N       | 1.2146698 | 2.108878  | 4.2699313 |
| N       | 0.9589653 | 2.1484331 | 3.4110072 |
| H       | 0.9589653 | 2.1484331 | 3.4110072 |
| C       | 2.3307625 | -2.5574969 | 1.6007779 |
| N       | 1.2130081 | -2.1082943 | -4.273820 |
| N       | 1.2146698 | 2.108878  | 4.2699313 |
| N       | 0.9589653 | 2.1484331 | 3.4110072 |
| H       | 0.9589653 | 2.1484331 | 3.4110072 |
$\text{H} \cdot -0.9538576 \ 5.2811604 \ -1.9100657$
$\text{H} \cdot -4.3772819 \ 3.9495683 \ -2.3182812$
$\text{H} \cdot -3.4175367 \ 5.4162445 \ -2.5414308$
$\text{H} \cdot -3.5837231 \ 4.2679962 \ -3.8798020$
$\text{H} \cdot -3.3404372 \ 1.8400387 \ -3.8597928$
$\text{H} \cdot -4.0138842 \ 0.3402751 \ -3.2141758$
$\text{H} \cdot -4.9545236 \ 1.8306046 \ -3.0947225$
$\text{H} \cdot -3.5568243 \ 1.2899717 \ 0.2878875$
$\text{H} \cdot -4.8735781 \ 0.7459156 \ -0.7502569$
$\text{H} \cdot -3.3654941 \ -0.1800310 \ -0.6957037$
$\text{H} \cdot -2.5388111 \ -0.6209908 \ -3.5900298$
$\text{H} \cdot -3.3054413 \ -2.1869945 \ -3.9782430$
$\text{H} \cdot 2.7373179 \ -1.1107850 \ -5.2716446$
$\text{H} \cdot 0.7479993 \ -2.4114180 \ -6.3150385$
$\text{H} \cdot 1.8587779 \ -3.5836798 \ -5.5812632$
$\text{H} \cdot 0.1376594 \ -3.6613087 \ -5.2004613$
$\text{H} \cdot -1.9679283 \ -2.6789845 \ -5.1949707$
$\text{H} \cdot -2.5520056 \ -1.2270116 \ -4.3715669$
$\text{H} \cdot -1.0306137 \ -1.1587672 \ -5.2610617$
$\text{H} \cdot -2.3774552 \ -1.9167708 \ -1.8463769$
$\text{H} \cdot -2.4882050 \ -3.4116790 \ -2.7871601$
$\text{H} \cdot -1.1877885 \ -3.2160045 \ -1.6082195$
$\text{H} \cdot -1.7678669 \ -2.2202088 \ -1.8328874$
$\text{H} \cdot -1.7615508 \ 2.2262510 \ 1.8288043$

$C_6H_4O_2 (BQ), \ \varepsilon_r = 40$

Illustration of the structure

Energy $= -381.4109504508$ hartree

Coordinates in Å

\begin{tabular}{cccc}
C & 1.4322862 & -0.0000050 & 0.0000412 \\
C & 0.6682407 & 1.2669082 & 0.0000734 \\
C & -0.6682460 & 1.2669415 & 0.0001413 \\
C & -1.4322858 & 0.0000205 & 0.0000912 \\
C & -0.6682328 & -1.2669005 & 0.0000484 \\
\end{tabular}
Illustration of the structure
(C₆H₄O₂+2H)(BF₄)₂, ɛᵣ = 40

Illustration of the structure
(almost symmetric F···H···O bonds with F-H 1.360 Å, O-H 1.059 Å)

Energy = -1231.573823076 hartree

Coordinates in Å

| Atom | X  | Y  | Z  |
|------|----|----|----|
| C    | 1.3529137 | -0.2923861 | 0.0135079 |
| C    | 0.9267697 | 1.1053189 | -0.0084731 |
| C    | -0.3801483 | 1.3838885 | -0.0260458 |
| O    | 2.5642423 | -0.6155185 | 0.0328176 |
| H    | 1.6812764 | 1.8805255 | -0.0106560 |
| H    | -0.7638064 | 2.3947898 | -0.0434775 |
| H    | -3.2670605 | -0.1784509 | -0.0408680 |
| B    | -5.4860508 | -1.0866713 | 0.5908817 |
| F    | -4.1447597 | -1.2171987 | -0.0529536 |
| F    | -5.5319656 | 0.1882712 | 1.1367553 |
| F    | -5.5622051 | -2.0712791 | 1.5584761 |
| F    | -6.4273490 | -1.2613427 | -0.4064217 |
| C    | -1.3544220 | 0.2916425 | -0.0236340 |
| C    | -0.9282725 | -1.1061400 | -0.0029225 |
| C    | 0.3786461 | -1.3847217 | 0.0142687 |
| O    | -2.5657934 | 0.6149600 | -0.0401522 |
| H    | -1.6826870 | -1.8814713 | -0.0008676 |
| H    | 0.7622450 | -2.3956728 | 0.0310449 |
| H    | 3.2650769 | 0.1783105 | 0.0373919 |
| B    | 5.4884010 | 1.0877479 | -0.5769266 |
| F    | 4.1424207 | 1.2172752 | 0.0573014 |
| F    | 5.5386536 | -0.1867746 | -1.1234538 |
| F    | 5.5716540 | 2.0730855 | -1.5431342 |
| F    | 6.4222211 | 1.2618122 | 0.4275413 |
$C_6Cl_4O_2 (CA), \varepsilon_r = 40$

Illustration of the structure

Energy = -2219.642096420 hartree

Coordinates in Å

|   |        |        |         |
|---|--------|--------|---------|
| C | 1.4482053 | -0.0000044 | 0.0000030 |
| C | 0.6716502 | 1.2755345 | -0.0000673 |
| C | -0.6716576 | 1.2755290 | -0.0000142 |
| C | -1.4481820 | 0.0000266 | -0.0000486 |
| C | -0.6716472 | -1.2755393 | -0.0000424 |
| C | 0.6716528 | -1.2755368 | -0.0000795 |
| O | 2.6569488 | -0.0000022 | 0.0001418 |
| Cl | 1.6046409 | 2.7092145 | -0.0001082 |
| Cl | -1.6046665 | 2.7092140 | 0.0002064 |
| O | -2.6569238 | 0.0000051 | -0.0001015 |
| Cl | -1.6046616 | -2.7092007 | 0.0001033 |
| Cl | 1.6046407 | -2.7092402 | 0.0000073 |
$\text{C}_6\text{Cl}_4\text{(OH)}_2, \varepsilon_r = 40$

Illustration of the structure

Energy = -2220.879308487 hartree

Coordinates in Å

|   |            |            |            |
|---|------------|------------|------------|
| C | 1.4108543  | -0.0313106 | -0.0002219 |
| C | 0.7174583  | 1.1826838  | -0.0001960 |
| C | -0.6754763 | 1.2188624  | -0.0002130 |
| C | -1.4108527 | 0.0313106  | -0.0001977 |
| C | -0.7174556 | -1.1826848 | -0.0002535 |
| C | 0.6754729  | -1.2188617 | -0.0002679 |
| O | 2.7588524  | -0.1051107 | -0.0002705 |
| Cl| 1.6534966  | 2.6441532  | -0.0001586 |
| Cl| -1.5308001 | 2.7226666  | -0.0003411 |
| O | -2.7588577 | 0.1051091  | -0.0001668 |
| Cl| -1.6534932 | -2.6441494 | -0.0001118 |
| Cl| 1.5308000  | -2.7226643 | -0.0002269 |
| H | 3.1373557  | 0.7883611  | 0.0013776  |
| H | -3.1373545 | -0.7883653 | 0.0012481  |
$C_6Cl_4O_2(HF)_2(BF_3)_2$, $\varepsilon_r = 40$

Illustration of the structure

Energy = -3069.779806366

Coordinates in Å

|   |    |    |    |
|---|----|----|----|
| C | -0.4401940 | 1.3106243 | 0.3375877 |
| C | -1.3113594 | 0.1202829 | 0.5458477 |
| C | -0.7690013 | -1.2159650 | 0.1877978 |
| Cl | -1.1155182 | 2.8143822 | 0.7678798 |
| O | -2.4312636 | 0.2627582 | 0.9972159 |
| Cl | -1.8041537 | -2.5455805 | 0.4521066 |
| H | -3.7464611 | -0.6009326 | 1.3711316 |
| B | -5.0873458 | -0.9025372 | 3.8928683 |
| F | -4.5819055 | -0.9763258 | 1.6527029 |
| F | -5.5989629 | -2.1210371 | 3.8748702 |
| F | -5.8847274 | 0.1441720 | 3.7643902 |
| F | -3.8278536 | -0.7247539 | 4.2568206 |
| C | 0.4729752 | -1.3445629 | -0.3137997 |
| C | 1.3429723 | -0.1539004 | -0.5252275 |
| C | 0.8019130 | 1.1819580 | -0.1636419 |
| Cl | 1.1490480 | -2.8486236 | -0.7419794 |
| O | 2.4607042 | -0.2955767 | -0.9822104 |
| Cl | 1.8379811 | 2.5115100 | -0.4248549 |
| H | 3.7700080 | 0.5722470 | -1.3705294 |
| B | 5.0304402 | 0.9644620 | -3.9248318 |
| F | 4.5997557 | 0.9517170 | -1.6630303 |
| F | 5.5348236 | 2.1851705 | -3.8788063 |
| F | 5.8378559 | -0.0803099 | -3.8608364 |
| F | 3.7602694 | 0.7908216 | -4.2514713 |
Illustration of the structure

Energy = -1484.973474636

Coordinates in Å

|    |      |      |     |
|----|------|------|-----|
| C  | 1.4506101 | 0.0524352 | -0.0000978 |
| C  | 0.6743583 | 1.3203734 | 0.0000527 |
| C  | -0.6743944 | 1.3203524 | -0.0000405 |
| C  | -1.4504768 | 0.0524349 | -0.0001888 |
| C  | -0.6776507 | -1.2299910 | -0.0000356 |
| C  | 0.6738629 | -1.2300236 | 0.0000396 |
| O  | 2.6582818 | 0.0273321 | -0.0003546 |
| Cl | 1.6030087 | 2.7518292 | 0.0001247 |
| Cl | -1.6031819 | 2.7517457 | 0.0000753 |
| O  | -2.6581552 | 0.0271383 | -0.0004127 |
| C  | -1.4387910 | -2.4307157 | -0.0000960 |
| C  | 1.4388319 | -2.4309394 | 0.0001928 |
| N  | -2.0591861 | -3.4001716 | -0.0001948 |
| N  | 2.0589633 | -3.4005649 | 0.0004129 |
$\text{C}_6\text{Cl}_2(\text{CN})_2(\text{OH})_2$, $\varepsilon_r = 40$

Illustration of the structure

Energy = -1486.228543189

Coordinates in Å

|   |   |    |    |
|---|---|---|---|
| C | 1.4146333 | 0.0478979 | -0.0002892 |
| C | 0.6945514 | 1.2539785 | -0.0000347 |
| C | -0.6945445 | 1.2539605 | -0.0001085 |
| C | -1.4145593 | 0.0478592 | 0.0002043 |
| C | -0.7064138 | -1.1550621 | 0.0002274 |
| C | 0.7065305 | -1.1550638 | -0.0002138 |
| O | 2.7543249 | -0.0040769 | 0.0007033 |
| Cl | 1.5928611 | 2.7270684 | -0.000252 |
| Cl | -1.5929076 | 2.7270230 | 0.0002598 |
| O | -2.7542670 | -0.0042104 | 0.0006277 |
| C | -1.4294776 | -2.3801921 | 0.0003187 |
| C | 1.4295033 | -2.3802829 | -0.0002804 |
| H | 3.1353995 | 0.8889105 | 0.0010331 |
| H | -3.1354172 | 0.8887405 | -0.0011090 |
| N | -2.0130494 | -3.3742128 | 0.0004294 |
| N | 2.0128323 | -3.3744493 | -0.0003362 |
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13) Acknowledgements

The authors gratefully acknowledge financial support by the Deutsche Forschungsgemeinschaft (DFG).