

Supporting Information for “Cyclic Benzobisimidazolium Derivative for the Selective Fluorescent Recognition of HSO_4^- via Combination of C-H Hydrogen Bondings and Charge Interactions”

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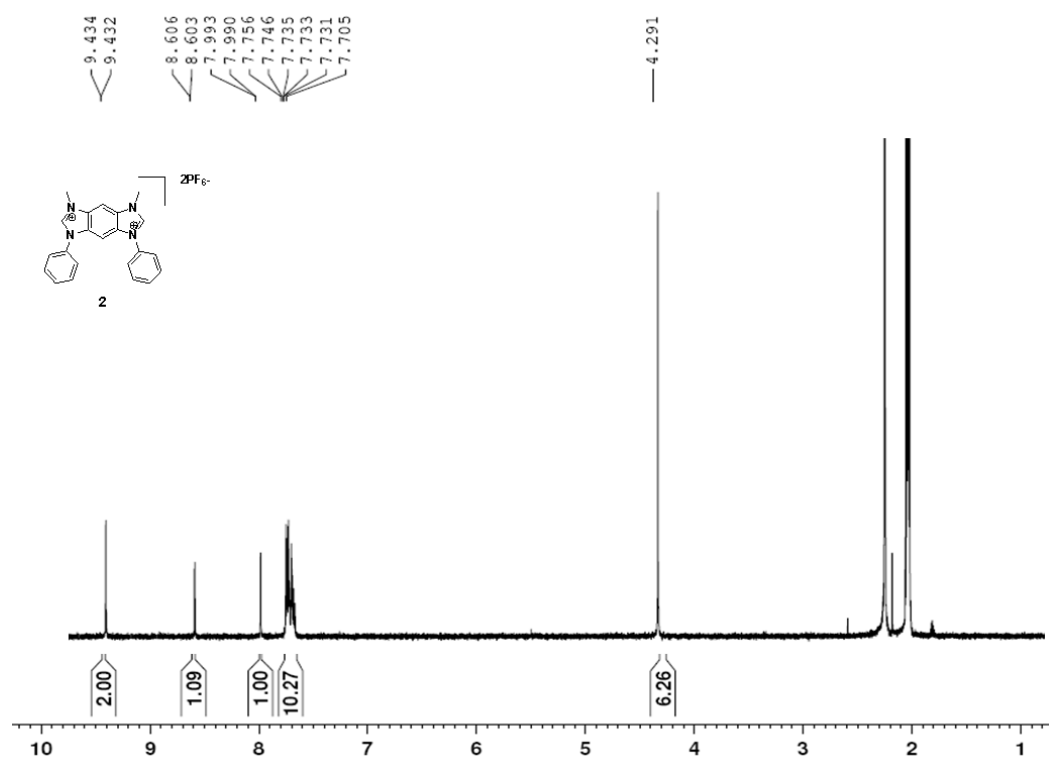


Fig S1. 1H NMR (300 MHz) of compound **2** in CD_3CN

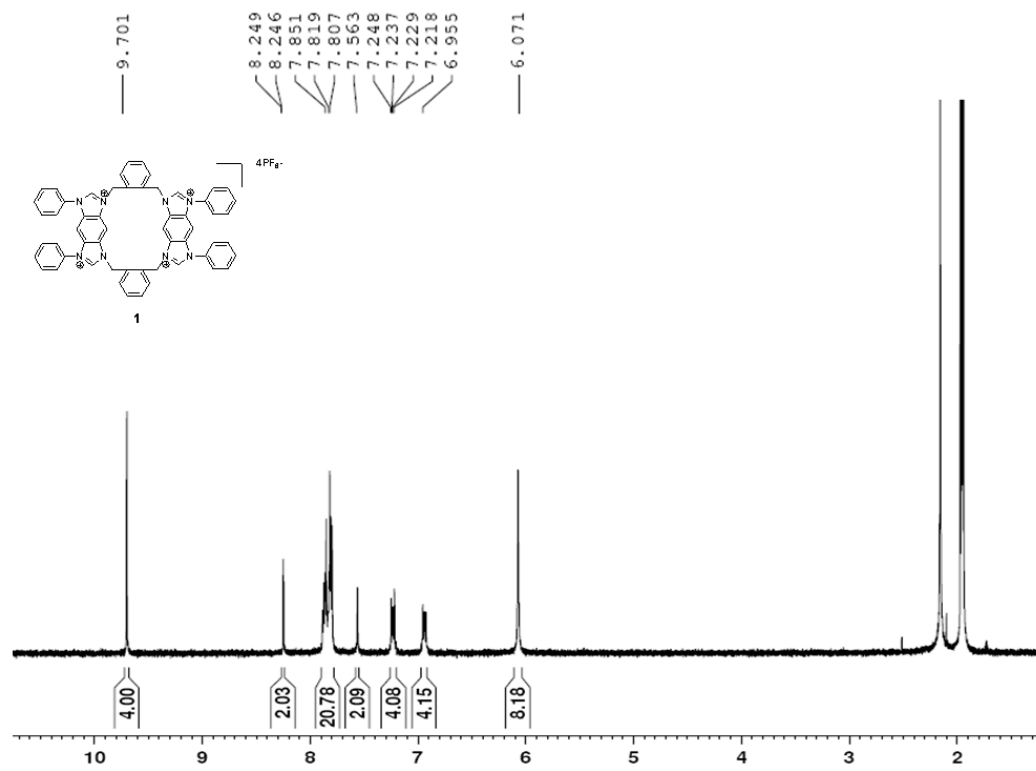


Fig S2. 1H NMR (300 MHz) of compound **1** in CD_3CN

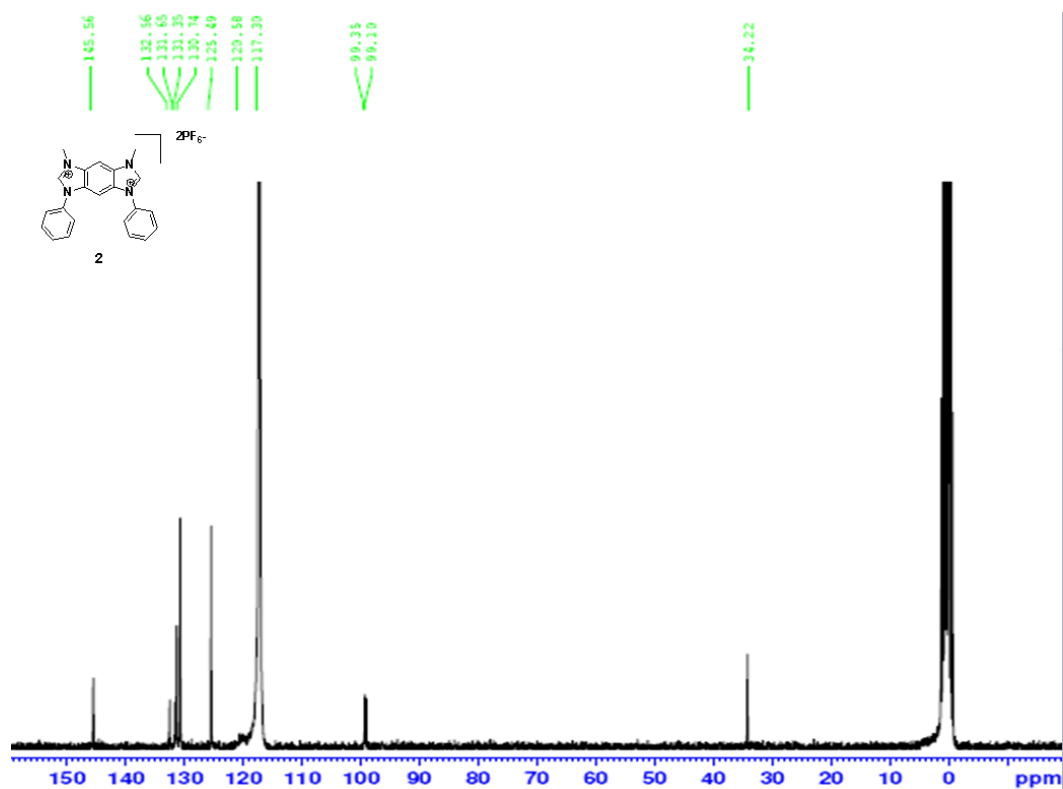


Fig S3. ¹³C NMR (300 MHz) of compound 2 in CD₃CN.

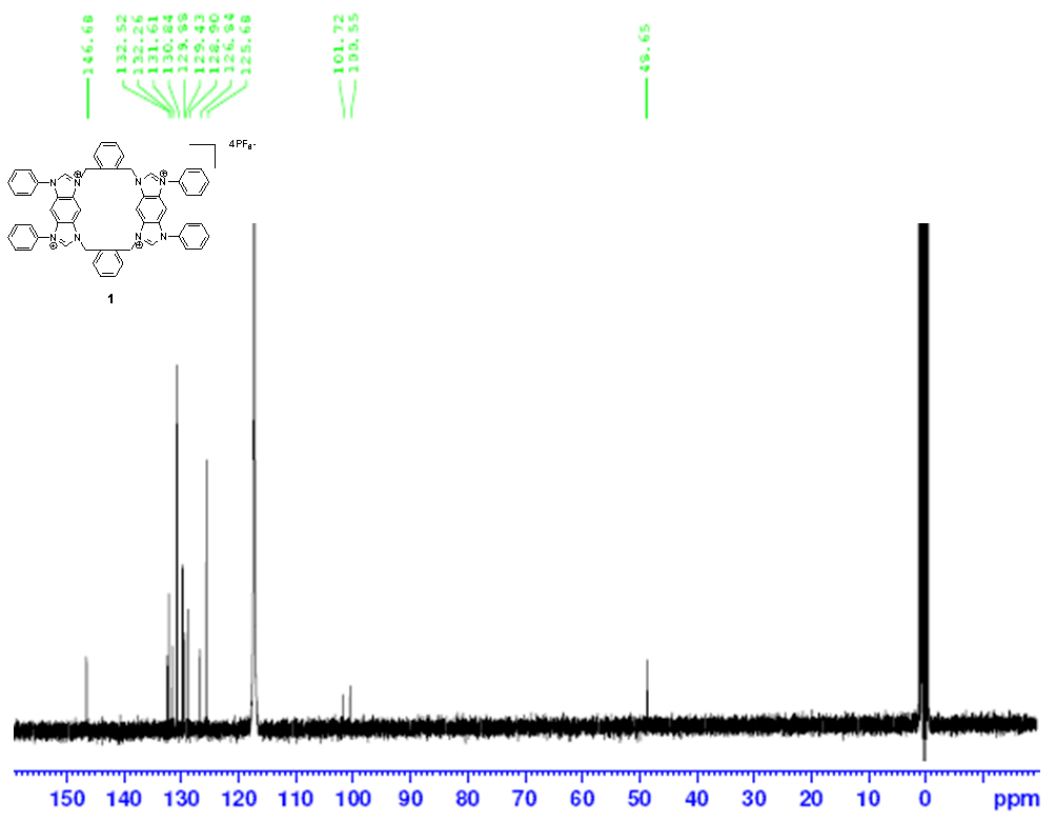


Fig S4. ¹³C NMR (300 MHz) of compound 1 in CD₃CN.

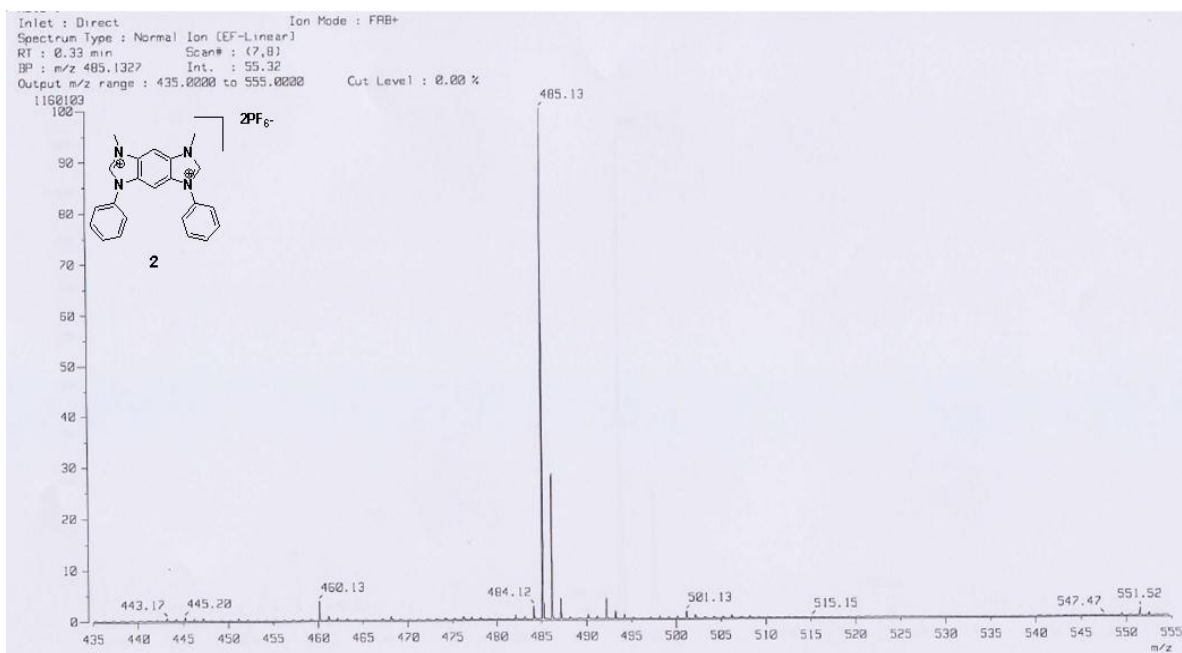


Fig S5. FAB MASS data of 2.

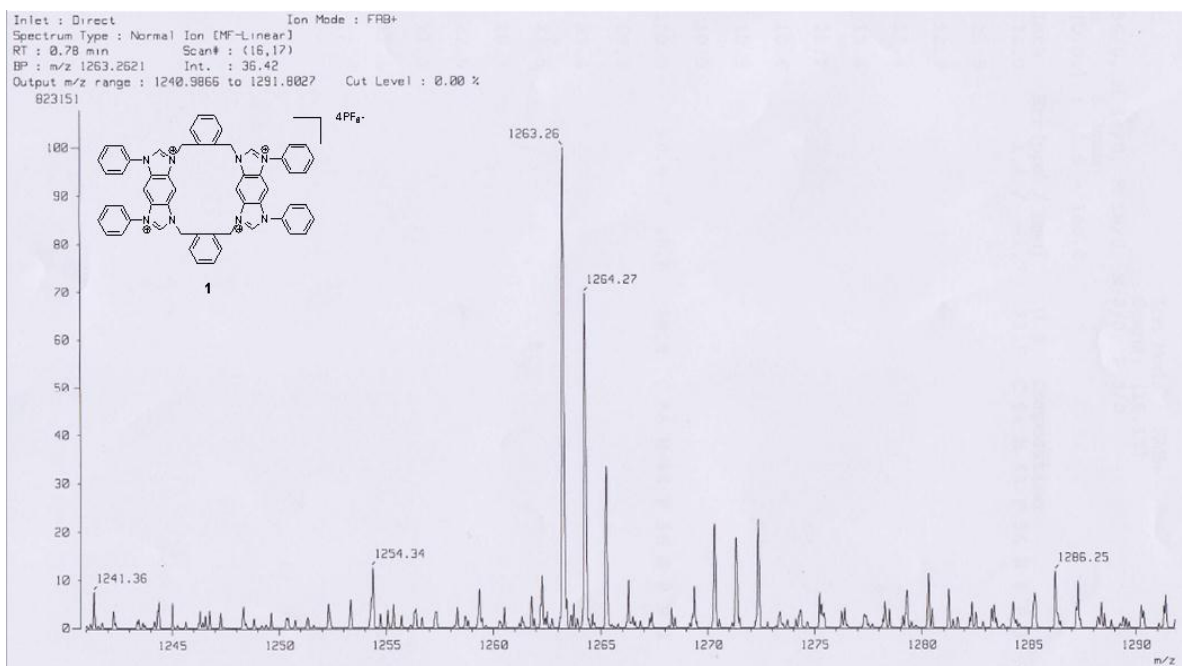


Fig S6. FAB MASS data of 1.

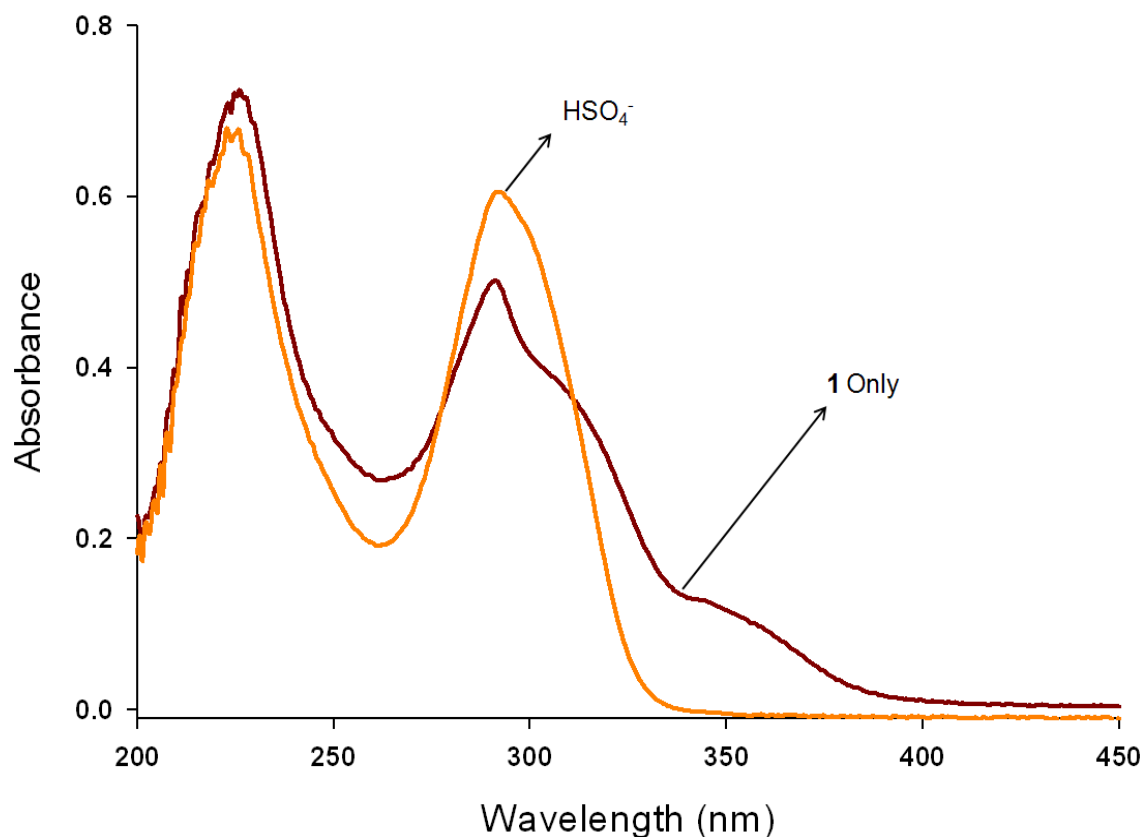


Fig S7. UV spectra of **1** (20.0 μM) upon addition of tetrabutylammonium salts HSO₄⁻ (10 equiv.) in CH₃CN.

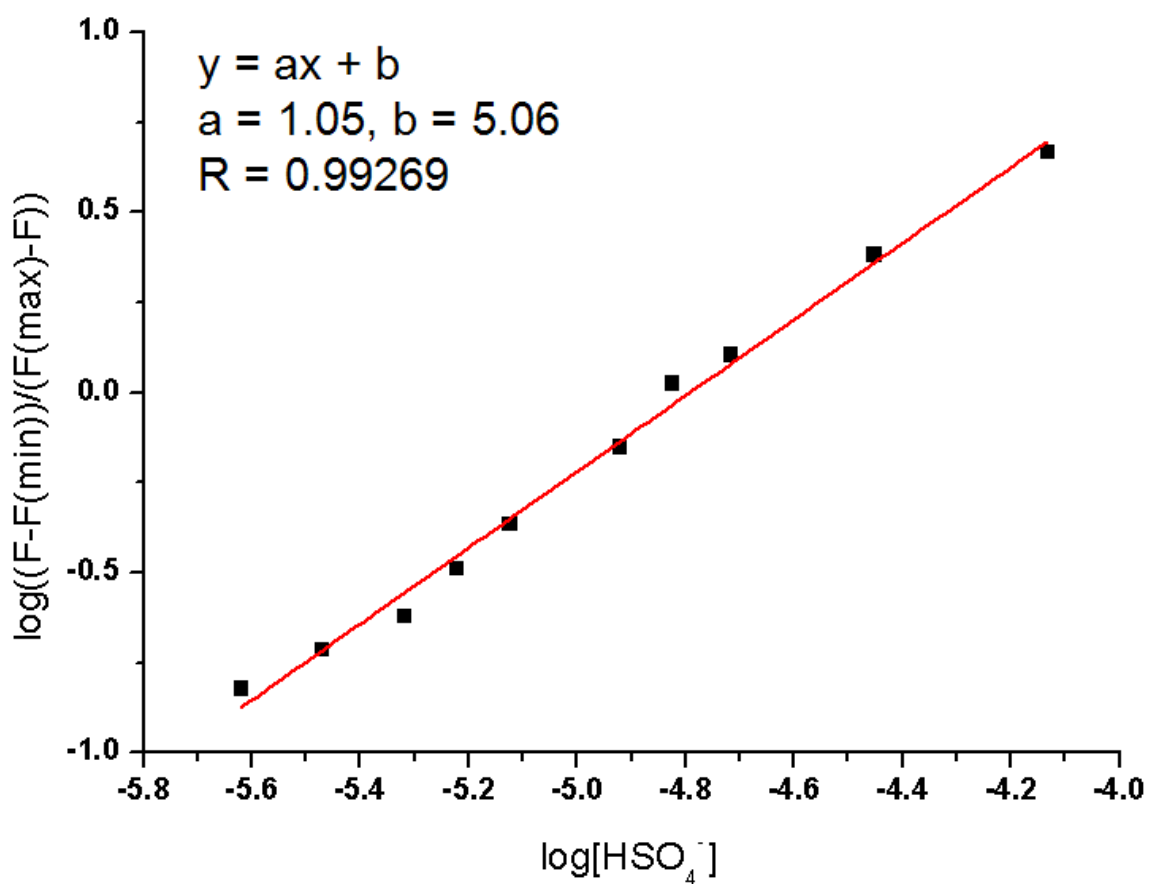


Fig S8. linear of $\log [(F-F_0)/(F_{\max}-F)]$ vs. $\log [\text{HSO}_4^-]$. (A present fluorescence of **1** at 290 nm).

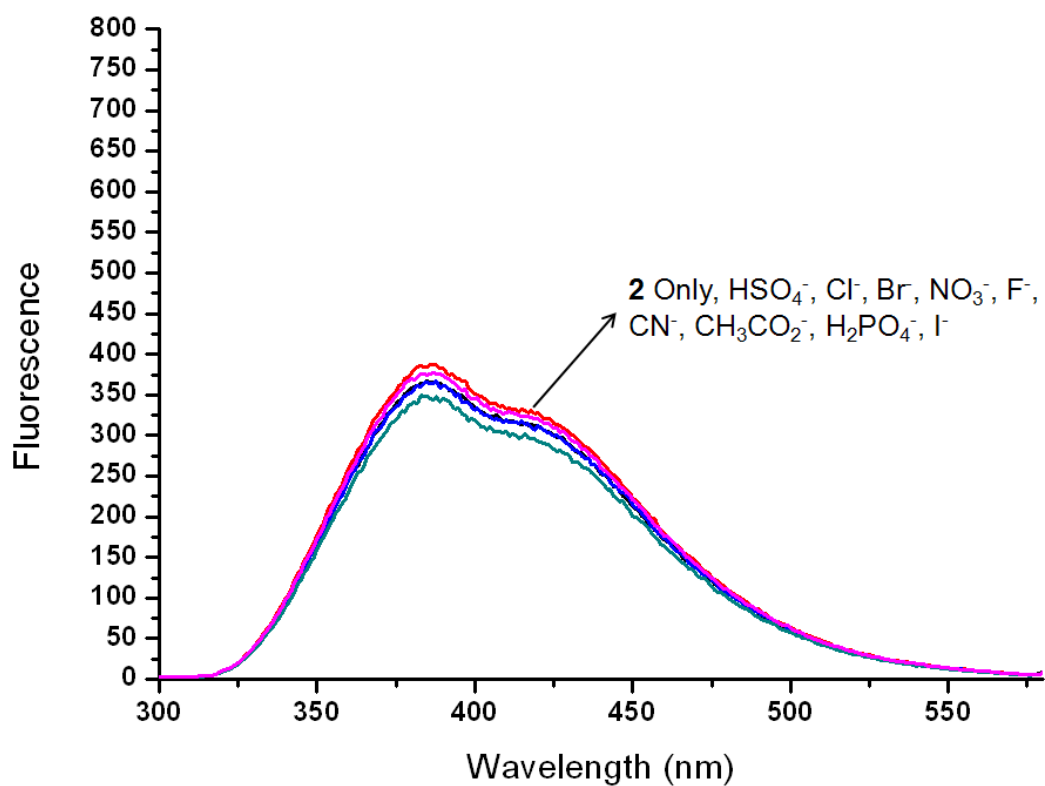


Fig S9. Fluorescence spectra **2** ($6.0 \mu\text{M}$) upon addition of TBA⁺ salts HSO_4^- , NO_3^- , Cl^- , Br^- , I^- , H_2PO_4^- , CH_3CO_2^- , F^- and CN^- (10 equiv) in 9 : 1 CH_3CN –HEPES v/v (pH7.4, 0.02M).

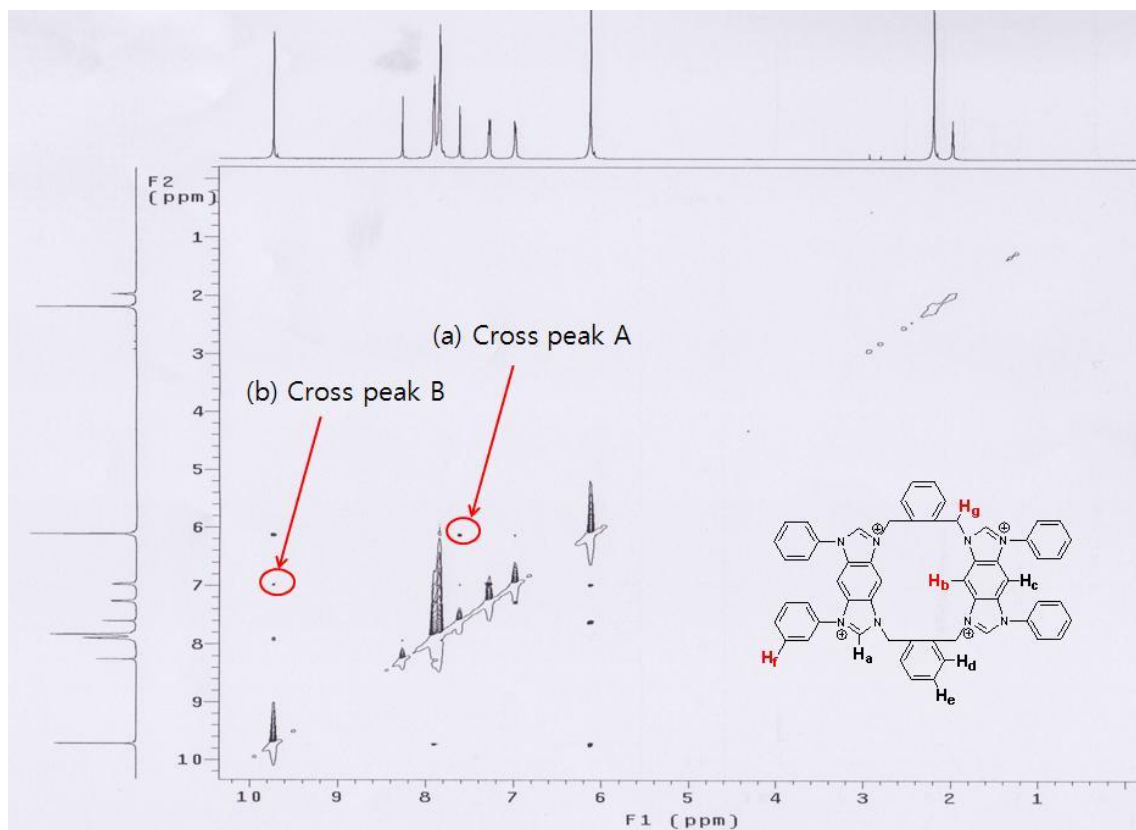


Fig S10. 2D-NOESY NMR spectra of **1** in CD₃CN (a) Cross peak **A** between H_b and H_g (b) Cross peak **B** between H_a and H_d.

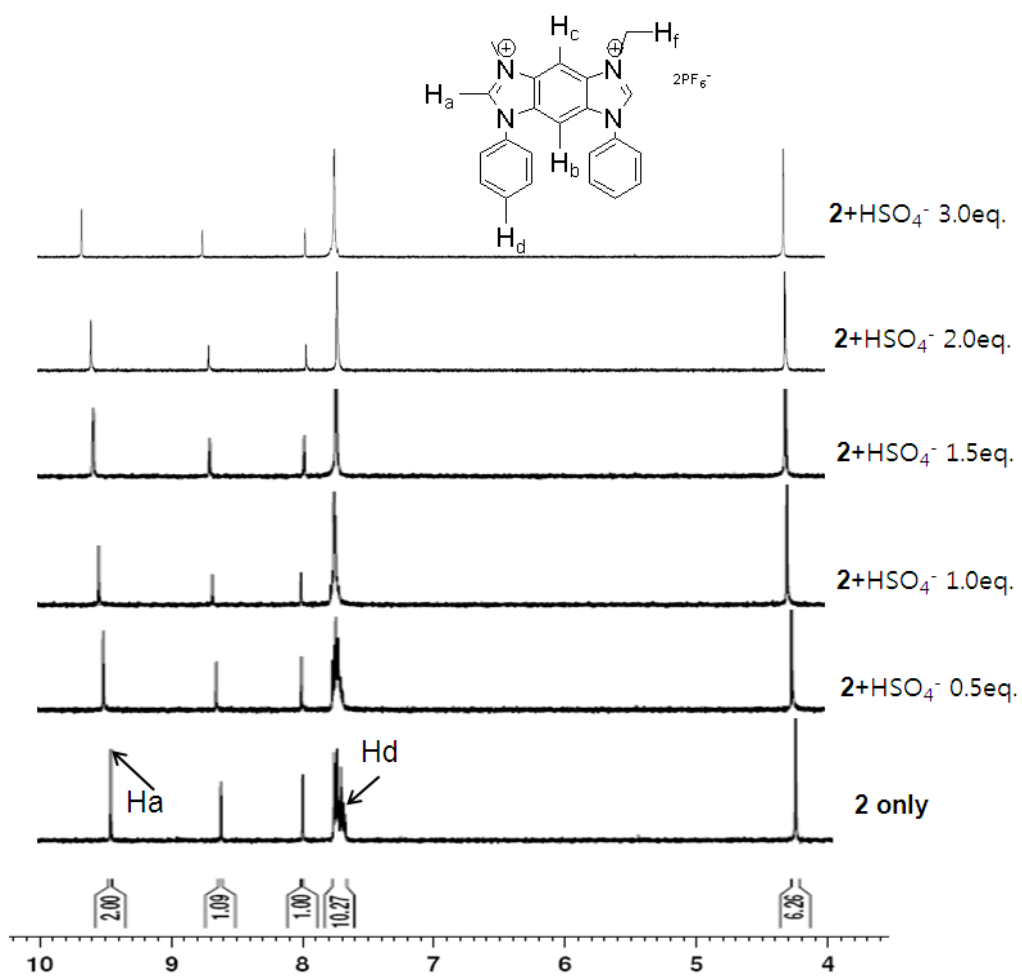


Fig S11. ¹H-NMR spectra of **2** (2 mM) upon the addition of HSO₄⁻ in CD₃CN at room temperature.

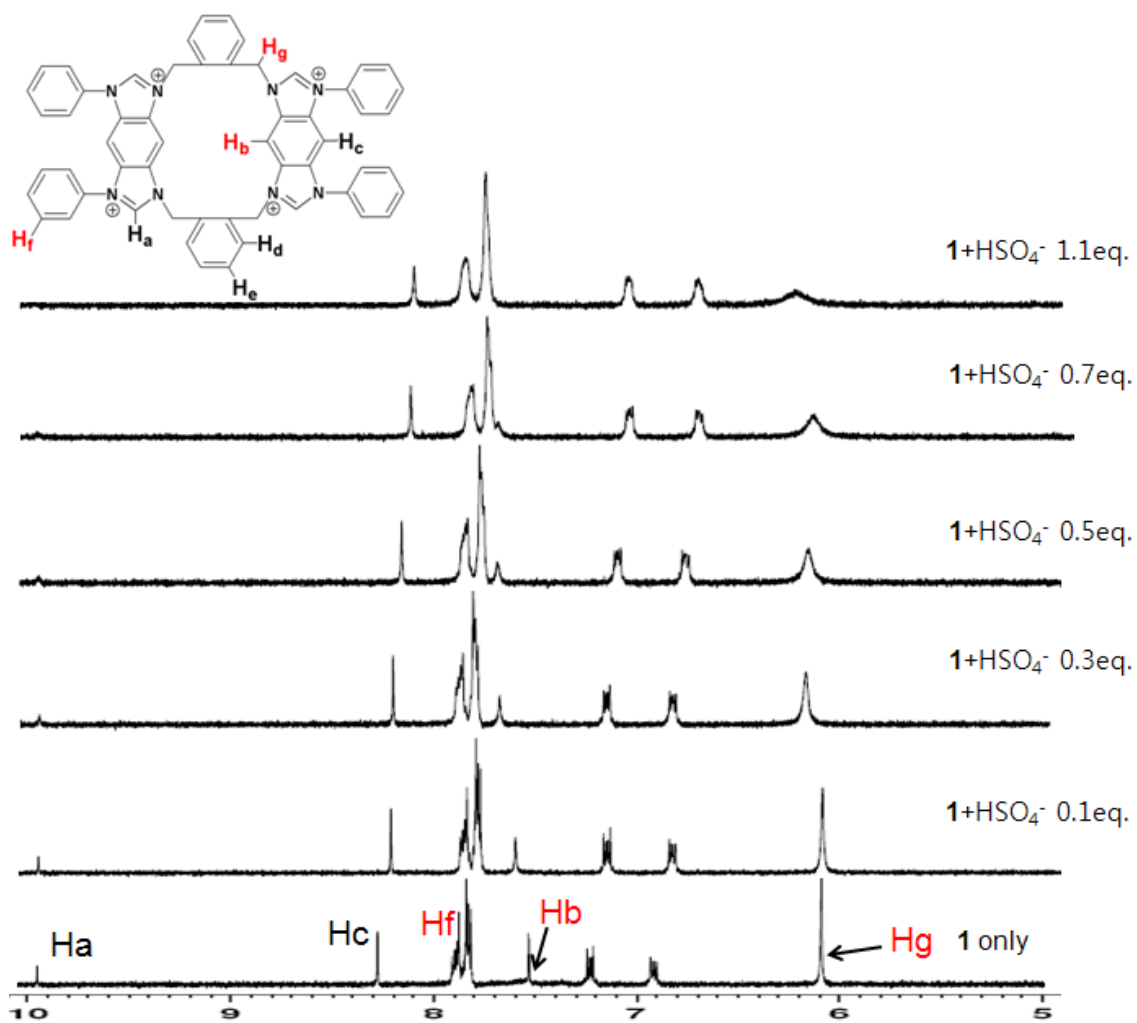


Fig S12. $^1\text{H-NMR}$ spectra of **1** (2 mM) upon the addition of HSO_4^- in $\text{CD}_3\text{CN} - \text{D}_2\text{O}$ (9:1, v/v) at room temperature.

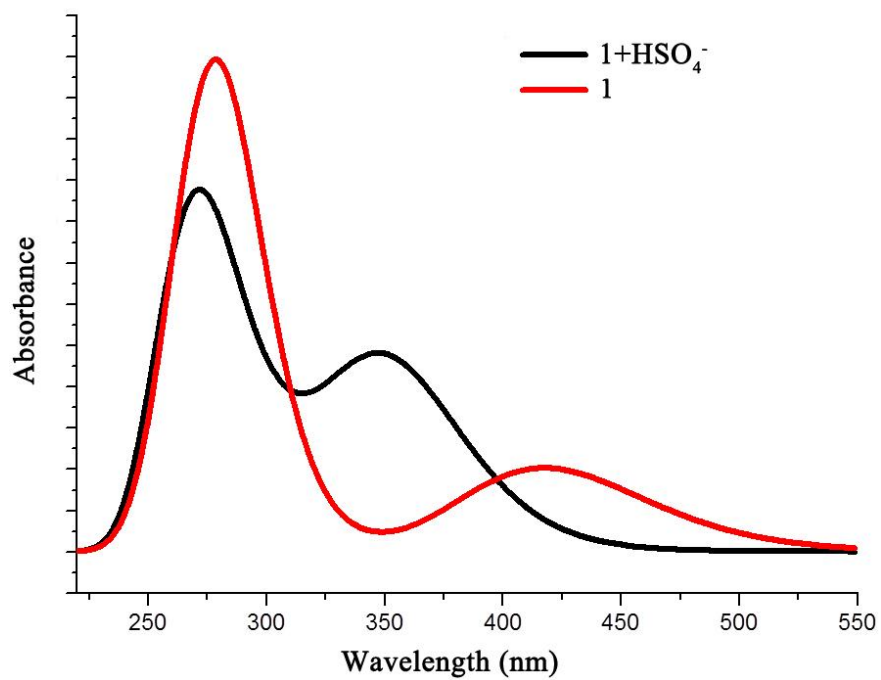
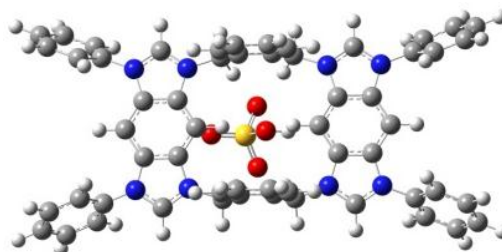


Fig S13. Simulated UV-absorbance spectra of **1** and **1+HSO₄⁻** by TDDFT calculations.

Table S1. Total energy and Cartesian coordinates of $1+\text{HSO}_4^-$ for several binding modes.

(a) $1+\text{HSO}_4^-$

Energy = -3297.32213a.u



C	-0.01268800	4.78391700	1.16650200
C	-0.12030100	3.36922200	1.16377700
C	0.03189800	5.54444600	0.00000000
C	0.11580900	4.04988800	3.25260500
H	0.13249300	6.62337700	0.00000000
N	-0.02148100	2.95409600	2.49507400
N	0.11390800	5.16314600	2.51015000
C	-0.01268800	4.78391700	-1.16650200
C	-0.12030100	3.36922200	-1.16377700
C	0.11580900	4.04988800	-3.25260500
N	-0.02148100	2.95409600	-2.49507400
N	0.11390800	5.16314600	-2.51015000
C	-0.22662700	2.61730100	0.00000000
H	-0.31638400	1.53972500	0.00000000
C	0.28512700	6.50858400	3.02551000
C	-0.75858500	7.42585700	2.88294000
C	1.48393000	6.83931300	3.66045700
C	-0.58925500	8.71152200	3.39688700
H	-1.69086100	7.13573700	2.40718800
C	1.63250000	8.12776300	4.17509500
H	2.28898500	6.11415100	3.73825300
C	0.60056600	9.06000600	4.04249900
H	-1.39254300	9.43554200	3.30512500
H	2.55671300	8.40184700	4.67352500
H	0.72267500	10.06060000	4.44507100
C	0.28512700	6.50858400	-3.02551000
C	1.48393000	6.83931300	-3.66045700

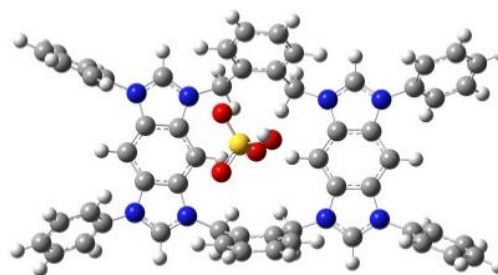
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C	1.63250000	8.12776300	-4.17509500
H	2.28898500	6.11415100	-3.73825300
C	-0.58925500	8.71152200	-3.39688700
H	-1.69086100	7.13573700	-2.40718800
C	0.60056600	9.06000600	-4.04249900
H	2.55671300	8.40184700	-4.67352500
H	-1.39254300	9.43554200	-3.30512500
H	0.72267500	10.06060000	-4.44507100
C	0.09556000	1.55145900	2.96176700
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H	0.49447100	1.60693200	3.98075600
C	0.09556000	1.55145900	-2.96176700
H	0.49447100	1.60693200	-3.98075600
H	0.86704200	1.08971700	-2.33729700
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C	-2.43571200	1.45353300	-2.97063700
C	-1.21484000	-0.64242300	-2.91038800
C	-3.65041200	0.77039600	-3.00132100
H	-2.44757100	2.53912600	-2.99248700
C	-2.44306700	-1.31234000	-2.95290200
C	-3.65336300	-0.62136100	-2.99251800
H	-4.58314600	1.32381600	-3.04450900
H	-2.46272400	-2.39750600	-2.95937900
H	-4.58908400	-1.17029900	-3.02848400
H	0.22157400	4.04662400	4.32888600
H	0.22157400	4.04662400	-4.32888600
C	-1.21376400	0.77306000	2.91939400
C	-1.21484000	-0.64242300	2.91038800
C	-2.43571200	1.45353300	2.97063700
C	-2.44306700	-1.31234000	2.95290200
C	-3.65041200	0.77039600	3.00132100
H	-2.44757100	2.53912600	2.99248700
C	-3.65336300	-0.62136100	2.99251800
H	-2.46272400	-2.39750600	2.95937900
H	-4.58314600	1.32381600	3.04450900

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C	0.08936800	-1.43571300	2.94239700
H	0.49225800	-1.48638900	3.96018200
H	0.87057500	-0.99776900	2.31336500
N	-0.05407700	-2.83210500	2.48737800
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C	0.07380700	-3.92659600	3.24622000
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C	1.40091600	-6.73954400	3.61493100
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C	0.07380700	-3.92659600	-3.24622000
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C	0.49009400	-8.94429100	4.02373300
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C	-0.87334900	-7.28495700	-2.90634900

H	0.60659300	-9.94750500	4.42148000
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H	2.22089800	-6.02891800	-3.66499100
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H	-1.81255800	-6.97804200	-2.45552900
C	0.49009400	-8.94429100	-4.02373300
H	2.47636400	-8.32207400	-4.59360700
H	-1.53018700	-9.28378100	-3.34535900
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O	2.36635600	-2.03740400	0.00000000
O	3.52735400	-0.21802900	-1.26082500
O	1.41206700	0.28338600	0.00000000
H	1.78285600	1.18259900	0.00000000

(b) $1+\text{HSO}_4^-$

Energy = -3297.31816 a.u



C	0.48283900	4.76885700	1.16551800
C	0.62644600	3.35805200	1.16112000
C	0.38434000	5.52581400	0.00000000
C	0.63890500	4.05748100	3.25870300
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N	0.72136200	2.95737200	2.50011100
N	0.48033500	5.15703100	2.51227100

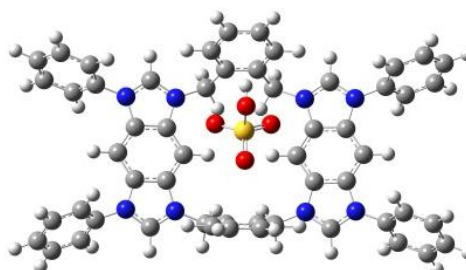
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N	0.72136200	2.95737200	-2.50011100
N	0.48033500	5.15703100	-2.51227100
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H	0.61824100	1.51486000	0.00000000
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C	1.35666000	7.42714500	2.82695000
C	-0.83100600	6.82890300	3.73636800
C	1.20875200	8.71415500	3.34434500
H	2.25993900	7.14150900	2.29590200
C	-0.95933700	8.11891700	4.25280300
H	-1.62280400	6.09681100	3.86618400
C	0.05608000	9.05777400	4.05621300
H	2.00006100	9.44326400	3.20230900
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C	1.35666000	7.42714500	-2.82695000
C	-0.83100600	6.82890300	-3.73636800
C	1.20875200	8.71415500	-3.34434500
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H	1.55815700	1.11911200	2.13836200
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H	1.55815700	1.11911200	-2.13836200
C	-0.12651300	0.75251000	-3.47161800

C	-1.26729700	1.38519800	-3.97576600
C	-0.04364400	-0.65948400	-3.52505500
C	-2.31617100	0.66187900	-4.53725600
H	-1.35724700	2.46551100	-3.92121600
C	-1.10082600	-1.36593600	-4.10281000
C	-2.22751700	-0.72419500	-4.60767000
H	-3.19187700	1.17968100	-4.91523300
H	-1.08286300	-2.44973200	-4.12533900
H	-3.03401500	-1.30765400	-5.03953200
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H	0.71399400	4.07274200	-4.33729900
C	-0.12651300	0.75251000	3.47161800
C	-0.04364400	-0.65948400	3.52505500
C	-1.26729700	1.38519800	3.97576600
C	-1.10082600	-1.36593600	4.10281000
C	-2.31617100	0.66187900	4.53725600
H	-1.35724700	2.46551100	3.92121600
C	-2.22751700	-0.72419500	4.60767000
H	-1.08286300	-2.44973200	4.12533900
H	-3.19187700	1.17968100	4.91523300
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C	1.20049200	-1.40235000	3.03239600
H	1.94262400	-1.49713600	3.83401400
H	1.68887900	-0.86771200	2.21767300
N	0.98643300	-2.77524900	2.51107300
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C	0.69423200	-4.56894400	1.16506300
C	1.09597500	-2.43769600	0.00000000
N	0.63754500	-4.96019500	2.50845300
H	0.83126500	-3.88885300	4.34240600
C	0.57591700	-5.32105600	0.00000000
C	0.92935400	-3.17132400	-1.16644800

H	1.17215100	-1.36070800	0.00000000
C	0.43586700	-6.30245100	3.01853300
H	0.40590800	-6.39087600	0.00000000
C	0.69423200	-4.56894400	-1.16506300
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C	-0.81166600	-6.90748900	2.85009600
N	0.63754500	-4.96019500	-2.50845300
C	0.81892400	-3.87082800	-3.26187700
C	1.28120700	-8.22876900	4.17457600
H	2.45596200	-6.45788400	3.77116300
C	-1.00061300	-8.19443400	3.35435700
H	-1.62097000	-6.37608200	2.35795600
C	0.43586700	-6.30245100	-3.01853300
H	0.83126500	-3.88885300	-4.34240600
C	0.04095800	-8.85137000	4.01538300
H	2.08901900	-8.74170000	4.68659400
H	-1.96579800	-8.67780400	3.24132200
C	1.49018700	-6.94460600	-3.67018200
C	-0.81166600	-6.90748900	-2.85009600
H	-0.11548100	-9.85061600	4.40947700
C	1.28120700	-8.22876900	-4.17457600
H	2.45596200	-6.45788400	-3.77116300
C	-1.00061300	-8.19443400	-3.35435700
H	-1.62097000	-6.37608200	-2.35795600
C	0.04095800	-8.85137000	-4.01538300
H	2.08901900	-8.74170000	-4.68659400
H	-1.96579800	-8.67780400	-3.24132200
H	-0.11548100	-9.85061600	-4.40947700
S	-1.65370800	-0.82071100	0.00000000
O	-1.86419800	-1.58622300	-1.24078700
O	-0.36366100	-0.04264000	0.00000000
O	-1.86419800	-1.58622300	1.24078700
O	-2.74056100	0.42725900	0.00000000
H	-3.63140700	0.02901500	0.00000000

(c) 1+HSO₄⁻

Energy = -3297.30329a.u



C	-1.32506000	-0.57424500	4.66615100
C	-1.33911800	-0.75288300	3.25778600
C	-0.15453800	-0.52753400	5.41409000
C	-3.42989800	-0.63045000	3.97877300
H	-0.14028700	-0.39887400	6.48950000
N	-2.68750500	-0.78552500	2.87535200
N	-2.66616900	-0.49749600	5.06776700
C	1.00084000	-0.67376800	4.64953300
C	0.99324800	-0.83281600	3.24164100
C	3.08967000	-0.86567200	3.94664300
N	2.33341200	-0.93616900	2.84424200
N	2.34397500	-0.69443500	5.04287800
C	-0.18357800	-0.87838400	2.50007000
H	-0.18543900	-0.91593600	1.42282200
C	-3.16447800	-0.32895500	6.41855000
C	-3.93614600	-1.34458500	6.98609600
C	-2.87083200	0.85177400	7.10491000
C	-4.43430900	-1.16359600	8.27684500
H	-4.13185900	-2.26256800	6.43926800
C	-3.36984100	1.01176300	8.39770100
H	-2.28887800	1.63754700	6.63228700
C	-4.15045500	0.00938200	8.98025200
H	-5.03802800	-1.94198400	8.73226500
H	-3.15964800	1.92617100	8.94323100

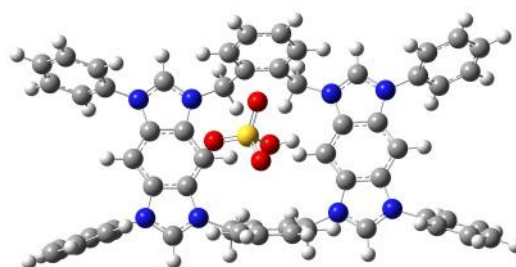
H	-4.54007400	0.14409600	9.98436500
C	2.86190300	-0.54848400	6.38983100
C	2.63203200	-1.56718800	7.31734700
C	3.58264400	0.60190200	6.71512400
C	3.14609300	-1.42374000	8.60620200
H	2.08483700	-2.46125400	7.03323400
C	4.09573700	0.72557700	8.00696700
H	3.72752200	1.38922200	5.98100100
C	3.87728000	-0.28286700	8.94857100
H	2.98559900	-2.20930400	9.33769000
H	4.66102800	1.61197000	8.27636400
H	4.27933500	-0.18076200	9.95164500
C	-3.22188500	-0.95974900	1.50685100
H	-2.55148600	-1.67462300	1.02221000
H	-4.18218900	-1.47543700	1.62575500
C	2.82937100	-1.25597000	1.48368000
H	3.49549700	-2.11962300	1.60097200
H	1.94880500	-1.61058700	0.95263000
C	3.52736000	-0.14217400	0.70752200
C	4.23599400	0.85669000	1.38092400
C	3.52736000	-0.14217400	-0.70752200
C	4.93563400	1.84821800	0.69696600
H	4.22138700	0.89762400	2.46471200
C	4.23599400	0.85669000	-1.38092400
C	4.93563400	1.84821800	-0.69696600
H	5.47298300	2.61283500	1.24892000
H	4.22138700	0.89762400	-2.46471200
H	5.47298300	2.61283500	-1.24892000
H	-4.51073700	-0.60749800	3.99678600
H	4.16578700	-0.96359900	3.96719900
C	-3.37849800	0.33153500	0.70761400
C	-3.37849800	0.33153500	-0.70761400
C	-3.62654800	1.53136300	1.38087900
C	-3.62654800	1.53136300	-1.38087900
C	-3.86333800	2.71875700	0.69492800
H	-3.61589300	1.55779600	2.46596100

C	-3.86333800	2.71875700	-0.69492800
H	-3.61589300	1.55779600	-2.46596100
H	-4.03528300	3.63739300	1.24579300
H	-4.03528300	3.63739300	-1.24579300
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H	3.49549700	-2.11962300	-1.60097200
H	1.94880500	-1.61058700	-0.95263000
C	-3.22188500	-0.95974900	-1.50685100
H	-4.18218900	-1.47543700	-1.62575500
H	-2.55148600	-1.67462300	-1.02221000
N	-2.68750500	-0.78552500	-2.87535200
C	-1.33911800	-0.75288300	-3.25778600
C	-3.42989800	-0.63045000	-3.97877300
C	-1.32506000	-0.57424500	-4.66615100
C	-0.18357800	-0.87838400	-2.50007000
N	-2.66616900	-0.49749600	-5.06776700
H	-4.51073700	-0.60749800	-3.99678600
C	-0.15453800	-0.52753400	-5.41409000
C	0.99324800	-0.83281600	-3.24164100
H	-0.18543900	-0.91593600	-1.42282200
C	-3.16447800	-0.32895500	-6.41855000
H	-0.14028700	-0.39887400	-6.48950000
C	1.00084000	-0.67376800	-4.64953300
N	2.33341200	-0.93616900	-2.84424200
C	-3.93614600	-1.34458500	-6.98609600
C	-2.87083200	0.85177400	-7.10491000
N	2.34397500	-0.69443500	-5.04287800
C	3.08967000	-0.86567200	-3.94664300
C	-4.43430900	-1.16359600	-8.27684500
H	-4.13185900	-2.26256800	-6.43926800
C	-3.36984100	1.01176300	-8.39770100
H	-2.28887800	1.63754700	-6.63228700
C	2.86190300	-0.54848400	-6.38983100
H	4.16578700	-0.96359900	-3.96719900
C	-4.15045500	0.00938200	-8.98025200
H	-5.03802800	-1.94198400	-8.73226500

H	-3.15964800	1.92617100	-8.94323100
C	3.58264400	0.60190200	-6.71512400
C	2.63203200	-1.56718800	-7.31734700
H	-4.54007400	0.14409600	-9.98436500
C	4.09573700	0.72557700	-8.00696700
H	3.72752200	1.38922200	-5.98100100
C	3.14609300	-1.42374000	-8.60620200
H	2.08483700	-2.46125400	-7.03323400
C	3.87728000	-0.28286700	-8.94857100
H	4.66102800	1.61197000	-8.27636400
H	2.98559900	-2.20930400	-9.33769000
H	4.27933500	-0.18076200	-9.95164500
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O	0.94467800	1.17665200	1.22824800
O	-0.81067700	2.45493600	0.00000000
O	0.94467800	1.17665200	-1.22824800
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H	2.41935100	3.01256500	0.00000000

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C	0.75584300	4.05066800	3.26139500

H	0.38478800	6.57203200	0.00000000
N	0.87343200	2.94715300	2.51158900
N	0.59805700	5.14213200	2.50649200
C	0.62758800	4.74346200	-1.16481200
C	0.80029200	3.33389200	-1.16784800
C	0.75584300	4.05066800	-3.26139500
N	0.87343200	2.94715300	-2.51158900
N	0.59805700	5.14213200	-2.50649200
C	0.88669800	2.58018500	0.00000000
H	0.93185200	1.49758000	0.00000000
C	0.41883800	6.49105800	3.01462500
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C	-0.77447700	6.81342000	3.66333700
C	1.27390700	8.70632900	3.35506800
H	2.37745600	7.13478300	2.35986700
C	-0.93087200	8.10497800	4.16803600
H	-1.56758400	6.07792600	3.76245300
C	0.08892000	9.04717400	4.01343500
H	2.06784700	9.43826800	3.24632700
H	-1.85046100	8.37306600	4.67814400
H	-0.03861400	10.04965800	4.40961700
C	0.41883800	6.49105800	-3.01462500
C	1.45015900	7.41830400	-2.84910000
C	-0.77447700	6.81342000	-3.66333700
C	1.27390700	8.70632900	-3.35506800
H	2.37745600	7.13478300	-2.35986700
C	-0.93087200	8.10497800	-4.16803600
H	-1.56758400	6.07792600	-3.76245300
C	0.08892000	9.04717400	-4.01343500
H	2.06784700	9.43826800	-3.24632700
H	-1.85046100	8.37306600	-4.67814400
H	-0.03861400	10.04965800	-4.40961700
C	1.11689400	1.58141800	3.03620400
H	1.73032700	1.09185300	2.27722900
H	1.76047000	1.71224300	3.91424700
C	1.11689400	1.58141800	-3.03620400

H	1.76047000	1.71224300	-3.91424700
H	1.73032700	1.09185300	-2.27722900
C	-0.13445500	0.78024500	-3.37757500
C	-1.28955100	1.44212500	-3.80434300
C	-0.11571000	-0.63444400	-3.38017200
C	-2.41728200	0.74260000	-4.22617900
H	-1.32933200	2.52760200	-3.79878700
C	-1.25435900	-1.31963100	-3.80877200
C	-2.39869300	-0.64681700	-4.22744900
H	-3.30554900	1.28180000	-4.53813300
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H	0.79924200	4.06930600	-4.34184000
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C	-1.28955100	1.44212500	3.80434300
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C	-2.41728200	0.74260000	4.22617900
H	-1.32933200	2.52760200	3.79878700
C	-2.39869300	-0.64681700	4.22744900
H	-1.27656400	-2.40387600	3.78444000
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H	-3.27501700	-1.20843200	4.53214300
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H	1.74319500	-0.89789200	-2.26167700
C	1.15300700	-1.40526000	3.02742300
H	1.80714800	-1.50735000	3.90167800
H	1.74319500	-0.89789200	2.26167700
N	0.95012200	-2.77355500	2.50783500
C	0.92048300	-3.16513400	1.16326300
C	0.82807600	-3.87472800	3.25991200
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N	0.70865800	-4.96887400	2.50325600

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C	0.92048300	-3.16513400	-1.16326300
H	0.96962500	-1.32822700	0.00000000
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C	0.76486500	-4.57410700	-1.16140000
N	0.95012200	-2.77355500	-2.50783500
C	1.60995000	-7.19434500	3.01359000
C	-0.73828700	-6.69453000	3.47238600
N	0.70865800	-4.96887400	-2.50325600
C	0.82807600	-3.87472800	-3.25991200
C	1.42205800	-8.48501500	3.50873200
H	2.58311200	-6.87077300	2.65613300
C	-0.90733000	-7.98821800	3.96750400
H	-1.56952200	-5.99627600	3.43979200
C	0.52288000	-6.31803900	-3.00736100
H	0.83993900	-3.89004700	-4.34083700
C	0.16863400	-8.87907500	3.98513200
H	2.25708400	-9.17798100	3.53053200
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C	-0.73828700	-6.69453000	-3.47238600
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C	-0.90733000	-7.98821800	-3.96750400
H	-1.56952200	-5.99627600	-3.43979200
C	1.42205800	-8.48501500	-3.50873200
H	2.58311200	-6.87077300	-2.65613300
C	0.16863400	-8.87907500	-3.98513200
H	-1.87977600	-8.29779600	-4.33673000
H	2.25708400	-9.17798100	-3.53053200
H	0.03086400	-9.88345600	-4.37315000
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O	-2.93030200	-0.42406400	-1.24752200
O	-1.67210900	-2.18846400	0.00000000
O	-2.93030200	-0.42406400	1.24752200

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H	-1.20842200	1.05140800	0.00000000