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Iodine Binding with Thiophene and Furan Based Dyes for DSCs

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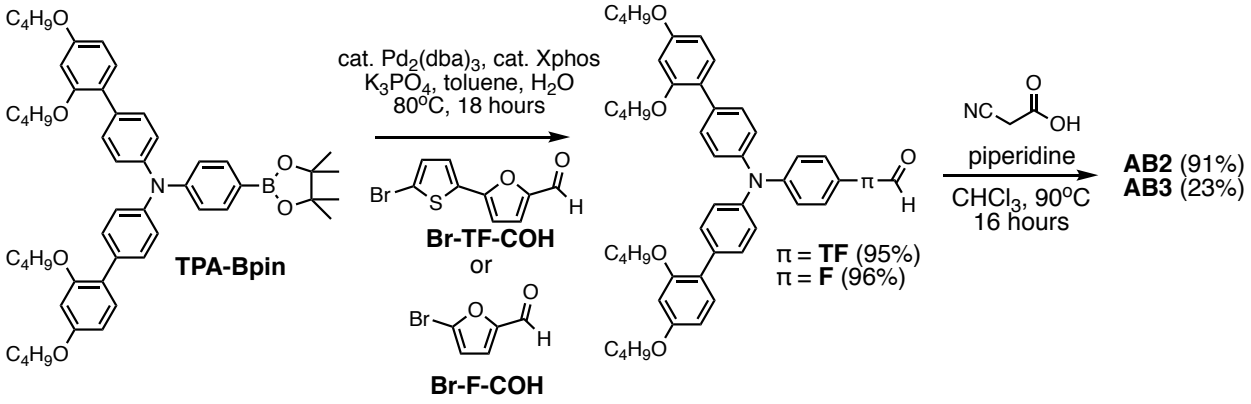
1. Synthetic Route



Scheme S1: Synthetic route to **AB2** and **AB3**.

2. Characterization Data

Table S1: Summary of optical and electrochemical properties of **AB1**, **AB2**, **AB3, D35**, **LD03** and **LD04.**

Dye	Absorbance Data					Electrochemical Data		
	λ_{onset} (nm)[a]	λ_{max} (nm)[a]	ε ($M^{-1}cm^{-1}$)[a]	λ_{max} (nm)[b]	ε ($M^{-1}cm^{-1}$)[b]	$E_{(S+/S)}$ (V)[c]	$E_{(S+/S^*)}$ (V)[d]	E_g^{opt} (eV)[e]
AB1	640	522	20000	437	25000	0.95	-0.99	1.94
AB2	633	497	15000	427	21000	1.00	-0.96	1.96
D35	613	508	32000	422	39000	1.04	-1.14	2.18
AB3	620	503	20000	423	23000	1.01	-1.13	2.14
LD03*	457	423	24000	373	28000	1.33[f]	-1.38	2.71
LD04	460	429	27000	371	36000	1.45[f]	-1.25	2.70

[a]Measured in CH_2Cl_2. [b]Measured in 0.1 M Bu_4NOH in DMF. [c]Measured with a 0.1 M Bu_4NPF_6 in CH_2Cl_2 solution using a glassy carbon working electrode, platinum reference electrode, and platinum counter electrode with ferrocene as an internal standard. Values are reported versus NHE. [d]Calculated from the equation $E_{(S+/S^*)} = E_{(S+/S)} - E_g^{opt}$. [e]Estimated from the onset of the absorption curve in CH_2Cl_2. Conversation from nanometers to eV was calculated by $E_g^{opt} = 1240/\lambda_{onset}$. [f]This process is irreversible. *We note that **LD03** is challenging to fully solubilize in CH_2Cl_2 for absorption measurements.

3. Computational Data

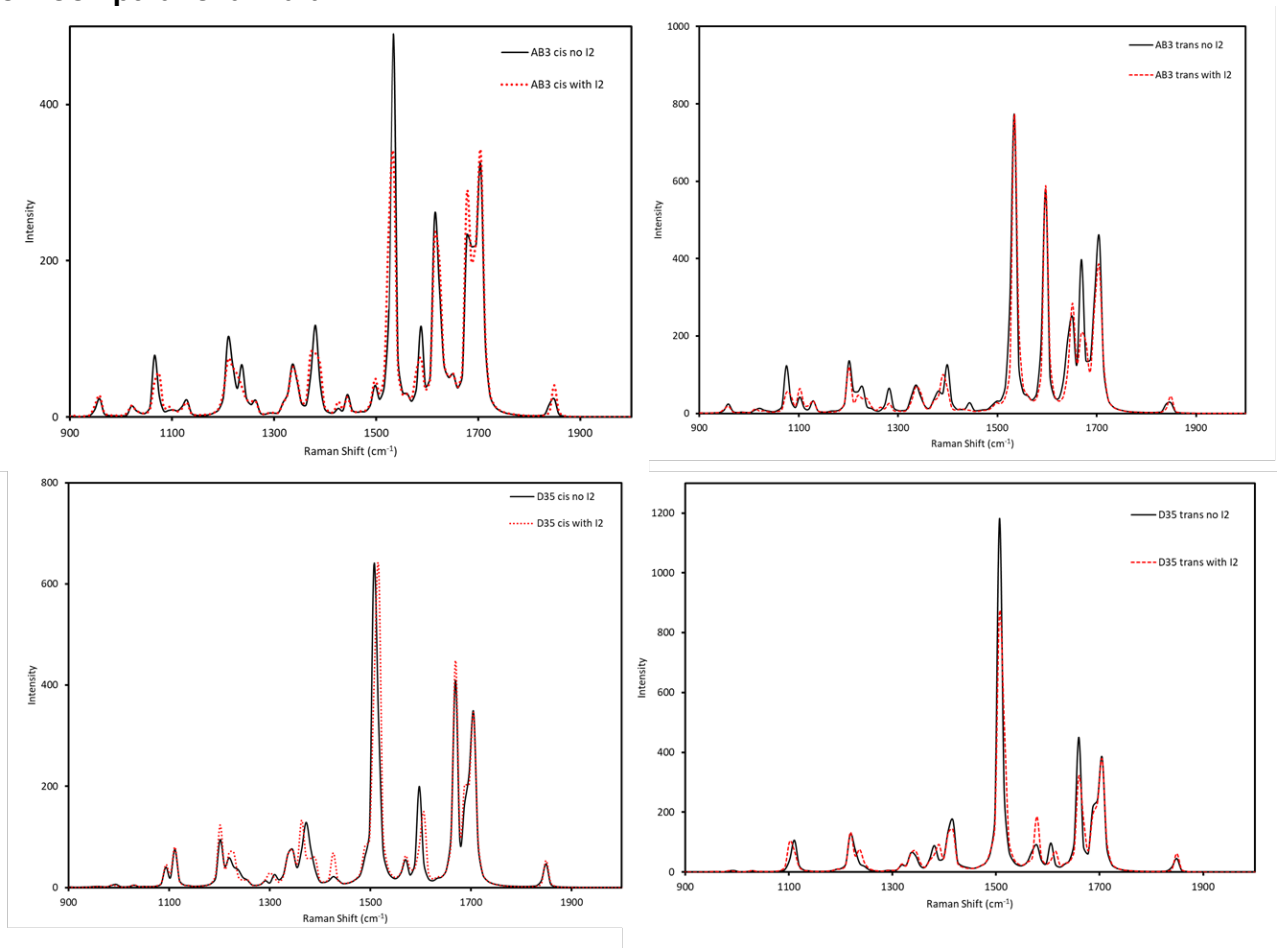


Figure S1: Simulated Raman spectra for cis and trans states of dyes **AB3** and **D35.** Calculations were done at wB97XD/6-31+G* level of theory and basis set.

Table S2: Excited state orbital transitions for cis **AB1**. Calculations were done at wB97XD/6-31+G* level of theory and basis set.

dye	State	transition orbitals	contribution (%)	vert. trans. (nm l eV)	oscillator strength	energy (Hartrees)
AB1 cis	1	219 (I_2) → 227 (I_2) 219 (I_2) → 228 (dye/I_2) 220 (dye/I_2) → 227 (I_2)	66 4 27	523 l 2.37	0.0004	-3310.9
AB1 cis	2	216 (dye/I_2) → 227 (I_2) 218 (I_2) → 227 (I_2) 218 (I_2) → 228 (dye/I_2) 219 (I_2) → 227 (I_2) 220 (dye/I_2) → 227 (I_2)	2 77 4 2 12	518 l 2.39	0.0004	-3310.9
AB1 cis	3	223 (dye) → 227 (I_2) 223 (dye) → 228 (dye/I_2) 224 (dye) → 227 (I_2) 224 (dye) → 228 (dye/I_2) 225 (dye) → 227 (I_2) 225 (dye) → 228 (dye/I_2) 226 (dye) → 227 (I_2) 226 (dye) → 228 (dye/I_2) 226 (dye) → 229 (dye)	6 3 14 7 15 7 27 12 4	423 l 2.93	0.9905	-3310.9
AB1 cis (no I_2)	1	216 (dye) → 220 (dye) 217 (dye) → 220 (dye) 218 (dye) → 220 (dye) 219 (dye) → 220 (dye) 219 (dye) → 221 (dye)	6 9 36 35 7	404 l 3.07	1.6582	-3288.1

Table S3: Excited state orbital transitions for trans **AB1**. Calculations were done at wB97XD/6-31+G* level of theory and basis set.

dye	State	transition orbitals	contribution (%)	vert. trans. (nm l eV)	oscillator strength	energy (Hartrees)
AB1 trans	1	216 (dye/I_2) → 227 (I_2) 217 (I_2) → 227 (I_2) 218 (I_2) → 227 (dye/I_2) 219 (dye/I_2) → 227 (I_2)	11 19 11 53	522 l 2.37	0.0005	-3310.9
AB1 trans	2	216 (dye/I_2) → 227 (I_2) 217 (I_2) → 227 (I_2) 217 (I_2) → 228 (dye/I_2) 219 (dye/I_2) → 227 (I_2)	4 77 3 14	520 l 2.38	0.0003	-3310.9
AB1 trans	3	223 (dye) → 227 (I_2) 223 (dye) → 228 (dye/I_2) 224 (dye) → 227 (I_2) 224 (dye) → 228 (dye/I_2) 225 (dye) → 227 (I_2) 225 (dye) → 228 (dye/I_2) 226 (dye) → 227 (I_2) 226 (dye) → 228 (dye/I_2) 226 (dye) → 229 (dye)	8 2 20 6 13 4 32 7 3	426 l 2.91	0.7251	-3310.9
AB1 trans (no I_2)	1	216 (dye) → 220 (dye) 217 (dye) → 220 (dye) 218 (dye) → 220 (dye) 219 (dye) → 220 (dye) 219 (dye) → 221 (dye)	8 13 31 34 8	401 l 3.09	1.7475	-3288.1

Table S4: Excited state orbital transitions for cis **AB2**. Calculations were done at wB97XD/6-31+G* level of theory and basis set.

dye	State	transition orbitals	contribution (%)	vert. trans. (nm l eV)	oscillator strength	energy (Hartrees)
AB2 cis	1	212 (dye/I_2) → 223 (I_2) 213 (I_2) → 223 (I_2) 215 (dye/I_2) → 223 (I_2) 216 (dye/I_2) → 223 (I_2)	12 5 72 8	522 l 2.37	0.0003	-2987.9
AB2 cis	2	214 (I_2) → 223 (I_2)	98	519 l 2.39	0.0007	-2987.9
AB2 cis	3	219 (dye) → 223 (I_2) 220 (dye) → 223 (I_2) 221 (dye) → 223 (I_2) 222 (dye) → 223 (I_2) 222 (dye) → 224 (dye)	5 10 32 44 2	429 l 2.89	0.1524	-2987.9
AB2 cis (no I_2)	1	212 (dye) → 216 (dye) 213 (dye) → 216 (dye) 214 (dye) → 216 (dye) 215 (dye) → 216 (dye) 215 (dye) → 217 (dye)	4 3 45 35 7	407 l 3.07	1.4447	-2965.1

Table S5: Excited state orbital transitions for trans **AB2**. Calculations were done at wB97XD/6-31+G* level of theory and basis set.

dye	State	transition orbitals	contribution (%)	vert. trans. (nm l eV)	oscillator strength	energy (Hartrees)
AB2 trans	1	209 (dye/I_2) → 223 (I_2) 212 (dye/I_2) → 223 (I_2) 214 (I_2) → 223 (I_2) 215 (I_2) → 223 (I_2)	3 7 57 33	522 l 2.38	0.0001	-2987.9
AB2 trans	2	213 (I_2) → 223 (I_2)	98	517 l 2.40	0.0003	-2987.9
AB2 trans	3	219 (dye) → 223 (I_2) 220 (dye) → 223 (I_2) 221 (dye) → 223 (I_2) 222 (dye) → 223 (I_2)	6 11 35 43	430 l 2.88	0.0248	-2987.9
AB2 trans (no I_2)	1	212 (dye) → 216 (dye) 213 (dye) → 216 (dye) 214 (dye) → 216 (dye) 215 (dye) → 216 (dye) 215 (dye) → 217 (dye)	5 4 43 34 8	400 l 3.10	1.8967	-2965.1

Table S6: Excited state orbital transitions for cis **D35**. Calculations were done at wB97XD/6-31+G* level of theory and basis set.

dye	State	transition orbitals	contribution (%)	vert. trans. (nm l eV)	oscillator strength	energy (Hartrees)
D35 cis	1	199 (I_2) → 206 (I_2) 199 (I_2) → 207 (dye/I_2)	94 3	523 l 2.37	0.0004	-2759.2
D35 cis	2	197 (I_2) → 206 (I_2) 198 (I_2) → 206 (I_2) 198 (I_2) → 207 (dye/I_2)	9 83 3	519 l 2.39	0.0007	-2759.2
D35 cis	3	202 (dye) → 206 (I_2) 203 (dye) → 206 (I_2) 203 (dye) → 207 (dye/I_2) 205 (dye) → 206 (I_2) 205 (dye) → 207 (dye/I_2) 205 (dye) → 208 (dye)	4 12 2 66 8 2	431 l 2.88	0.4107	-2759.2
D35 cis (no I_2)	1	195 (dye) → 199 (dye) 196 (dye) → 199 (dye) 198 (dye) → 199 (dye) 198 (dye) → 200 (dye)	8 18 61 7	393 l 3.16	1.2567	-2736.3

Table S7: Excited state orbital transitions for trans **D35**. Calculations were done at wB97XD/6-31+G* level of theory and basis set.

dye	State	transition orbitals	contribution (%)	vert. trans. (nm l eV)	oscillator strength	energy (Hartrees)
D35 trans	1	196 (I_2) → 206 (I_2) 197 (I_2) → 206 (I_2) 198 (I_2) → 206 (dye/I_2) 199 (dye/I_2) → 206 (I_2)	13 46 30 5	521 l 2.38	0.0009	-2759.2
D35 trans	2	197 (I_2) → 206 (I_2) 198 (I_2) → 206 (I_2)	32 64	520 l 2.38	0.0004	-2759.2
D35 trans	3	202 (dye) → 206 (I_2) 203 (dye) → 206 (I_2) 205 (dye) → 206 (I_2) 205 (dye) → 207 (dye/I_2)	4 12 74 4	437 l 2.84	0.2797	-2759.2
D35 trans (no I_2)	1	195 (dye) → 199 (dye) 196 (dye) → 199 (dye) 198 (dye) → 199 (dye) 198 (dye) → 200 (dye)	9 19 59 8	390 l 3.18	1.4418	-2736.3

Table S8: Excited state orbital transitions for cis **AB3**. Calculations were done at wB97XD/6-31+G* level of theory and basis set.

dye	State	transition orbitals	contribution (%)	vert. trans. (nm l eV)	oscillator strength	energy (Hartrees)
AB3 cis	1	192 (I_2) → 202 (I_2) 193 (I_2) → 202 (I_2)	2 93	528 l 2.35	0.0021	-2436.2
AB3 cis	2	192 (I_2) → 202 (I_2) 193 (I_2) → 202 (I_2)	97 3	523 l 2.37	0.0003	-2436.2
AB3 cis	3	193 (I_2) → 202 (I_2) 198 (dye) → 202 (I_2) 199 (dye) → 202 (I_2) 201 (dye) → 202 (I_2) 201 (dye) → 203 (dye)	3 5 14 67 4	447 l 2.77	0.1710	-2436.2
AB3 cis (no I_2)	1	191 (dye) → 195 (dye) 192 (dye) → 195 (dye) 193 (dye) → 195 (dye) 194 (dye) → 195 (dye) 194 (dye) → 196 (dye)	5 15 3 66 6	407 l 3.04	1.0472	-2413.4

Table S9: Excited state orbital transitions for trans **AB3**. Calculations were done at wB97XD/6-31+G* level of theory and basis set.

dye	State	transition orbitals	contribution (%)	vert. trans. (nm l eV)	oscillator strength	energy (Hartrees)
AB3 trans	1	190 (dye/I_2) → 202 (I_2) 192 (I_2) → 202 (I_2) 193 (I_2) → 202 (I_2) 194 (I_2) → 202 (I_2) 195 (dye) → 202 (I_2)	3 18 3 72 4	521 l 2.38	0.0004	-2436.2
AB3 trans	2	192 (I_2) → 202 (I_2) 193 (I_2) → 202 (I_2)	3 96	516 l 2.40	0.0003	-2436.2
AB3 trans	3	198 (dye) → 202 (I_2) 199 (dye) → 202 (I_2) 201 (dye) → 202 (I_2)	6 11 35	458 l 2.71	0.0042	-2436.2
AB3 trans (no I_2)	1	191 (dye) → 195 (dye) 192 (dye) → 195 (dye) 194 (dye) → 195 (dye) 194 (dye) → 196 (dye)	6 19 64 7	397 l 3.12	1.5510	-2413.4

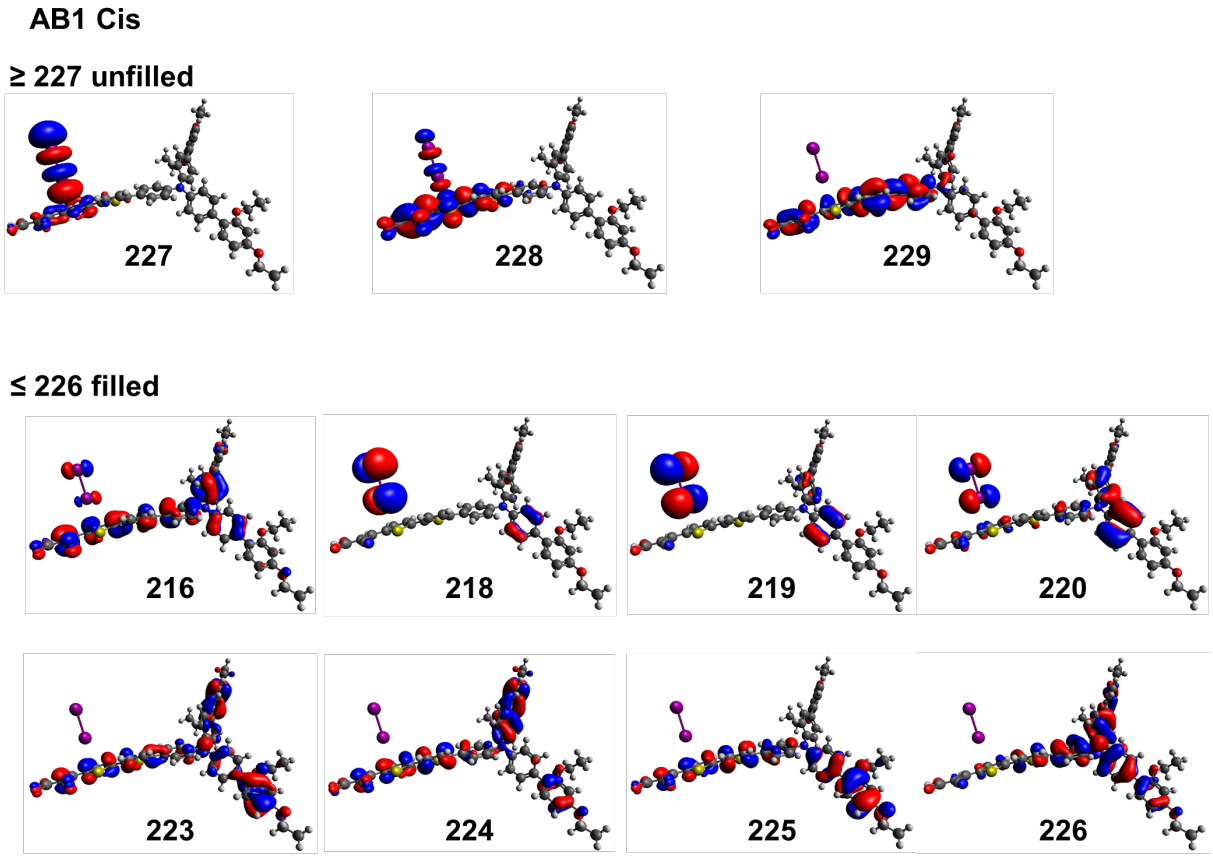


Figure S2: Orbitals contributing to TD-DFT predicted transitions for **AB1**. Calculations were done at wB97XD/6-31+G* level of theory and basis set.

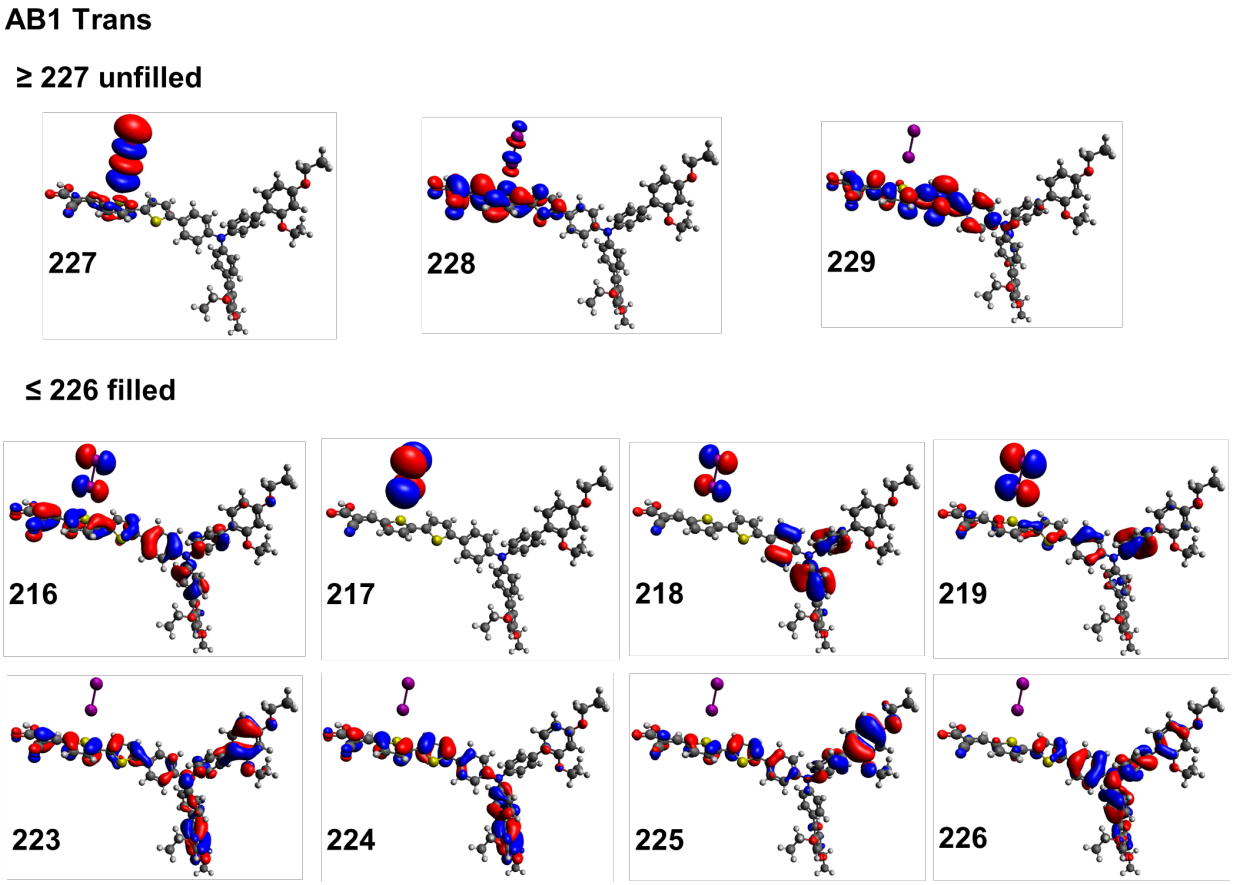


Figure S3: Orbitals contributing to TD-DFT predicted transitions for trans **AB1**. Calculations were done at wB97XD/6-31+G* level of theory and basis set.

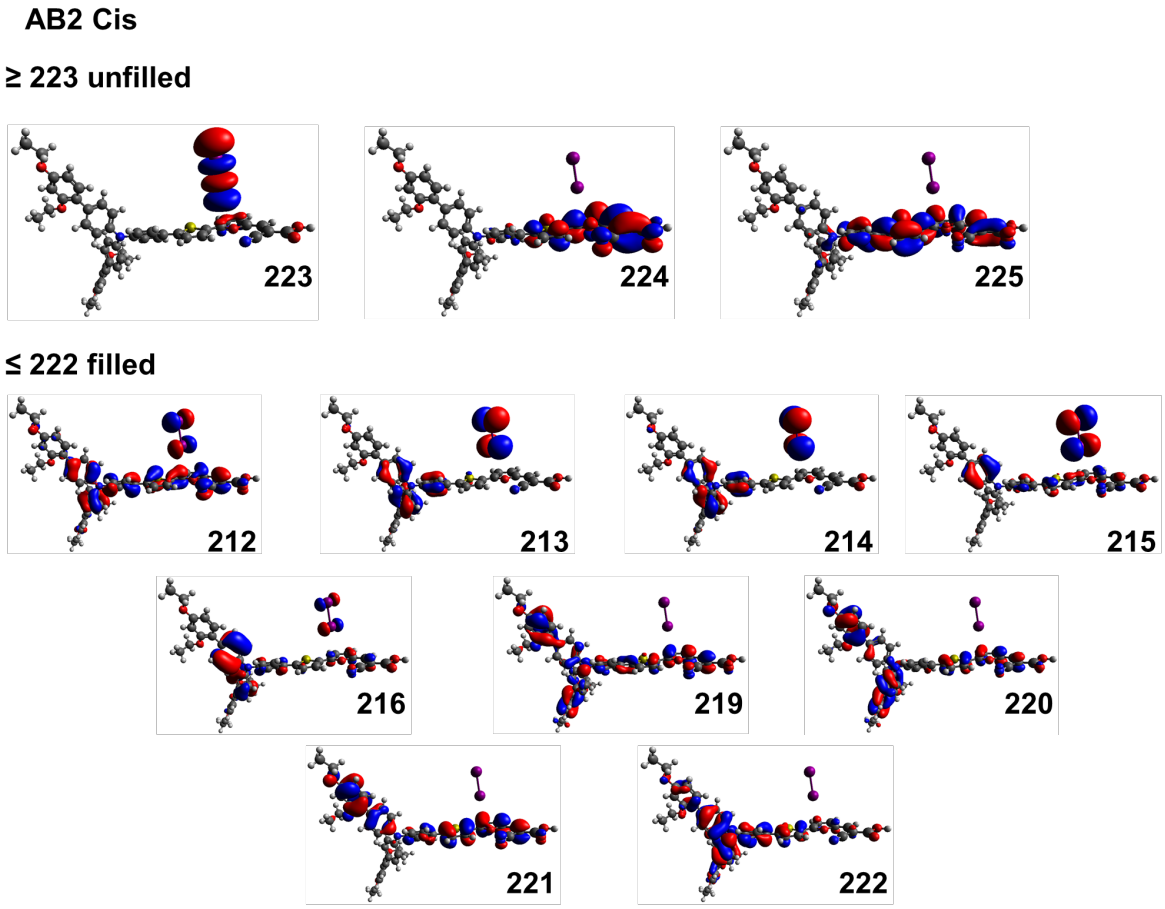


Figure S4: Orbitals contributing to TD-DFT predicted transitions for cis **AB2**. Calculations were done at wB97XD/6-31+G* level of theory and basis set.

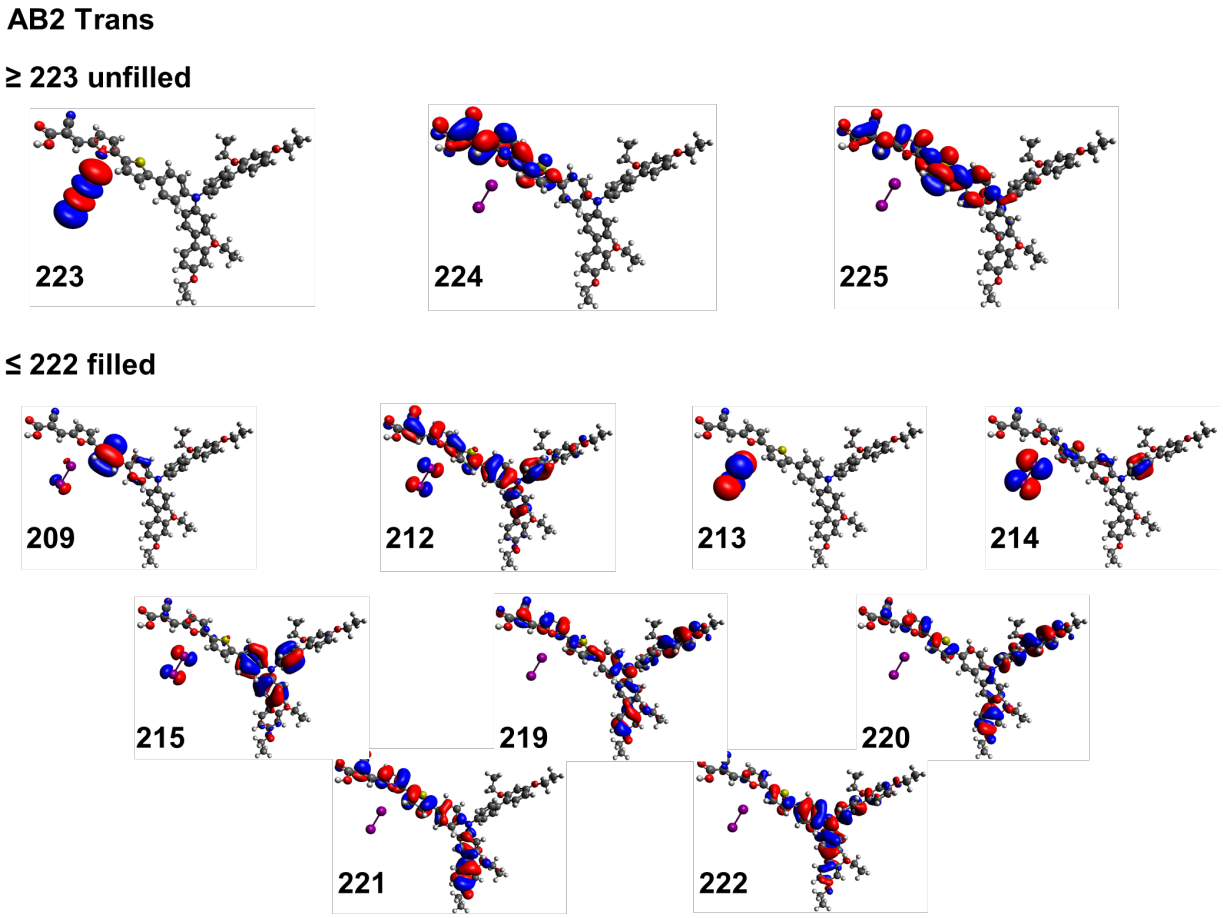


Figure S5: Orbitals contributing to TD-DFT predicted transitions for **AB2**. Calculations were done at wB97XD/6-31+G* level of theory and basis set.

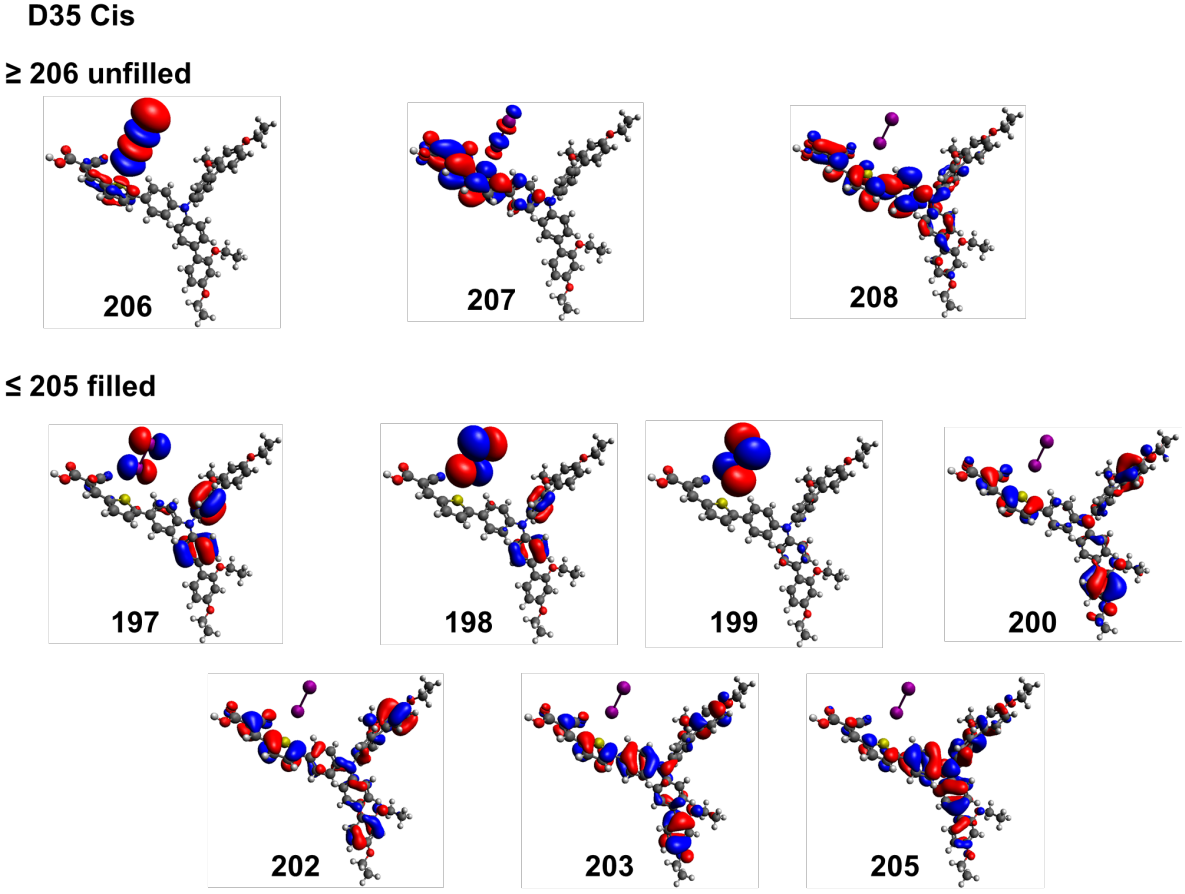


Figure S6: Orbitals contributing to TD-DFT predicted transitions for cis **D35**. Calculations were done at wB97XD/6-31+G* level of theory and basis set.

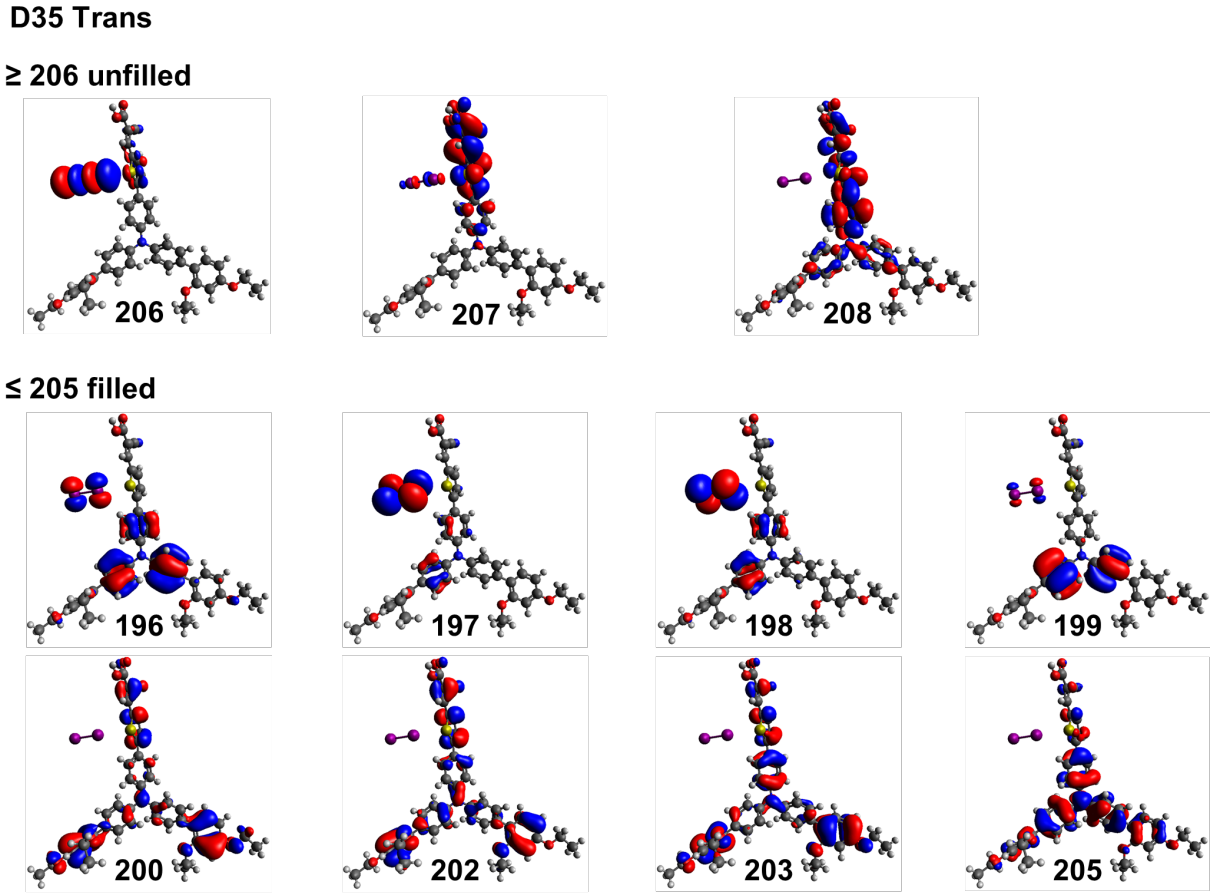
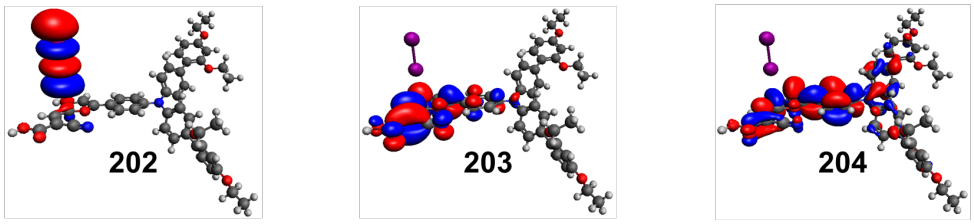


Figure S7: Orbitals contributing to TD-DFT predicted transitions for trans **D35**. Calculations were done at wB97XD/6-31+G* level of theory and basis set.

AB3 Cis

≥ 202 unfilled



≤ 201 filled

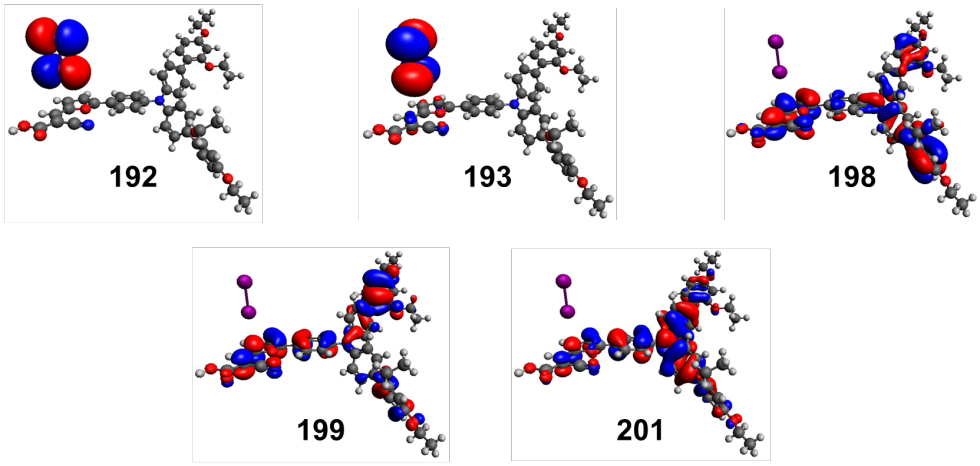
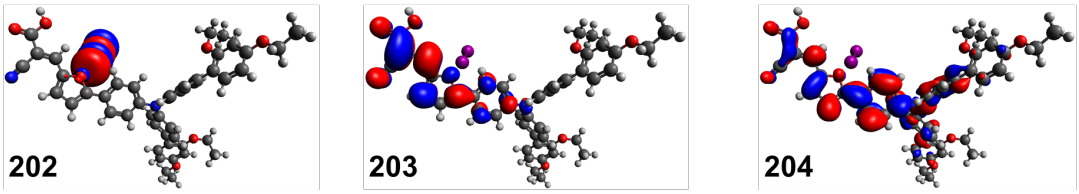


Figure S8: Orbitals contributing to TD-DFT predicted transitions for cis **AB3**. Calculations were done at wB97XD/6-31+G* level of theory and basis set.

AB3 Trans

≥ 202 unfilled



≤ 201 filled

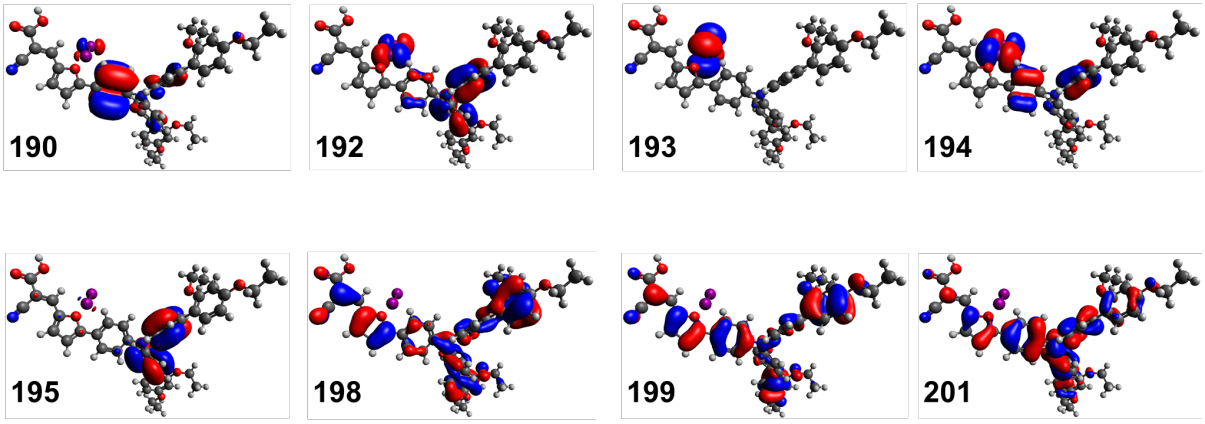


Figure S9: Orbitals contributing to TD-DFT predicted transitions for trans **AB3**. Calculations were done at wB97XD/6-31+G* level of theory and basis set.

Optimized coordinates for I_2 coordinated cis-AB1 at wB97XD/6-31+G* level of theory and basis set

I	8.824000	2.397000	-2.750000
I	8.102000	0.336000	-1.189000
H	13.007000	-1.984000	3.377000
O	12.065000	-1.818000	3.218000
C	11.709000	-2.588000	2.167000
O	12.487000	-3.317000	1.599000
C	10.280000	-2.437000	1.800000
C	9.843000	-3.223000	0.688000
N	9.453000	-3.846000	-0.209000
C	9.452000	-1.599000	2.479000
C	4.419000	-1.107000	0.865000
C	4.183000	-1.545000	-0.416000
C	2.818000	-1.465000	-0.789000
C	2.009000	-0.967000	0.203000
H	4.970000	-1.880000	-1.085000
H	2.448000	-1.730000	-1.773000
C	-0.054000	0.306000	0.849000
C	-1.428000	0.499000	0.800000
C	-2.241000	-0.355000	0.042000
C	-1.635000	-1.413000	-0.652000
C	-0.265000	-1.612000	-0.578000
C	0.556000	-0.752000	0.164000
H	0.552000	1.000000	1.426000
H	-1.876000	1.322000	1.346000
H	-2.248000	-2.089000	-1.240000
H	0.176000	-2.456000	-1.102000
N	-3.632000	-0.161000	-0.020000
C	-4.175000	3.459000	-0.667000
C	-5.303000	3.733000	0.115000
C	-5.863000	2.680000	0.850000
C	-5.310000	1.407000	0.816000
C	-4.185000	1.143000	0.026000
C	-3.628000	2.182000	-0.725000
H	-3.714000	4.260000	-1.240000
H	-5.756000	0.604000	1.395000
H	-2.757000	1.989000	-1.345000
C	-6.443000	-2.354000	-1.068000
C	-6.273000	-3.473000	-0.242000
C	-5.202000	-3.464000	0.659000
C	-4.333000	-2.380000	0.740000
C	-4.508000	-1.277000	-0.098000
C	-5.570000	-1.276000	-1.007000
H	-5.063000	-4.308000	1.330000
H	-3.519000	-2.385000	1.460000
H	-5.710000	-0.421000	-1.662000
H	9.905000	-1.050000	3.301000

S	2.937000	-0.609000	1.625000
H	-6.735000	2.867000	1.469000
H	-7.263000	-2.336000	-1.779000
C	-5.893000	5.096000	0.139000
C	-6.246000	5.749000	1.338000
C	-6.138000	5.780000	-1.052000
C	-6.830000	7.007000	1.323000
C	-6.718000	7.048000	-1.087000
H	-5.893000	5.292000	-1.992000
C	-7.075000	7.664000	0.114000
H	-7.093000	7.487000	2.260000
H	-6.895000	7.523000	-2.045000
C	-7.166000	-4.656000	-0.331000
C	-6.628000	-5.934000	-0.445000
C	-8.575000	-4.541000	-0.284000
C	-7.416000	-7.085000	-0.520000
H	-5.547000	-6.037000	-0.495000
C	-9.377000	-5.674000	-0.360000
C	-8.801000	-6.944000	-0.478000
H	-6.940000	-8.053000	-0.619000
H	-10.458000	-5.620000	-0.326000
O	-7.652000	8.888000	0.214000
O	-6.061000	5.150000	2.558000
O	-9.060000	-3.283000	-0.128000
O	-9.686000	-7.971000	-0.548000
C	-7.922000	9.612000	-0.976000
C	-8.557000	10.929000	-0.579000
H	-8.600000	9.030000	-1.617000
H	-6.986000	9.780000	-1.527000
H	-8.782000	11.520000	-1.473000
H	-9.488000	10.758000	-0.030000
H	-7.880000	11.507000	0.058000
C	-4.707000	5.065000	3.013000
C	-4.151000	6.419000	3.427000
H	-4.082000	4.606000	2.237000
H	-4.747000	4.381000	3.864000
H	-3.135000	6.297000	3.819000
H	-4.108000	7.106000	2.576000
H	-4.773000	6.871000	4.206000
C	-10.461000	-3.047000	-0.121000
C	-11.059000	-3.051000	-1.521000
H	-10.562000	-2.057000	0.331000
H	-10.964000	-3.764000	0.541000
H	-12.128000	-2.815000	-1.469000
H	-10.569000	-2.295000	-2.142000
H	-10.946000	-4.023000	-2.011000
C	-9.184000	-9.293000	-0.664000
C	-10.371000	-10.234000	-0.716000
H	-8.542000	-9.522000	0.198000

H	-8.578000	-9.379000	-1.577000
H	-10.023000	-11.268000	-0.806000
H	-10.971000	-10.147000	0.195000
H	-11.008000	-10.004000	-1.575000
C	5.685000	-1.019000	1.565000
C	6.028000	-0.203000	2.623000
S	7.015000	-2.022000	1.081000
C	7.369000	-0.369000	3.024000
H	5.345000	0.511000	3.068000
C	8.064000	-1.305000	2.282000
H	7.835000	0.198000	3.823000

Optimized coordinates for I_2 coordinated trans-AB1 at wB97XD/6-31+G* level of theory and basis set

H	12.899000	-3.677000	0.983000
O	11.977000	-3.461000	0.775000
C	11.837000	-3.596000	-0.561000
O	12.747000	-3.932000	-1.282000
C	10.464000	-3.292000	-1.032000
C	10.258000	-3.420000	-2.441000
N	10.047000	-3.513000	-3.578000
C	9.480000	-2.918000	-0.171000
C	4.460000	-1.413000	0.409000
C	4.223000	-0.791000	1.611000
C	2.857000	-0.469000	1.812000
C	2.049000	-0.839000	0.764000
H	5.005000	-0.558000	2.327000
H	2.476000	0.003000	2.710000
C	-0.209000	-1.587000	-0.035000
C	-1.579000	-1.400000	-0.151000
C	-2.196000	-0.276000	0.414000
C	-1.395000	0.659000	1.086000
C	-0.023000	0.476000	1.178000
C	0.598000	-0.654000	0.629000
H	0.237000	-2.481000	-0.465000
H	-2.180000	-2.134000	-0.678000
H	-1.852000	1.540000	1.526000
H	0.579000	1.229000	1.679000
N	-3.584000	-0.083000	0.307000
C	-5.178000	-3.320000	1.203000
C	-6.250000	-3.380000	0.305000
C	-6.414000	-2.317000	-0.593000
C	-5.535000	-1.242000	-0.601000
C	-4.471000	-1.190000	0.306000
C	-4.306000	-2.237000	1.217000
H	-5.021000	-4.137000	1.904000
H	-5.677000	-0.428000	-1.306000
H	-3.486000	-2.206000	1.929000

C	-5.765000	2.888000	0.781000
C	-5.207000	3.813000	-0.109000
C	-4.094000	3.411000	-0.858000
C	-3.559000	2.134000	-0.730000
C	-4.118000	1.226000	0.171000
C	-5.226000	1.617000	0.929000
H	-3.659000	4.101000	-1.577000
H	-2.707000	1.836000	-1.334000
H	-5.665000	0.915000	1.633000
H	9.779000	-2.865000	0.873000
S	2.984000	-1.594000	-0.488000
H	-7.234000	-2.342000	-1.304000
H	-6.626000	3.173000	1.377000
C	-7.190000	-4.530000	0.325000
C	-7.584000	-5.209000	-0.846000
C	-7.737000	-4.973000	1.530000
C	-8.493000	-6.256000	-0.796000
C	-8.647000	-6.027000	1.601000
H	-7.466000	-4.455000	2.446000
C	-9.034000	-6.669000	0.424000
H	-8.780000	-6.760000	-1.713000
H	-9.048000	-6.316000	2.566000
C	-5.738000	5.194000	-0.242000
C	-4.878000	6.285000	-0.175000
C	-7.110000	5.455000	-0.462000
C	-5.315000	7.605000	-0.309000
H	-3.822000	6.101000	0.005000
C	-7.566000	6.762000	-0.594000
C	-6.672000	7.836000	-0.518000
H	-4.599000	8.415000	-0.236000
H	-8.610000	6.996000	-0.763000
O	-9.916000	-7.699000	0.358000
O	-7.113000	-4.835000	-2.080000
O	-7.911000	4.364000	-0.565000
O	-7.236000	9.063000	-0.658000
C	-10.498000	-8.175000	1.562000
C	-11.428000	-9.316000	1.203000
H	-11.050000	-7.361000	2.052000
H	-9.707000	-8.516000	2.245000
H	-11.899000	-9.712000	2.109000
H	-12.214000	-8.973000	0.523000
H	-10.876000	-10.125000	0.715000
C	-5.751000	-5.171000	-2.356000
C	-5.554000	-6.663000	-2.569000
H	-5.105000	-4.802000	-1.549000
H	-5.510000	-4.610000	-3.263000
H	-4.510000	-6.866000	-2.832000
H	-5.792000	-7.227000	-1.661000
H	-6.194000	-7.027000	-3.380000

C	-9.313000	4.512000	-0.737000
C	-10.027000	4.848000	0.565000
H	-9.640000	3.537000	-1.107000
H	-9.523000	5.250000	-1.522000
H	-11.108000	4.902000	0.392000
H	-9.835000	4.071000	1.311000
H	-9.697000	5.807000	0.976000
C	-6.396000	10.206000	-0.604000
C	-7.270000	11.428000	-0.798000
H	-5.635000	10.141000	-1.393000
H	-5.884000	10.243000	0.368000
H	-6.657000	12.335000	-0.763000
H	-7.779000	11.389000	-1.766000
H	-8.028000	11.490000	-0.010000
C	5.725000	-1.866000	-0.136000
C	6.062000	-2.096000	-1.454000
S	7.075000	-2.181000	0.902000
C	7.402000	-2.500000	-1.633000
H	5.370000	-1.945000	-2.274000
C	8.111000	-2.585000	-0.450000
H	7.835000	-2.703000	-2.604000
I	8.462000	3.781000	0.385000
I	7.906000	1.171000	0.678000

Optimized coordinates for I_2 coordinated cis-AB2 at wB97XD/6-31+G* level of theory and basis set

I	-7.012000	0.493000	1.741000
I	-7.366000	3.060000	2.439000
H	-12.947000	-2.914000	-2.626000
O	-12.095000	-2.891000	-2.163000
C	-11.187000	-2.426000	-3.048000
O	-11.478000	-2.125000	-4.182000
C	-9.822000	-2.332000	-2.476000
C	-8.814000	-1.845000	-3.370000
N	-7.990000	-1.453000	-4.085000
C	-9.568000	-2.690000	-1.188000
C	-4.904000	-1.838000	-0.786000
C	-4.649000	-1.360000	-2.051000
C	-3.290000	-1.004000	-2.231000
C	-2.516000	-1.206000	-1.113000
H	-5.414000	-1.281000	-2.816000
H	-2.886000	-0.636000	-3.167000
C	-0.269000	-1.745000	-0.134000
C	1.086000	-1.485000	0.011000
C	1.684000	-0.415000	-0.670000
C	0.878000	0.390000	-1.488000
C	-0.480000	0.136000	-1.610000
C	-1.081000	-0.941000	-0.945000

H	-0.699000	-2.596000	0.389000
H	1.691000	-2.119000	0.651000
H	1.320000	1.227000	-2.019000
H	-1.088000	0.792000	-2.228000
N	3.057000	-0.149000	-0.534000
C	4.814000	-3.396000	-0.972000
C	5.857000	-3.295000	-0.044000
C	5.945000	-2.124000	0.719000
C	5.021000	-1.098000	0.568000
C	3.987000	-1.206000	-0.369000
C	3.898000	-2.364000	-1.146000
H	4.715000	-4.299000	-1.569000
H	5.105000	-0.197000	1.170000
H	3.102000	-2.460000	-1.879000
C	5.132000	2.841000	-1.285000
C	4.497000	3.840000	-0.536000
C	3.371000	3.480000	0.213000
C	2.895000	2.173000	0.222000
C	3.530000	1.190000	-0.539000
C	4.653000	1.538000	-1.297000
H	2.876000	4.230000	0.825000
H	2.030000	1.911000	0.825000
H	5.151000	0.778000	-1.892000
H	-10.407000	-3.046000	-0.599000
S	-3.472000	-1.835000	0.193000
H	6.741000	-2.022000	1.450000
H	6.006000	3.092000	-1.878000
C	6.847000	-4.393000	0.103000
C	7.236000	-4.904000	1.358000
C	7.450000	-4.953000	-1.024000
C	8.191000	-5.905000	1.460000
C	8.407000	-5.964000	-0.943000
H	7.183000	-4.565000	-2.004000
C	8.787000	-6.438000	0.314000
H	8.473000	-6.278000	2.438000
H	8.849000	-6.349000	-1.854000
C	4.964000	5.249000	-0.552000
C	4.064000	6.284000	-0.785000
C	6.314000	5.599000	-0.314000
C	4.439000	7.629000	-0.798000
H	3.025000	6.030000	-0.982000
C	6.709000	6.932000	-0.326000
C	5.775000	7.946000	-0.567000
H	3.694000	8.390000	-0.996000
H	7.735000	7.233000	-0.147000
O	9.710000	-7.409000	0.528000
O	6.712000	-4.405000	2.524000
O	7.154000	4.567000	-0.048000
O	6.281000	9.206000	-0.557000

C	10.350000	-7.999000	-0.593000
C	11.319000	-9.042000	-0.074000
H	10.880000	-7.225000	-1.166000
H	9.597000	-8.459000	-1.249000
H	11.835000	-9.521000	-0.913000
H	12.067000	-8.582000	0.578000
H	10.789000	-9.812000	0.494000
C	5.359000	-4.770000	2.808000
C	5.225000	-6.233000	3.200000
H	4.721000	-4.536000	1.947000
H	5.067000	-4.115000	3.633000
H	4.183000	-6.453000	3.461000
H	5.514000	-6.892000	2.374000
H	5.856000	-6.463000	4.064000
C	8.540000	4.799000	0.156000
C	9.293000	5.007000	-1.151000
H	8.892000	3.892000	0.654000
H	8.688000	5.636000	0.850000
H	10.363000	5.130000	-0.948000
H	9.164000	4.137000	-1.803000
H	8.942000	5.893000	-1.689000
C	5.399000	10.294000	-0.787000
C	6.213000	11.570000	-0.712000
H	4.605000	10.292000	-0.028000
H	4.931000	10.187000	-1.776000
H	5.565000	12.436000	-0.886000
H	6.676000	11.675000	0.273000
H	7.003000	11.569000	-1.469000
C	-6.176000	-2.274000	-0.276000
C	-6.614000	-2.748000	0.948000
C	-7.999000	-3.000000	0.798000
H	-6.004000	-2.919000	1.824000
C	-8.326000	-2.659000	-0.495000
H	-8.682000	-3.375000	1.547000
O	-7.207000	-2.221000	-1.137000

Optimized coordinates for I_2 coordinated trans-AB2 at wB97XD/6-31+G* level of theory and basis set

H	-12.475000	-1.798000	-2.080000
O	-11.599000	-1.966000	-1.699000
C	-11.791000	-2.734000	-0.606000
O	-12.886000	-3.101000	-0.248000
C	-10.527000	-3.068000	0.090000
C	-10.650000	-3.886000	1.255000
N	-10.682000	-4.549000	2.207000
C	-9.320000	-2.621000	-0.352000
C	-4.629000	-2.013000	-0.332000
C	-4.456000	-1.381000	-1.541000

C	-3.119000	-0.963000	-1.756000
C	-2.275000	-1.273000	-0.717000
H	-5.259000	-1.242000	-2.255000
H	-2.780000	-0.476000	-2.663000
C	0.034000	-1.853000	0.074000
C	1.389000	-1.572000	0.175000
C	1.926000	-0.419000	-0.416000
C	1.057000	0.447000	-1.097000
C	-0.300000	0.170000	-1.173000
C	-0.839000	-0.989000	-0.599000
H	-0.346000	-2.767000	0.524000
H	2.042000	-2.254000	0.710000
H	1.450000	1.348000	-1.557000
H	-0.955000	0.873000	-1.682000
N	3.298000	-0.131000	-0.325000
C	5.108000	-3.276000	-1.135000
C	6.186000	-3.233000	-0.244000
C	6.282000	-2.134000	0.619000
C	5.330000	-1.123000	0.600000
C	4.258000	-1.173000	-0.298000
C	4.162000	-2.257000	-1.175000
H	5.003000	-4.123000	-1.808000
H	5.419000	-0.279000	1.279000
H	3.338000	-2.306000	-1.881000
C	5.263000	2.970000	-0.903000
C	4.652000	3.877000	-0.027000
C	3.580000	3.419000	0.748000
C	3.133000	2.105000	0.659000
C	3.742000	1.216000	-0.229000
C	4.810000	1.662000	-1.012000
H	3.107000	4.095000	1.456000
H	2.311000	1.764000	1.282000
H	5.288000	0.974000	-1.704000
H	-9.322000	-2.004000	-1.246000
S	-3.141000	-2.077000	0.556000
H	7.106000	-2.079000	1.323000
H	6.094000	3.299000	-1.517000
C	7.204000	-4.315000	-0.237000
C	7.656000	-4.925000	0.951000
C	7.770000	-4.759000	-1.433000
C	8.636000	-5.907000	0.925000
C	8.751000	-5.749000	-1.480000
H	7.455000	-4.292000	-2.363000
C	9.193000	-6.323000	-0.287000
H	8.966000	-6.359000	1.854000
H	9.162000	-6.042000	-2.439000
C	5.087000	5.294000	0.064000
C	4.153000	6.321000	-0.018000
C	6.441000	5.655000	0.255000

C	4.498000	7.671000	0.075000
H	3.110000	6.059000	-0.177000
C	6.807000	6.994000	0.348000
C	5.839000	8.001000	0.257000
H	3.727000	8.427000	-0.006000
H	7.834000	7.304000	0.495000
O	10.145000	-7.287000	-0.198000
O	7.172000	-4.543000	2.177000
O	7.318000	4.626000	0.373000
O	6.317000	9.268000	0.358000
C	10.748000	-7.760000	-1.391000
C	11.758000	-8.822000	-1.006000
H	11.239000	-6.926000	-1.913000
H	9.977000	-8.177000	-2.055000
H	12.248000	-9.214000	-1.904000
H	12.523000	-8.404000	-0.346000
H	11.267000	-9.651000	-0.488000
C	5.841000	-4.967000	2.483000
C	5.758000	-6.461000	2.753000
H	5.163000	-4.679000	1.670000
H	5.568000	-4.392000	3.371000
H	4.733000	-6.730000	3.036000
H	6.028000	-7.041000	1.865000
H	6.429000	-6.745000	3.570000
C	8.708000	4.877000	0.521000
C	9.379000	5.228000	-0.800000
H	9.108000	3.938000	0.912000
H	8.875000	5.649000	1.283000
H	10.455000	5.362000	-0.645000
H	9.233000	4.418000	-1.522000
H	8.977000	6.149000	-1.231000
C	5.400000	10.348000	0.285000
C	6.190000	11.633000	0.433000
H	4.654000	10.253000	1.086000
H	4.875000	10.322000	-0.680000
H	5.514000	12.493000	0.382000
H	6.711000	11.656000	1.395000
H	6.931000	11.724000	-0.366000
C	-5.849000	-2.561000	0.206000
C	-6.133000	-3.354000	1.293000
C	-7.534000	-3.542000	1.300000
H	-5.418000	-3.759000	1.994000
C	-8.036000	-2.855000	0.217000
H	-8.110000	-4.116000	2.012000
O	-6.990000	-2.253000	-0.448000
I	-8.059000	3.454000	0.184000
I	-7.389000	0.887000	-0.174000

Optimized coordinates for I_2 coordinated cis-D35 at wB97XD/6-31+G* level of theory and basis set

H	10.197000	-5.506000	1.434000
O	9.294000	-5.272000	1.171000
C	8.842000	-4.387000	2.087000
O	9.513000	-4.022000	3.024000
C	7.460000	-3.928000	1.813000
C	6.928000	-2.986000	2.747000
N	6.465000	-2.220000	3.486000
C	6.758000	-4.376000	0.737000
C	5.435000	-4.057000	0.292000
C	4.884000	-4.548000	-0.877000
C	3.590000	-4.058000	-1.146000
C	3.134000	-3.184000	-0.182000
H	5.422000	-5.227000	-1.530000
H	3.026000	-4.303000	-2.038000
C	1.720000	-1.232000	0.499000
C	0.508000	-0.561000	0.518000
C	-0.621000	-1.102000	-0.118000
C	-0.491000	-2.344000	-0.762000
C	0.721000	-3.015000	-0.764000
C	1.855000	-2.473000	-0.141000
H	2.576000	-0.771000	0.985000
H	0.434000	0.396000	1.025000
H	-1.350000	-2.784000	-1.258000
H	0.783000	-3.983000	-1.252000
N	-1.844000	-0.422000	-0.112000
C	-1.139000	3.160000	-0.823000
C	-1.985000	3.812000	0.081000
C	-2.781000	3.023000	0.921000
C	-2.729000	1.637000	0.865000
C	-1.884000	0.999000	-0.047000
C	-1.095000	1.772000	-0.900000
H	-0.501000	3.750000	-1.477000
H	-3.352000	1.039000	1.524000
H	-0.436000	1.285000	-1.613000
C	-5.316000	-1.390000	-1.010000
C	-5.543000	-2.494000	-0.179000
C	-4.508000	-2.896000	0.674000
C	-3.292000	-2.221000	0.704000
C	-3.075000	-1.131000	-0.141000
C	-4.099000	-0.722000	-1.000000
H	-4.669000	-3.732000	1.350000
H	-2.510000	-2.536000	1.389000
H	-3.936000	0.128000	-1.656000

H	7.278000	-5.085000	0.097000
S	4.305000	-2.984000	1.083000
H	-3.445000	3.503000	1.633000
H	-6.100000	-1.058000	-1.682000
C	-2.052000	5.296000	0.106000
C	-1.912000	6.034000	1.304000
C	-2.235000	6.011000	-1.073000
C	-1.969000	7.424000	1.286000
C	-2.292000	7.405000	-1.114000
H	-2.355000	5.455000	-2.000000
C	-2.159000	8.109000	0.080000
H	-1.865000	8.019000	2.185000
H	-2.447000	7.907000	-2.062000
C	-6.820000	-3.252000	-0.213000
C	-6.812000	-4.638000	-0.334000
C	-8.077000	-2.613000	-0.101000
C	-7.978000	-5.405000	-0.356000
H	-5.853000	-5.141000	-0.433000
C	-9.251000	-3.358000	-0.124000
C	-9.203000	-4.751000	-0.252000
H	-7.909000	-6.481000	-0.464000
H	-10.229000	-2.901000	-0.041000
O	-2.200000	9.462000	0.190000
O	-1.691000	5.303000	2.426000
O	-8.043000	-1.266000	0.061000
O	-10.413000	-5.368000	-0.265000
C	-2.377000	10.234000	-0.987000
C	-2.374000	11.695000	-0.585000
H	-3.328000	9.963000	-1.467000
H	-1.562000	10.022000	-1.694000
H	-2.509000	12.326000	-1.470000
H	-3.186000	11.903000	0.118000
H	-1.426000	11.961000	-0.109000
C	-1.566000	5.941000	3.689000
C	-2.915000	6.322000	4.283000
H	-0.893000	6.804000	3.614000
H	-1.074000	5.194000	4.317000
H	-2.772000	6.761000	5.277000
H	-3.446000	7.048000	3.661000
H	-3.545000	5.433000	4.387000
C	-9.249000	-0.518000	0.136000
C	-9.873000	-0.283000	-1.233000
H	-8.945000	0.432000	0.582000
H	-9.951000	-0.998000	0.829000
H	-10.769000	0.340000	-1.130000
H	-9.164000	0.238000	-1.885000
H	-10.161000	-1.220000	-1.718000
C	-10.454000	-6.781000	-0.384000
C	-11.909000	-7.203000	-0.362000

H	-9.903000	-7.237000	0.451000
H	-9.972000	-7.087000	-1.323000
H	-11.983000	-8.292000	-0.453000
H	-12.385000	-6.898000	0.574000
H	-12.455000	-6.748000	-1.194000
I	5.819000	-0.362000	-0.576000
I	6.878000	1.529000	-2.160000

Optimized coordinates for I_2 coordinated trans-D35 at wB97XD/6-31+G* level of theory and basis set

H	10.016000	-3.776000	3.307000
O	9.166000	-3.701000	2.845000
C	9.253000	-4.478000	1.745000
O	10.245000	-5.114000	1.473000
C	8.017000	-4.463000	0.927000
C	8.052000	-5.272000	-0.251000
N	8.038000	-5.918000	-1.215000
C	6.931000	-3.726000	1.285000
C	5.668000	-3.589000	0.619000
C	5.192000	-4.099000	-0.575000
C	3.880000	-3.675000	-0.878000
C	3.329000	-2.840000	0.071000
H	5.774000	-4.739000	-1.225000
H	3.364000	-3.945000	-1.792000
C	1.766000	-0.979000	0.683000
C	0.511000	-0.391000	0.657000
C	-0.558000	-1.016000	-0.005000
C	-0.324000	-2.253000	-0.628000
C	0.930000	-2.840000	-0.584000
C	2.005000	-2.214000	0.065000
H	2.574000	-0.454000	1.186000
H	0.356000	0.565000	1.146000
H	-1.135000	-2.757000	-1.143000
H	1.074000	-3.808000	-1.056000
N	-1.825000	-0.422000	-0.046000
C	-1.337000	3.187000	-0.799000
C	-2.269000	3.795000	0.051000
C	-3.047000	2.967000	0.869000
C	-2.896000	1.586000	0.846000
C	-1.966000	0.992000	-0.013000
C	-1.194000	1.805000	-0.845000
H	-0.712000	3.808000	-1.436000
H	-3.508000	0.958000	1.487000
H	-0.470000	1.352000	-1.517000
C	-5.191000	-1.671000	-0.999000
C	-5.357000	-2.766000	-0.142000
C	-4.319000	-3.064000	0.748000

C	-3.158000	-2.300000	0.788000
C	-3.000000	-1.220000	-0.083000
C	-4.028000	-0.914000	-0.980000
H	-4.435000	-3.891000	1.445000
H	-2.373000	-2.535000	1.500000
H	-3.911000	-0.073000	-1.658000
H	7.043000	-3.161000	2.208000
S	4.445000	-2.588000	1.371000
H	-3.776000	3.411000	1.539000
H	-5.980000	-1.419000	-1.701000
C	-2.440000	5.270000	0.038000
C	-2.425000	6.039000	1.225000
C	-2.601000	5.948000	-1.165000
C	-2.577000	7.421000	1.172000
C	-2.752000	7.335000	-1.242000
H	-2.627000	5.369000	-2.085000
C	-2.740000	8.069000	-0.058000
H	-2.570000	8.038000	2.062000
H	-2.885000	7.806000	-2.208000
C	-6.571000	-3.621000	-0.185000
C	-6.452000	-5.005000	-0.262000
C	-7.877000	-3.079000	-0.129000
C	-7.555000	-5.861000	-0.291000
H	-5.456000	-5.435000	-0.318000
C	-8.988000	-3.914000	-0.160000
C	-8.830000	-5.302000	-0.241000
H	-7.400000	-6.931000	-0.362000
H	-10.001000	-3.531000	-0.119000
O	-2.882000	9.417000	0.018000
O	-2.223000	5.348000	2.375000
O	-7.952000	-1.729000	-0.011000
O	-9.987000	-6.011000	-0.268000
C	-3.040000	10.152000	-1.185000
C	-3.161000	11.617000	-0.817000
H	-3.940000	9.807000	-1.714000
H	-2.171000	9.984000	-1.837000
H	-3.286000	12.220000	-1.723000
H	-4.027000	11.781000	-0.168000
H	-2.264000	11.958000	-0.292000
C	-2.240000	6.015000	3.629000
C	-3.653000	6.306000	4.114000
H	-1.627000	6.924000	3.585000
H	-1.743000	5.317000	4.308000
H	-3.618000	6.772000	5.105000
H	-4.187000	6.980000	3.438000
H	-4.224000	5.375000	4.191000
C	-9.213000	-1.075000	-0.005000
C	-9.805000	-0.938000	-1.401000
H	-8.999000	-0.089000	0.414000

H	-9.901000	-1.583000	0.683000
H	-10.749000	-0.384000	-1.351000
H	-9.116000	-0.388000	-2.049000
H	-10.002000	-1.912000	-1.858000
C	-9.915000	-7.426000	-0.343000
C	-11.333000	-7.960000	-0.350000
H	-9.357000	-7.813000	0.521000
H	-9.383000	-7.721000	-1.258000
H	-11.320000	-9.054000	-0.407000
H	-11.860000	-7.666000	0.563000
H	-11.887000	-7.573000	-1.211000
I	6.700000	2.264000	-1.651000
I	5.731000	0.170000	-0.279000

Optimized coordinates for I_2 coordinated cis-AB3 at wB97XD/6-31+G* level of theory and basis set

H	-9.532000	-4.423000	-1.133000
O	-8.874000	-3.756000	-1.385000
C	-7.703000	-4.145000	-0.835000
O	-7.597000	-5.154000	-0.177000
C	-6.591000	-3.210000	-1.129000
C	-5.322000	-3.568000	-0.570000
N	-4.291000	-3.850000	-0.122000
C	-6.789000	-2.089000	-1.875000
C	-1.847000	-1.093000	-1.201000
C	-0.502000	-1.027000	-0.876000
C	0.297000	0.034000	-1.333000
C	-0.299000	1.029000	-2.129000
C	-1.644000	0.964000	-2.444000
C	-2.442000	-0.096000	-1.989000
H	-2.445000	-1.920000	-0.827000
H	-0.064000	-1.802000	-0.255000
H	0.304000	1.851000	-2.501000
H	-2.075000	1.745000	-3.065000
N	1.656000	0.102000	-1.008000
C	3.096000	-3.302000	-1.416000
C	3.915000	-3.413000	-0.286000
C	3.962000	-2.329000	0.599000
C	3.215000	-1.181000	0.369000
C	2.406000	-1.082000	-0.766000
C	2.359000	-2.149000	-1.664000
H	3.031000	-4.136000	-2.111000
H	3.261000	-0.349000	1.066000
H	1.732000	-2.080000	-2.549000
C	4.232000	2.765000	-1.276000
C	3.656000	3.813000	-0.546000
C	2.395000	3.599000	0.022000

C	1.731000	2.386000	-0.124000
C	2.311000	1.355000	-0.865000
C	3.568000	1.557000	-1.443000
H	1.939000	4.385000	0.619000
H	0.763000	2.233000	0.344000
H	4.025000	0.756000	-2.017000
H	-7.795000	-1.911000	-2.240000
H	4.586000	-2.391000	1.485000
H	5.208000	2.903000	-1.728000
C	4.731000	-4.635000	-0.072000
C	4.708000	-5.347000	1.150000
C	5.533000	-5.134000	-1.093000
C	5.474000	-6.497000	1.310000
C	6.307000	-6.288000	-0.954000
H	5.567000	-4.591000	-2.034000
C	6.272000	-6.968000	0.261000
H	5.478000	-7.066000	2.232000
H	6.920000	-6.623000	-1.782000
C	4.332000	5.126000	-0.391000
C	3.645000	6.307000	-0.649000
C	5.675000	5.235000	0.040000
C	4.224000	7.570000	-0.501000
H	2.616000	6.242000	-0.994000
C	6.271000	6.481000	0.194000
C	5.548000	7.649000	-0.078000
H	3.640000	8.455000	-0.725000
H	7.295000	6.592000	0.529000
O	6.975000	-8.096000	0.537000
O	3.882000	-4.853000	2.106000
O	6.314000	4.069000	0.305000
O	6.235000	8.806000	0.103000
C	7.799000	-8.648000	-0.478000
C	8.450000	-9.895000	0.085000
H	8.559000	-7.912000	-0.778000
H	7.187000	-8.890000	-1.359000
H	9.097000	-10.352000	-0.672000
H	9.058000	-9.650000	0.961000
H	7.692000	-10.626000	0.381000
C	3.788000	-5.484000	3.375000
C	4.943000	-5.114000	4.295000
H	3.694000	-6.571000	3.251000
H	2.844000	-5.118000	3.785000
H	4.801000	-5.582000	5.275000
H	5.906000	-5.442000	3.894000
H	4.981000	-4.029000	4.433000
C	7.647000	4.100000	0.788000
C	8.080000	2.665000	1.012000
H	7.688000	4.672000	1.725000
H	8.297000	4.595000	0.052000

H	9.108000	2.639000	1.388000
H	7.428000	2.176000	1.741000
H	8.038000	2.098000	0.077000
C	5.571000	10.036000	-0.143000
C	6.553000	11.154000	0.141000
H	4.690000	10.116000	0.508000
H	5.232000	10.070000	-1.188000
H	6.077000	12.124000	-0.038000
H	6.888000	11.118000	1.182000
H	7.430000	11.072000	-0.509000
C	-3.853000	-0.157000	-2.320000
C	-4.701000	0.664000	-3.037000
O	-4.543000	-1.212000	-1.847000
C	-5.976000	0.063000	-2.984000
H	-4.438000	1.589000	-3.527000
C	-5.841000	-1.093000	-2.238000
H	-6.892000	0.420000	-3.436000
I	-6.818000	1.002000	0.295000
I	-7.401000	2.163000	2.642000

Optimized coordinates for I_2 coordinated trans-AB3 at wB97XD/6-31+G* level of theory and basis set

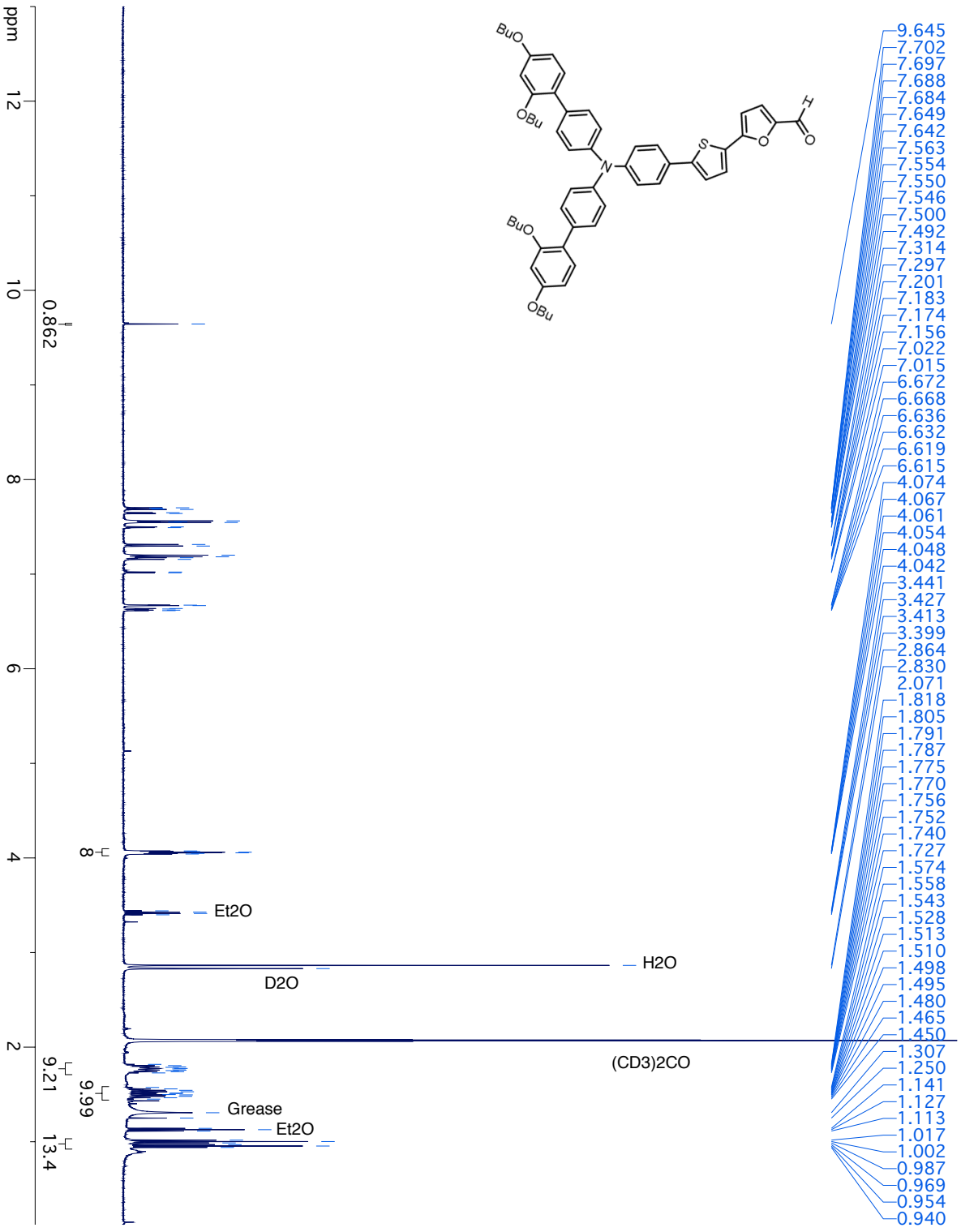
I	4.895000	-1.550000	3.767000
I	4.812000	-0.719000	1.223000
H	9.846000	2.614000	0.261000
O	9.128000	2.135000	-0.181000
C	9.707000	1.301000	-1.070000
O	10.906000	1.238000	-1.221000
C	8.724000	0.490000	-1.823000
C	9.263000	-0.413000	-2.790000
N	9.638000	-1.164000	-3.591000
C	7.385000	0.597000	-1.606000
C	2.323000	0.697000	-1.411000
C	0.984000	0.837000	-1.084000
C	0.040000	-0.110000	-1.512000
C	0.488000	-1.202000	-2.277000
C	1.829000	-1.343000	-2.588000
C	2.772000	-0.397000	-2.163000
H	3.031000	1.445000	-1.068000
H	0.662000	1.685000	-0.489000
H	-0.226000	-1.944000	-2.621000
H	2.147000	-2.205000	-3.167000
N	-1.313000	0.023000	-1.186000
C	-2.250000	3.589000	-1.676000
C	-3.054000	3.839000	-0.558000
C	-3.264000	2.791000	0.347000
C	-2.686000	1.544000	0.148000

C	-1.890000	1.305000	-0.975000
C	-1.684000	2.337000	-1.893000
H	-2.062000	4.388000	-2.388000
H	-2.860000	0.741000	0.860000
H	-1.069000	2.160000	-2.772000
C	-4.213000	-2.291000	-1.377000
C	-3.785000	-3.371000	-0.595000
C	-2.514000	-3.298000	-0.015000
C	-1.696000	-2.188000	-0.202000
C	-2.131000	-1.125000	-0.996000
C	-3.397000	-1.187000	-1.584000
H	-2.170000	-4.110000	0.621000
H	-0.721000	-2.140000	0.273000
H	-3.740000	-0.360000	-2.200000
H	7.065000	1.309000	-0.850000
H	-3.883000	2.957000	1.222000
H	-5.194000	-2.323000	-1.840000
C	-3.691000	5.169000	-0.379000
C	-3.592000	5.893000	0.832000
C	-4.397000	5.755000	-1.424000
C	-4.194000	7.141000	0.957000
C	-5.005000	7.008000	-1.321000
H	-4.491000	5.205000	-2.357000
C	-4.899000	7.699000	-0.116000
H	-4.137000	7.722000	1.870000
H	-5.551000	7.409000	-2.166000
C	-4.623000	-4.583000	-0.405000
C	-4.085000	-5.848000	-0.617000
C	-5.972000	-4.508000	0.013000
C	-4.817000	-7.024000	-0.440000
H	-3.052000	-5.921000	-0.950000
C	-6.720000	-5.667000	0.191000
C	-6.145000	-6.923000	-0.035000
H	-4.346000	-7.981000	-0.631000
H	-7.755000	-5.645000	0.510000
O	-5.444000	8.918000	0.128000
O	-2.859000	5.309000	1.813000
O	-6.449000	-3.260000	0.252000
O	-6.975000	-7.979000	0.168000
C	-6.168000	9.558000	-0.911000
C	-6.652000	10.893000	-0.381000
H	-7.016000	8.928000	-1.213000
H	-5.514000	9.699000	-1.784000
H	-7.217000	11.420000	-1.157000
H	-7.302000	10.750000	0.487000
H	-5.805000	11.519000	-0.082000
C	-2.738000	5.927000	3.086000
C	-3.971000	5.717000	3.954000
H	-2.495000	6.990000	2.970000

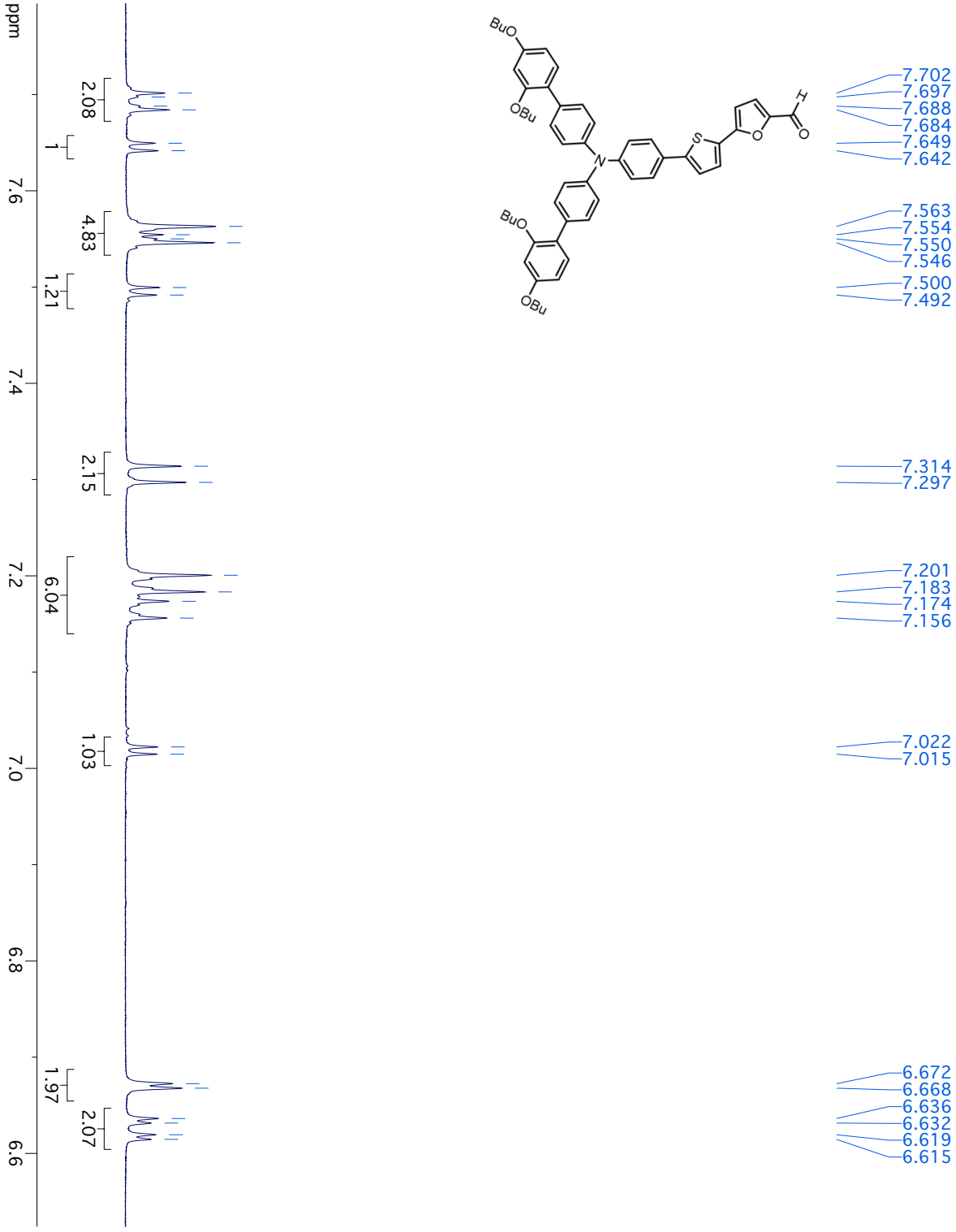
H	-1.870000	5.438000	3.537000
H	-3.810000	6.165000	4.941000
H	-4.863000	6.171000	3.513000
H	-4.160000	4.648000	4.088000
C	-7.806000	-3.066000	0.626000
C	-8.754000	-3.146000	-0.563000
H	-7.822000	-2.062000	1.056000
H	-8.086000	-3.770000	1.420000
H	-9.779000	-2.940000	-0.235000
H	-8.476000	-2.402000	-1.316000
H	-8.736000	-4.133000	-1.034000
C	-6.468000	-9.289000	-0.032000
C	-7.587000	-10.266000	0.269000
H	-5.611000	-9.459000	0.634000
H	-6.125000	-9.397000	-1.071000
H	-7.234000	-11.292000	0.125000
H	-7.926000	-10.156000	1.303000
H	-8.439000	-10.094000	-0.396000
C	4.181000	-0.560000	-2.489000
C	4.856000	-1.363000	-3.379000
O	5.066000	0.194000	-1.801000
C	6.231000	-1.082000	-3.223000
H	4.413000	-2.061000	-4.075000
C	6.332000	-0.117000	-2.245000
H	7.054000	-1.526000	-3.765000

4. NMR Spectrum

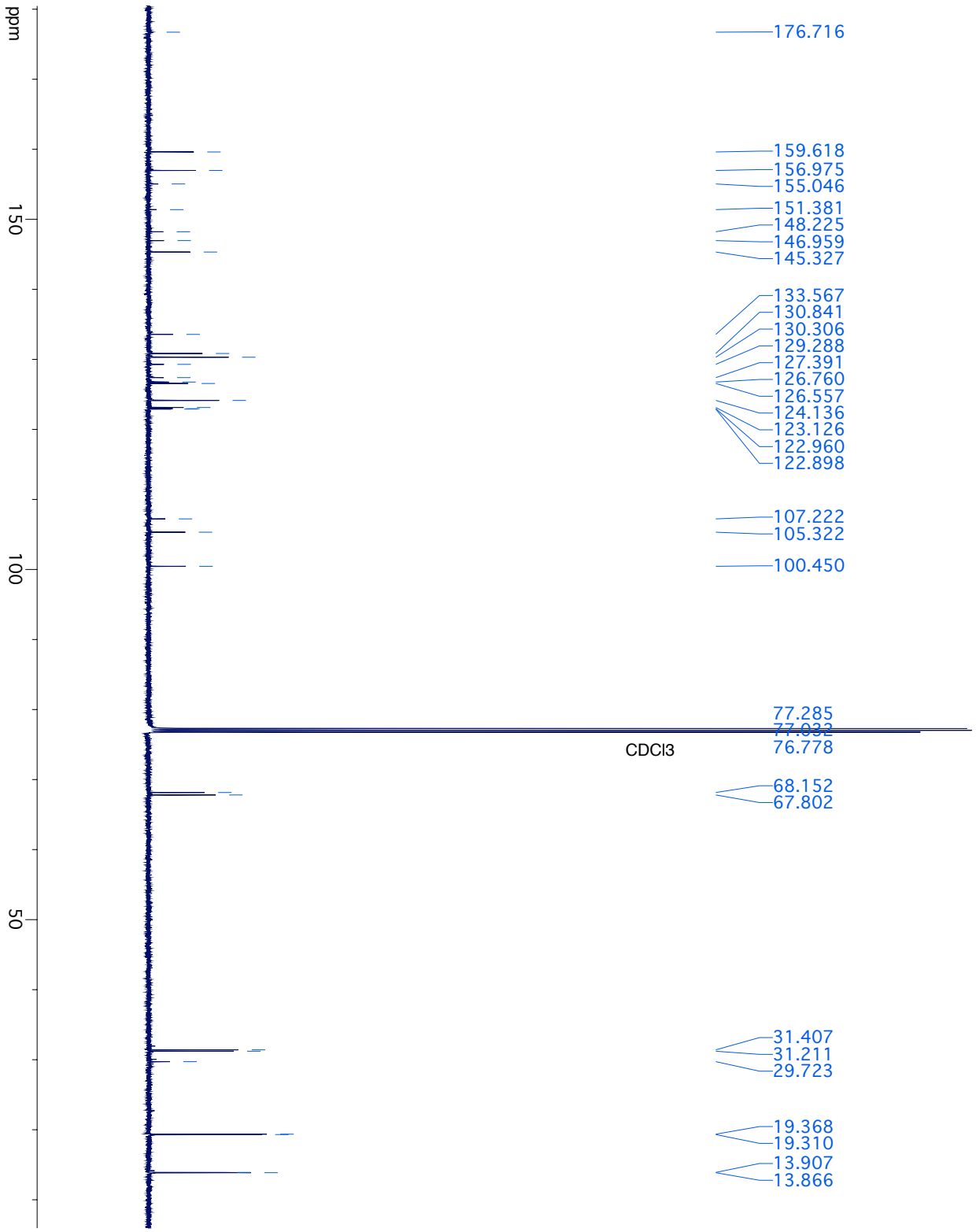
500 MHz, $(CD_3)_2CO$, room temperature



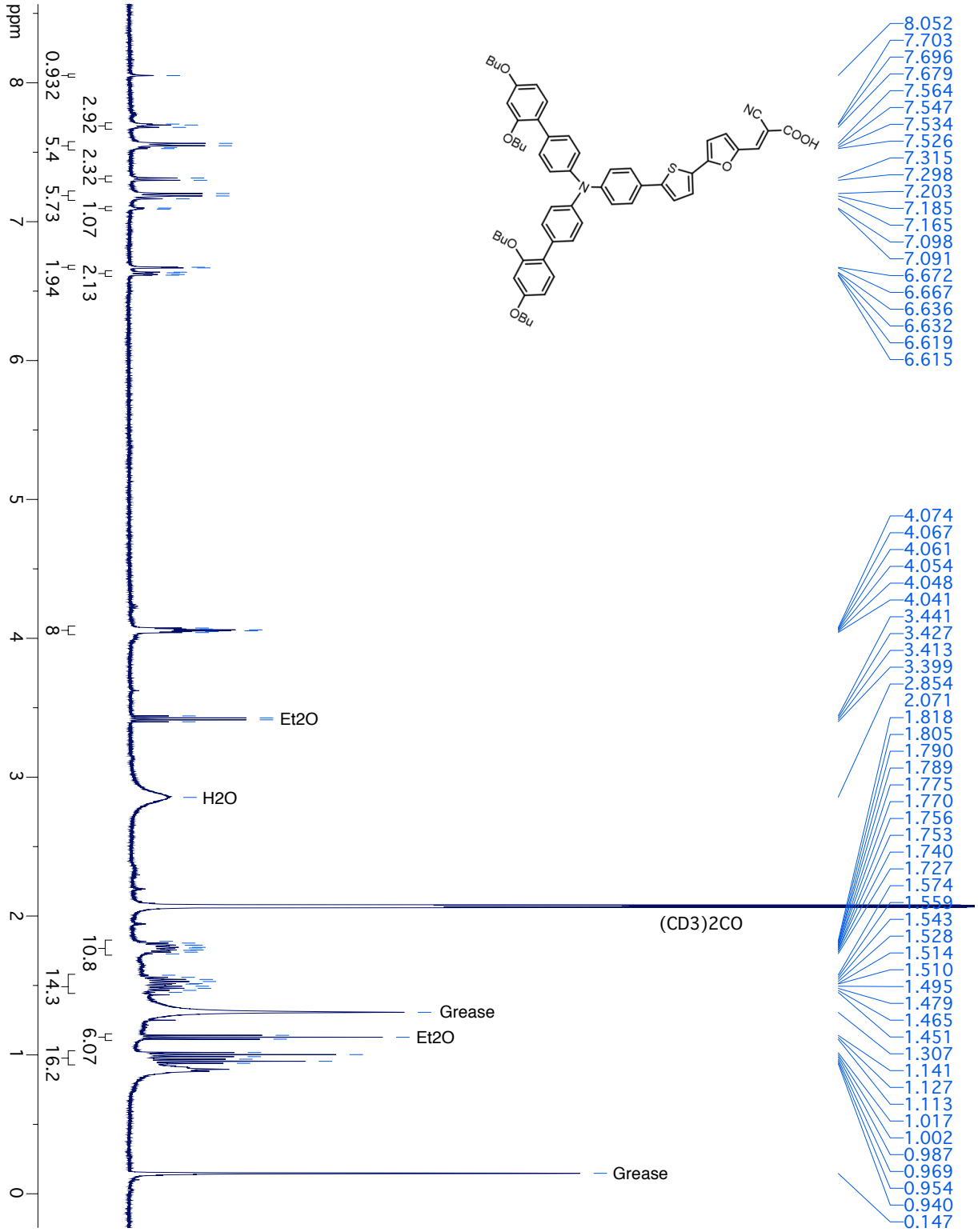
500 MHz, $(CD_3)_2CO$, room temperature



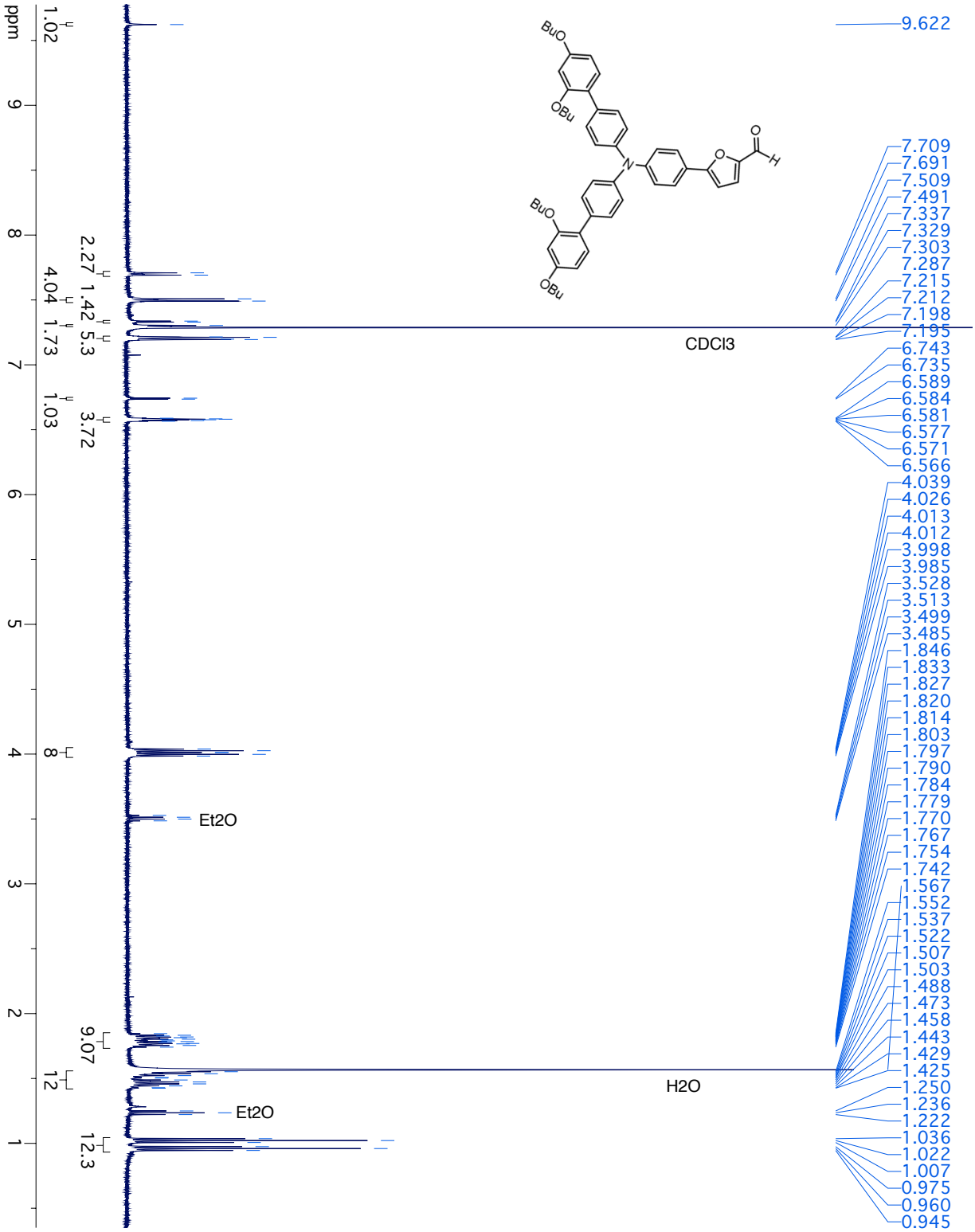
500 MHz, $CDCl_3$, room temperature



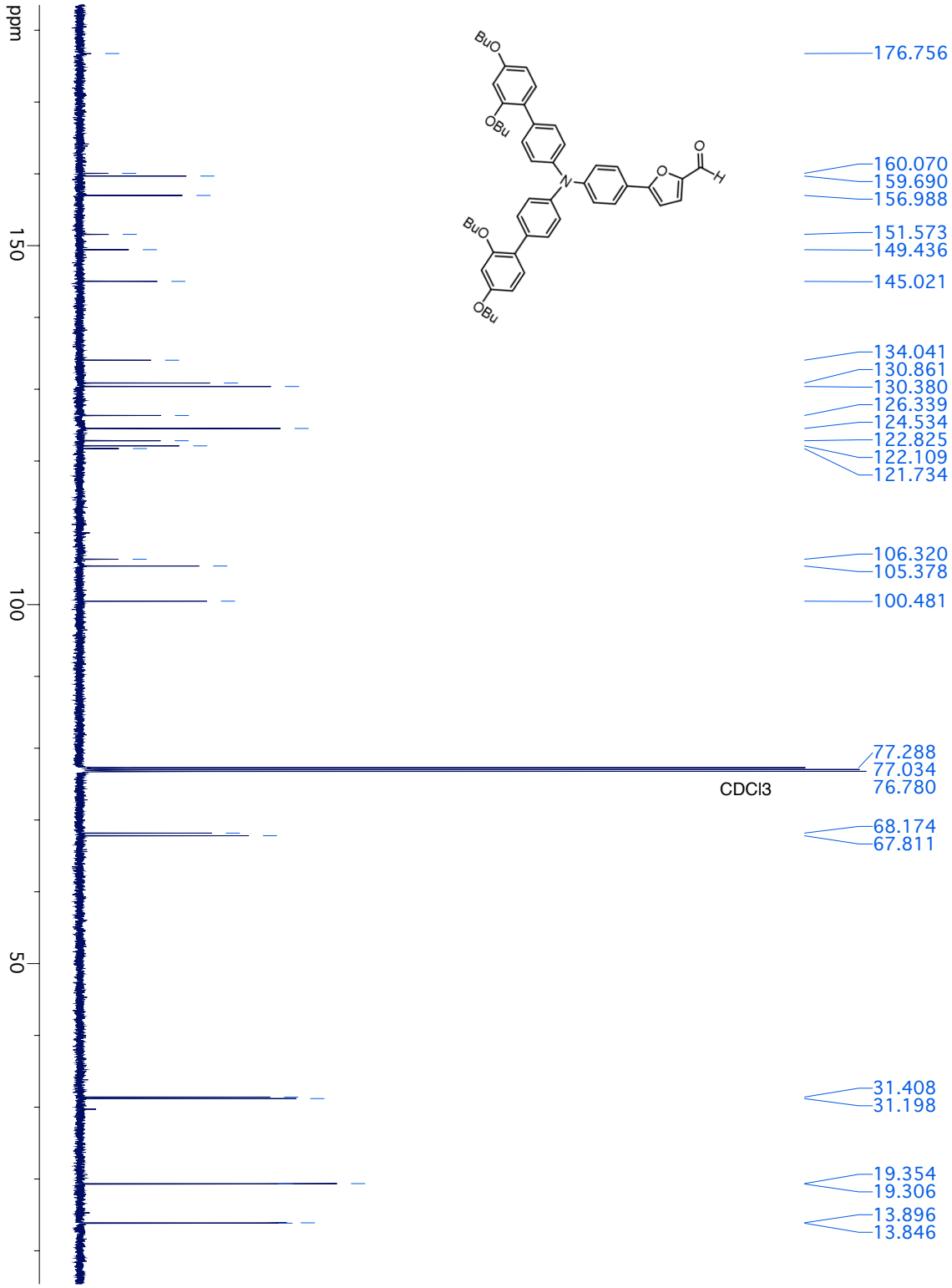
500 MHz, $(CD_3)_2CO$, room temperature



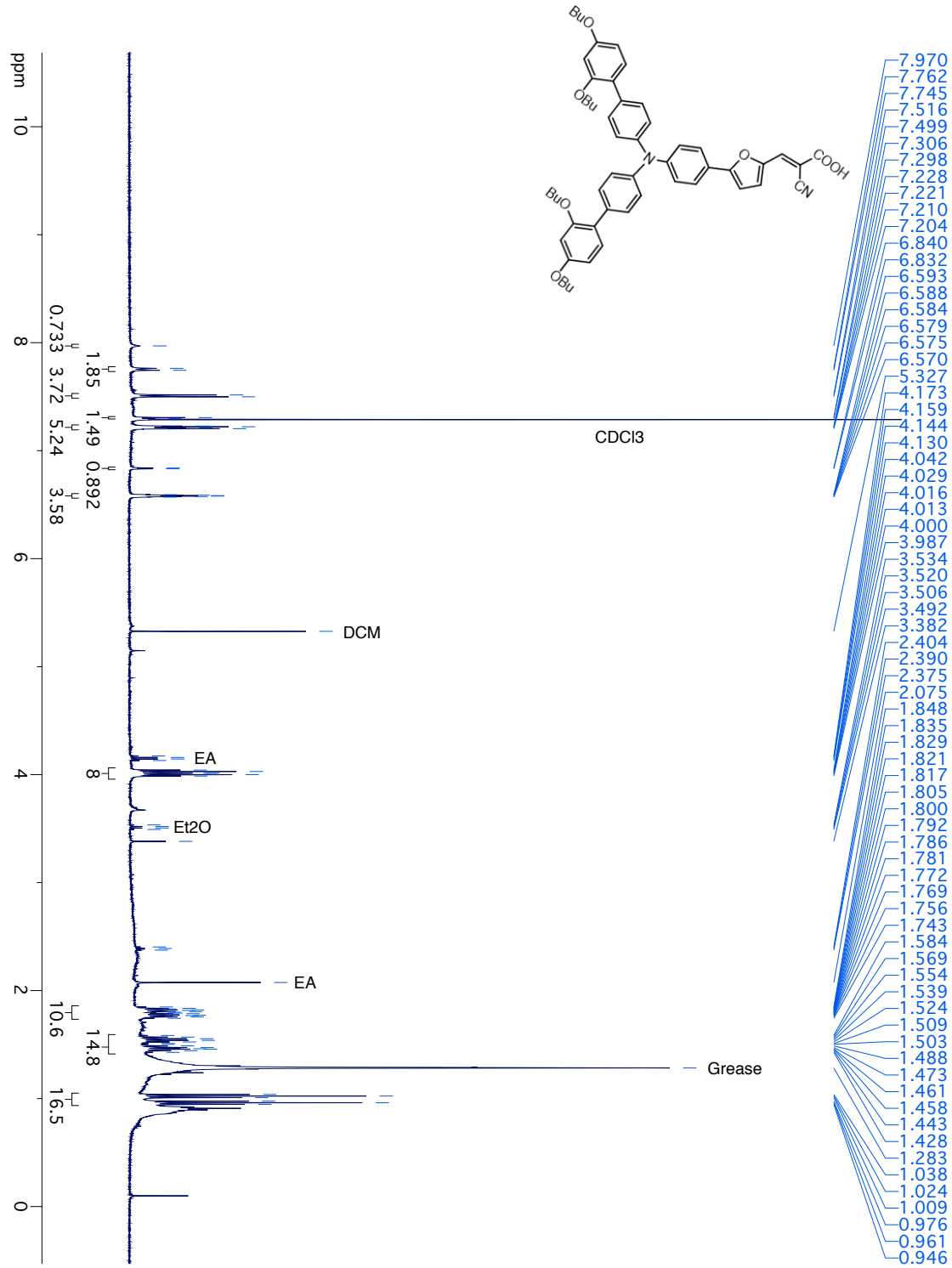
500 MHz, $CDCl_3$, room temperature



500 MHz, $CDCl_3$, room temperature



500 MHz, $CDCl_3$, room temperature, Note: We have found that with grease added we get a well resolved spectrum such as the one below to allow us to establish purity. The spectrum after this one has no grease added, leading to broad peaks, but shows evidence for the lack of grease in the sample.



500 MHz, $CDCl_3$, room temperature, See the note with the spectrum above.