

Electronic Supporting Information.

Borenum Cations Derived from BODIPY Dyes

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General Experimental Procedures

All operations were performed under a purified argon atmosphere using glovebox or vacuum line techniques. Toluene and hexanes solvents were dried and purified by passing through activated alumina, and vacuum distilled from Na/benzophenone. Et₂O was dried over Na/K alloy and vacuum distilled from Na/benzophenone. Pentane was dried and vacuum distilled from Na/benzophenone. NEt₃ and CH₂Cl₂ were dried over and distilled from CaH₂. Phenylacetylene was purchased from Aldrich and passed through a column of alumina immediately prior to use. [Ph₃C][B(C₆F₅)₄] was generously given by Nova Chemicals Inc. Silica gel column chromatography was carried out on Geduran Silica 60 silica gel (particle size 40-63 μm). Diisobutylaluminum chloride (25 % w/w in hexanes) and lithium deuteride were purchased from Alfa Aesar and used as received. Diisobutylaluminum hydride (DIBAL-H, 1.0 M in CH₂Cl₂) was purchased from Aldrich and used as received. Et₃SiH was purchased from Aldrich and vacuum distilled prior to use. *trans*-crotonaldehyde was purchased from Aldrich and distilled under argon prior to use. All NMR spectra were recorded in dry, oxygen-free CD₂Cl₂ on a Bruker AMX-300 MHz (operating at 300 MHz (¹H), 46 MHz (²H), 96 MHz (¹¹B), 75 MHz (¹³C) or 282 MHz (¹⁹F)) at 25 °C unless otherwise specified. Chemical shifts were reported relative to residual solvent signal (¹H, ²H and ¹³C{¹H}), BF₃•OEt₂ (¹¹B) and C₆F₆ (¹⁹F) standards. Infrared spectra (FTIR) were recorded on a Nicolet Nexus 470 as thin film (KBr pellets). Low-resolution mass spectra were obtained on a Bruker Esquire 3000 spectrometer operating in electrospray ionization (ESI) mode. Fluorescence spectra were obtained on a Yvon-Jobin spectrophotometer with excitation and emission set to 1.0 nm bandpass, and λ_{max} values for absorption taken from the excitation spectra. Fluorescence quantum yield values were measured in CH₂Cl₂ and reported relative to rhodamine 6G in methanol (φ_f = 0.80),^{1a} corrected for the difference in solvent refractive index.^{1b} X-ray crystallographic analyses were performed on suitable crystals coated in perfluoropolyalkyl ether oil (1600 cSt) and mounted on a Nonius Kappa CCD diffractometer. Elemental analyses were performed on a Perkin Elmer Model 2400 series II by Johnson Li (University of Calgary).

[Et₃Si][B(C₆F₅)₄] was prepared according to Scott et al. and immediately used in the next step.² N,N'-difluoroboryl-4,4'-diethyl-3,3',5,5'-tetramethyldipyromethene (**1**) was synthesized as previously reported³ by using toluene and NEt₃ as solvent and base respectively. Diisobutylaluminum deuteride (DIBAL-D) was prepared according to Eisch et al.⁴

Methods

The determination of the Lewis acidity was made according to a modification of Childs' method.⁵ The studied compound was loaded in a thick wall 5 mm J Young NMR tube. The correct amount of *trans*-crotonaldehyde was added to the NMR tube to have an

excess of approximately 75 % of the borenium compound. CD_2Cl_2 was then condensed at $-78\text{ }^\circ\text{C}$ and the NMR spectra were recorded at $-20\text{ }^\circ\text{C}$.

Syntheses

Synthesis of [**2-F**]: Under an argon atmosphere, **1** (0.304 g, 1.0 mmol) and $[\text{Et}_3\text{Si}][\text{B}(\text{C}_6\text{F}_5)_4]$ (0.936 g, 1.18 mmol) were mixed together. The flask was evacuated and CH_2Cl_2 ($\approx 50\text{ mL}$) was condensed into the flask. The purple solution was stirred 15 minutes at room temperature and solvent and other volatile compounds were removed *in vacuo*. Pentane ($\approx 50\text{ mL}$) was condensed onto the residue and was sonicated for 30 minutes. The solid was filtered, washed with pentane and volatiles were removed *in vacuo* to afford a dark purple solid. Two crops of suitable X-ray crystals obtained from a concentrated CH_2Cl_2 solution layered with hexanes gave 0.856 g (0.89 mmol) of [**1-F**] (yield: 89 %). ^1H NMR (CD_2Cl_2 , 300 MHz, 203 K): 7.42 (s, 1H), 2.50 (s, 6H), 2.38 (q, 4H, $^3J_{\text{HH}} = 7.6\text{ Hz}$), 2.29 (s, 6H), 1.00 (t, 6H, $^3J_{\text{HH}} = 7.5\text{ Hz}$); partial $^{13}\text{C}\{^1\text{H}\}$ NMR (CD_2Cl_2 , 75 MHz, 203 K): 159.40, 153.63, 139.04, 136.00, 121.29, 19.28, 17.34, 13.89, 11.25 (signals for the $\text{B}(\text{C}_6\text{F}_5)_4$ anion were not assigned); ^{19}F NMR (CD_2Cl_2 , 282 MHz, 203 K): -118.4 (s, broad, 1F, BF), -131.6 (s, 2F), -160.9 (t, 1F, $^3J_{\text{FF}} = 28\text{ Hz}$), -164.9 (m, 2F); ^{11}B NMR (CD_2Cl_2 , 96 MHz, 203 K) 1.2 (broad, BF), -15.8 (s, [$\text{B}(\text{C}_6\text{F}_5)_4$]). λ_{max} : 413, 592 nm; λ_{em} : 609. Anal. Calcd for $\text{C}_{41}\text{H}_{23}\text{F}_{21}\text{B}_2\text{N}_2$: C, 51.07; H, 2.40; N, 2.91. Found: C, 51.09; H, 2.67; N, 2.92.

Synthesis of [**2-H**]: Under an argon atmosphere, a CH_2Cl_2 solution of DIBAL-H (0.115 mL, 0.115 mmol) was added to [**2-F**] (111 g, 0.115 mmol) and the solution was diluted with CH_2Cl_2 (20 mL). The solution was stirred 15 minutes and the solvent and other volatile byproducts were removed *in vacuo*. Pentane ($\approx 20\text{ mL}$) was condensed onto the residue and was sonicated for 30 minutes. The solid was decanted and dried *in vacuo* to afford a dark blue solid. Suitable X-ray crystals obtained from a concentrated CH_2Cl_2 solution layered with hexanes gave 92 g (0.097 mmol) of [**2-H**] (yield: 85 %). ^1H NMR (CD_2Cl_2 , 300 MHz): 7.40 (s, 1H), 2.55 (s, 6H), 2.45 (q, 4H, $^3J_{\text{HH}} = 7.6\text{ Hz}$), 2.33 (s, 6H), 1.11 (t, 6H, $^3J_{\text{HH}} = 7.6\text{ Hz}$); partial $^{13}\text{C}\{^1\text{H}\}$ NMR (CD_2Cl_2 , 75 MHz): 160.43, 154.04, 139.18, 135.06, 121.72, 17.65, 13.88, 12.71, 11.15 (signals for the $\text{B}(\text{C}_6\text{F}_5)_4$ anion were not assigned); ^{19}F NMR (CD_2Cl_2 , 282 MHz): -133.1 (s, 2F), -163.7 (t, 1F, $^3J_{\text{FF}} = 28\text{ Hz}$), -167.5 (m, 2F); ^{11}B NMR (CD_2Cl_2 , 96 MHz): 24.0 (broad, BH), -16.9 (s, [$\text{B}(\text{C}_6\text{F}_5)_4$]). λ_{max} : 409, 589 nm; λ_{em} : 599. Anal. Calcd for $\text{C}_{41}\text{H}_{24}\text{F}_{20}\text{B}_2\text{N}_2$: C, 52.04; H, 2.56; N, 2.96. Found: C, 51.35 ; H, 2.63; N, 2.90.

Synthesis of [**2-D**]: Performed according to the preparation of [**2-H**] by adding the appropriate amount of a 1 M CH_2Cl_2 solution of DIBAL-D. Yield: 89 %. ^2H NMR (CH_2Cl_2 , 46 MHz): 7.45 (broad).

Synthesis of [**3-H**]: Under an argon atmosphere, [**2-H**] (80 mg, 0.085 mmol) and DMAP (11 g, 0.085 mmol) were mixed together. CH_2Cl_2 ($\approx 20\text{ mL}$) was condensed onto the solids and the solution was stirred 15 minutes at room temperature. The solvent was removed *in vacuo* and pentane ($\approx 20\text{ mL}$) was condensed onto the oily residue. The suspension was sonicated 15 minutes and volatiles were decanted to leave 51 mg (0.048

mmol) of an orange-red powder (yield: 56 %). $^1\text{H}\{^{11}\text{B}\}$ NMR (CD_2Cl_2 , 300 MHz): 7.70 (d, 2H, $^3J_{\text{HH}} = 7.6$ Hz), 7.31 (s, 1H), 6.56 (d, 2H, $^3J_{\text{HH}} = 7.6$ Hz), 4.40 (s, BH), 3.10 (s, 6H), 2.38 (q, 4H, $^3J_{\text{HH}} = 7.6$ Hz), 2.25 (s, 6H), 2.13 (s, 6H), 1.01 (t, 6H, $^3J_{\text{HH}} = 7.6$ Hz); ^{11}B NMR (CD_2Cl_2 , 96 MHz): -1.9 ppm (d, BH, $^1J_{\text{BH}} = 96$ Hz), -15.4 (s, $[\text{B}(\text{C}_6\text{F}_5)_4]$); $^{11}\text{B}\{^1\text{H}\}$ NMR (CD_2Cl_2 , 96 MHz): -1.6 (s, broad, BH), -15.0 (s, $[\text{B}(\text{C}_6\text{F}_5)_4]$); partial $^{13}\text{C}\{^1\text{H}\}$ NMR (CD_2Cl_2 , 75 MHz): 175.30, 155.43, 144.00 (DMAP), 138.60, 133.54, 132.03, 120.77, 108.00 (DMAP), 40.24 (DMAP-NMe₂), 17.82, 14.79, 12.90, 9.87 (signals for the $\text{B}(\text{C}_6\text{F}_5)_4$ anion were not assigned); ^{19}F NMR (CD_2Cl_2 , 282 MHz): -133.12 (s, 2F), -163.72 (t, 1F, $^3J_{\text{FF}} = 20$ Hz), -167.54 (m, 2F). ESI⁺ (*m/z*, nature of peak): 388.97, $[\text{M}]^+$; 266.94, $[[\text{M}]-\text{DMAP}]^+$; 122.91, $[\text{DMAP}+\text{H}]^+$. λ_{max} : 360, 532 nm; λ_{em} : 542. $\phi_{\text{fl}} = 0.81$. Anal. Calcd for $\text{C}_{48}\text{H}_{34}\text{F}_{20}\text{B}_2\text{N}_4$: C, 53.96; H, 3.21; N, 5.24. Found: C, 53.61; H, 3.49; N, 5.02.

Synthesis of **[3-D]**: Performed according to the preparation of **[3-H]**. Yield: 59 %. ^2H NMR (CD_2Cl_2 , 46 MHz): 4.36 (broad).

Molecular Orbital Calculations (MO)

MO calculations employed the Gaussian03 suite of programs.⁶ For the B-H and B-F cations involved in this study, the B3LYP/6-311+G** method was used for both optimization and NICS(1) calculations. Structures were fully optimized and verified as ground-states. Two conformations exist for each cation, with the ethyl-substituent of these on the same or opposite faces, the latter marginally more stable and in agreement with the X-ray data, $E_{\text{B-H}} = -796.717020$, $E_{\text{B-F}} = -896.052223$ Hartrees. NICS(1) calculations⁷ were carried out for both the 5- and 6-membered rings, and the values reported are averages of the quite similar +1 and -1 z-axis values. C_4N -ring = -9.8 (**2-H**), -4.3 (**2-F**); $\text{C}_3\text{N}_2\text{B}$ -ring = +0.70 (**2-H**); +0.3 (**2-F**).

X-Ray Crystallography.

Data were collected on a Bruker P4/RA/SMART 1000 CCD diffractometer⁸ using Mo $K\alpha$ radiation at -80°C . Unit cell parameters were obtained from a least-squares refinement of the setting angles of the number of reflections from the data collection. An empirical absorption correction was applied to the data through use of the *SADABS* procedure. The structures were solved using the direct methods program *SHELXS-86*,⁹ and full-matrix least-squares refinement on F^2 was completed using the program *SHELXL-93*.¹⁰

Supporting Information References

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(8) Programs for diffractometer operation, data collection, data reduction and absorption correction were those supplied by Bruker.

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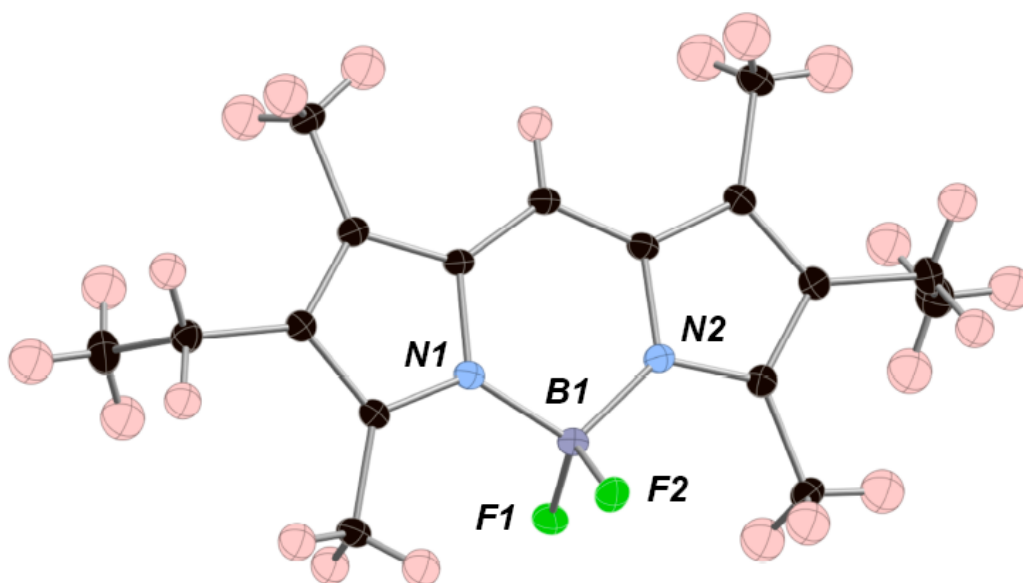


Figure S1. Thermal Ellipsoid Diagram of **1**. Selected bond distances (Å): F1-B1, 1.3891(19); F2-B1, 1.3938(19); N1-B1, 1.552(2); N2-B1, 1.554(2). Selected bond angles (°): F1-B1-F2, 108.79(12); F1-B1-N1, 110.40(12); F2-B1-N1, 110.04(12); F1-B1-N2, 110.35(12); F2-B1-N2, 110.22(12); N1-B1-N2, 107.05(11). Crystal data for **1**

$C_{17}H_{23}BF_2N_2$, $M = 304.18$, $T = 173(2)$ K, space group $P-1$, triclinic, $a = 8.554(2)$, $b = 9.258(4)$, $c = 12.068(5)$, $\alpha = 100.439(18)$, $\beta = 103.76(2)$, $\gamma = 113.981(19)$, $V = 805.5(5)$ Å³, $Z = 2$, $D_c = 1.254$ g cm⁻³, $\mu(\text{Mo-K}\alpha) = 0.089$ mm⁻¹, 6894 reflections measured, 3646 unique ($R_{\text{int}} = 0.0226$) which were used in all calculations. The final R and $wR(F^2)$ were 0.0430 and 0.1069, respectively.

Table S1. Final Coordinates for Optimized **2-F**

Atomic No.	x	y	z
7	-1.220843	-0.557360	0.110691
6	-1.206179	0.854318	0.108331
6	-2.537469	1.302417	0.230109
6	-2.540299	-0.968518	0.232441
6	-3.363179	0.158006	0.307761
5	0.000015	-1.312007	-0.000001
7	1.220854	-0.557334	-0.110707
6	2.540322	-0.968464	-0.232445
6	3.363177	0.158075	-0.307766
6	2.537443	1.302471	-0.230109
6	1.206163	0.854344	-0.108333
6	-0.000016	1.533117	0.000002
1	-0.000027	2.615084	0.000001
6	2.928252	-2.404255	-0.272561
1	2.449728	-2.923736	-1.107745
1	2.626440	-2.923393	0.641688
1	4.006911	-2.501435	-0.379933
6	2.988733	2.723153	-0.282738
1	3.504155	2.929043	-1.226042
1	3.699259	2.936558	0.520983
1	2.160513	3.426293	-0.194096
6	4.862831	0.155658	-0.423610
1	5.176919	1.050235	-0.968336
1	5.182273	-0.691828	-1.036099
6	5.582827	0.107100	0.936985
1	6.665448	0.124961	0.795235
1	5.330941	-0.802143	1.488680
1	5.312482	0.960985	1.563171
6	-2.988787	2.723089	0.282781
1	-2.160613	3.426249	0.193866
1	-3.503943	2.929014	1.226225
1	-3.699550	2.936430	-0.520744
6	-2.928202	-2.404317	0.272544
1	-2.626245	-2.923470	-0.641647
1	-4.006874	-2.501517	0.379765
1	-2.449788	-2.923766	1.107811
6	-4.862832	0.155566	0.423615

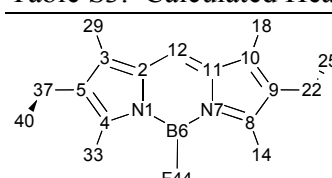
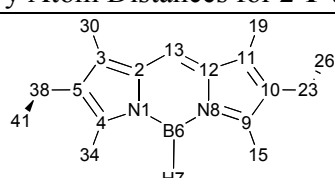
1	-5.176915	1.050051	0.968498
1	-5.182270	-0.692023	1.035963
6	-5.582837	0.107232	-0.936984
1	-5.312525	0.961234	-1.563023
1	-6.665458	0.125037	-0.795223
1	-5.330929	-0.801907	-1.488840
9	0.000025	-2.639668	-0.000021

Table S2. Final Coordinates for Optimized **2-H**

Atomic No.	x	y	z
7	1.208324	-0.690749	-0.109334
6	1.204122	0.719327	-0.108869
6	2.537976	1.159828	-0.232344
6	2.524701	-1.109257	-0.231215
6	3.357403	0.008351	-0.309015
5	0.000038	-1.460971	-0.000109
1	0.000129	-2.638765	-0.000178
7	-1.208260	-0.690881	0.109236
6	-2.524643	-1.109531	0.231104
6	-3.357410	0.007975	0.309007
6	-2.538047	1.159564	0.232435
6	-1.204192	0.719185	0.108939
6	-0.000055	1.402483	0.000073
1	-0.000123	2.484622	0.000140
6	-2.892076	-2.550911	0.263753
1	-2.374782	-3.077001	1.071275
1	-2.624533	-3.048959	-0.673465
1	-3.964033	-2.668044	0.412475
6	-2.999101	2.576633	0.288335
1	-3.514381	2.777302	1.232978
1	-3.713018	2.786690	-0.513394
1	-2.175656	3.285364	0.199356
6	-4.856848	-0.004505	0.425194
1	-5.177419	0.885943	0.972986
1	-5.170440	-0.856565	1.034551
6	-5.576841	-0.053749	-0.935392
1	-6.659610	-0.043394	-0.793732
1	-5.318764	-0.959827	-1.489487
1	-5.312034	0.803550	-1.559282
6	2.998864	2.576960	-0.288160
1	2.175416	3.285580	-0.198338
1	3.513385	2.777969	-1.233149
1	3.713378	2.786847	0.513077
6	2.892388	-2.550575	-0.263901
1	2.625846	-3.048435	0.673711

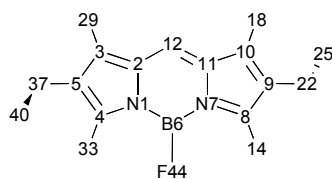
1	3.964236	-2.667521	-0.413586
1	2.374433	-3.076976	-1.070778
6	4.856843	-0.004073	-0.425176
1	5.177461	0.886833	-0.972188
1	5.170429	-0.855630	-1.035248
6	5.576788	-0.054475	0.935398
1	5.312146	0.802444	1.559880
1	6.659563	-0.044266	0.793780
1	5.318491	-0.960886	1.488845

Table S3. Calculated Heavy Atom Distances for **2-F** and **2-H**.

2-F	Distance (Å)	2-H	Distance Å
N1-C2	1.411756	N1-C2	1.410082
C2-C3	1.409948	C2-C3	1.410125
C3-C5	1.413331	C3-C5	1.415358
C4-C5	1.397090	C4-C5	1.395884
N1-C4	1.387386	N1-C4	1.386670
N1-B6	1.439528	N1-B6	1.437055
B6-F44	1.327661	B6-H7	1.177793
B6-N7	1.439526	B6-N8	1.437004
N7-C8	1.387388	N8-C9	1.386716
C8-C9	1.397088	C9-C10	1.395847
C9-C10	1.413333	C10-C11	1.415407
C10-C11	1.409948	C11-C12	1.410089
C11-C12	1.388286	C12-C13	1.388775
C2-C12	1.388284	C2-C13	1.388745
C3-C29	1.491567	C3-C30	1.491240
C4-C33	1.487816	C4-C34	1.487837
C5-C37	1.504123	C5-C38	1.503984
C37-C40	1.540121	C38-C41	1.540137
C8-C14	1.487815	C9-C15	1.487834
C9-C22	1.504123	C10-C23	1.503984
C10-C18	1.491567	C11-C19	1.491235
C22-C25	1.540121	C23-C26	1.540133

Table S4. Mulliken Population Analysis for Cation **2-F**

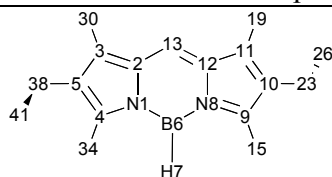


Atom	Charge	Charge with hydrogens summed into heavy atoms
1N	0.013893	0.013893
2C	0.036472	0.036472
3C	0.114078	0.114078
4C	-0.257283	-0.257283
5C	0.476421	0.476421
6B	0.802926	0.802926
7N	0.013905	0.013905
8C	-0.257313	-0.257313
9C	0.476495	0.476495
10C	0.114011	0.114011
11C	0.036415	0.036415
12C	-0.298980	-0.151412
13H	0.147569	0.000000
14C	-0.722671	-0.154597
15H	0.195280	0.000000
16H	0.200075	0.000000
17H	0.172719	0.000000
18C	-0.521100	0.004761
19H	0.192053	0.000000
20H	0.184636	0.000000
21H	0.149173	0.000000
22C	-0.284544	0.019134
23H	0.147877	0.000000
24H	0.155801	0.000000
25C	-0.526266	-0.073446
26H	0.165861	0.000000
27H	0.145359	0.000000
28H	0.141600	0.000000
29C	-0.521105	0.004757
30H	0.149172	0.000000
31H	0.192070	0.000000
32H	0.184620	0.000000
33C	-0.722667	-0.154599
34H	0.200063	0.000000
35H	0.172715	0.000000
36H	0.195290	0.000000
37C	-0.284555	0.019128
38H	0.147893	0.000000
39H	0.155790	0.000000

40C	-0.526270	-0.073452
41H	0.141597	0.000000
42H	0.165861	0.000000
43H	0.145360	0.000000
44F	-0.010295	-0.010295

Sum of Mulliken charges= 1.00000

Table S5. Mulliken Population Analysis for Cation of **2-H**



Atom	Charge	Charge with hydrogens summed into heavy atoms
1N	0.274305	0.274305
2C	-0.044241	-0.044241
3C	0.230307	0.230307
4C	-0.255025	-0.255025
5C	0.504366	0.504366
6B	0.409020	0.420715
7H	0.011695	0.000000
8N	0.274177	0.274177
9C	-0.254742	-0.254742
10C	0.504314	0.504314
11C	0.230168	0.230168
12C	-0.044229	-0.044229
13C	-0.325808	-0.176739
14H	0.149069	0.000000
15C	-0.839534	-0.283044
16H	0.185314	0.000000
17H	0.198327	0.000000
18H	0.172848	0.000000
19C	-0.515468	0.009333
20H	0.191460	0.000000
21H	0.183890	0.000000
22H	0.149451	0.000000
23C	-0.284048	0.018432
24H	0.148233	0.000000
25H	0.154247	0.000000
26C	-0.528198	-0.076454
27H	0.165410	0.000000
28H	0.144691	0.000000
29H	0.141643	0.000000
30C	-0.515613	0.009227

31H	0.149448	0.000000
32H	0.191512	0.000000
33H	0.183880	0.000000
34C	-0.839511	-0.282988
35H	0.198428	0.000000
36H	0.172870	0.000000
37H	0.185225	0.000000
38C	-0.284005	0.018536
39H	0.148252	0.000000
40H	0.154289	0.000000
41C	-0.528170	-0.076416
42H	0.141670	0.000000
43H	0.165410	0.000000
44H	0.144675	0.000000

Sum of Mulliken charges = 1.00000