

Electronic supplementary information

A 2,6-diamidopyridine-based macrocyclic aromatic amide receptor with cascade ion pair recognition

Xinguo Mao, Rui Zhang, Yulong Sun, Xuping Wang,* Qinggang Li, Han Zuilhof,*
Leyong Wang and Qiang Shi*

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1. Characterization of compounds 1 and MAA

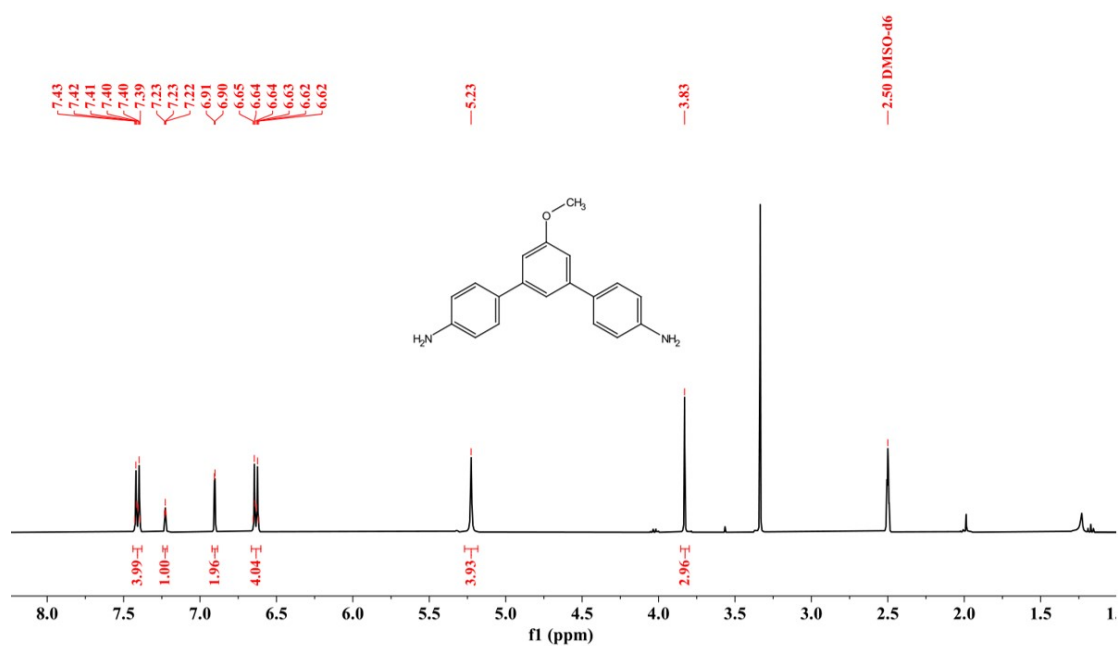


Fig. S1 ¹H NMR spectrum (400 MHz, DMSO-*d*₆, 298 K) of compound 1.

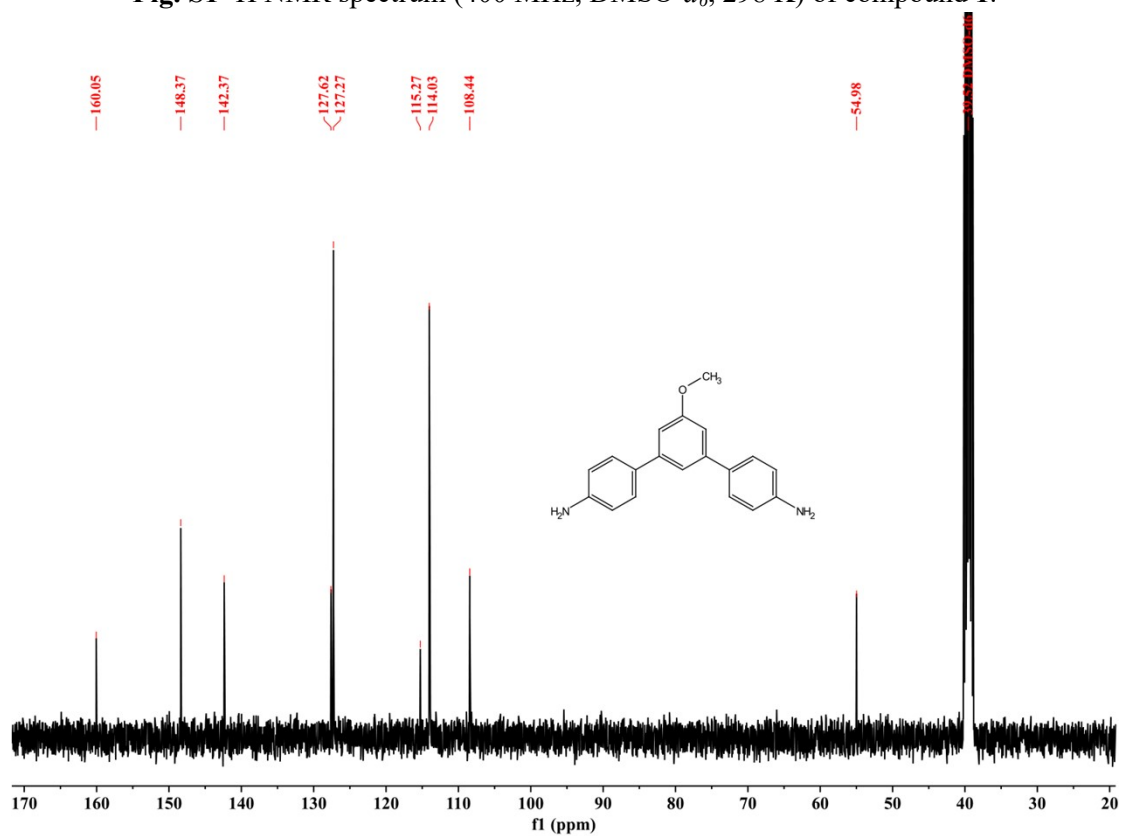


Fig. S2 ¹³C NMR spectrum (101 MHz, DMSO-*d*₆, 298 K) of compound 1.

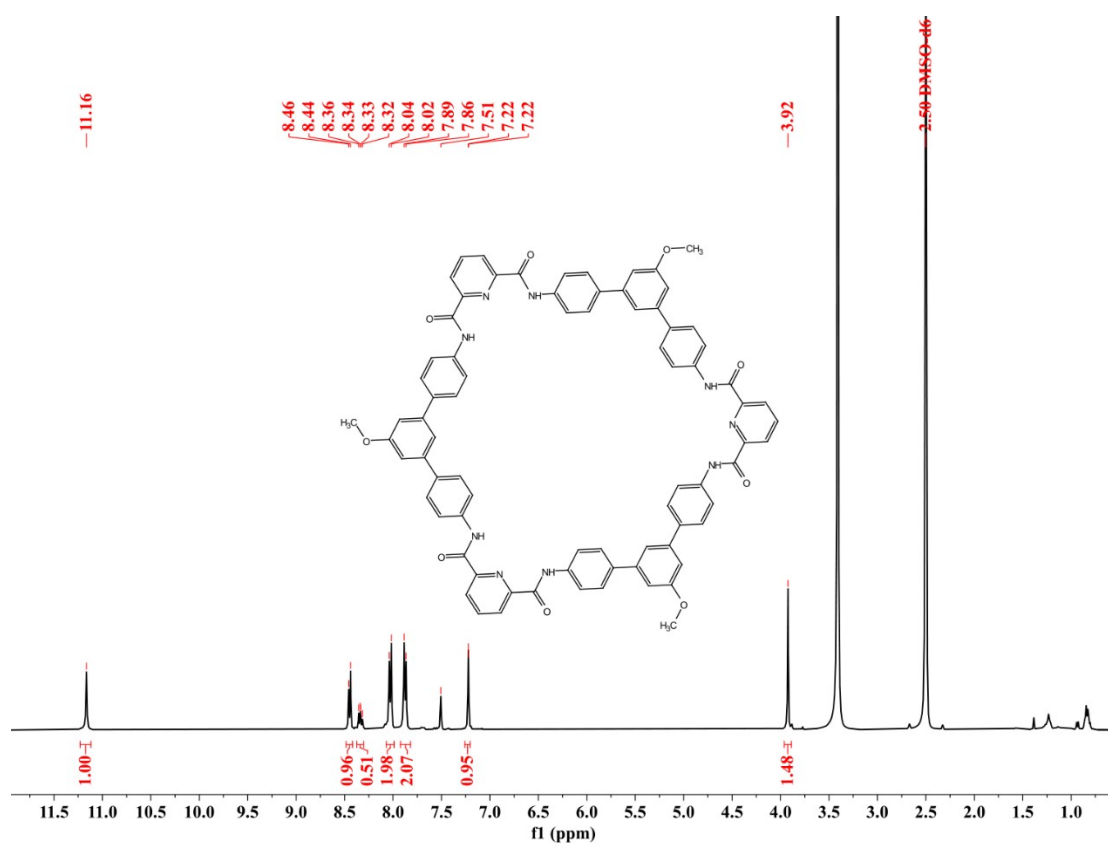


Fig. S3 ¹H NMR spectrum (400 MHz, DMSO-*d*₆, 298 K) of compound MAA.

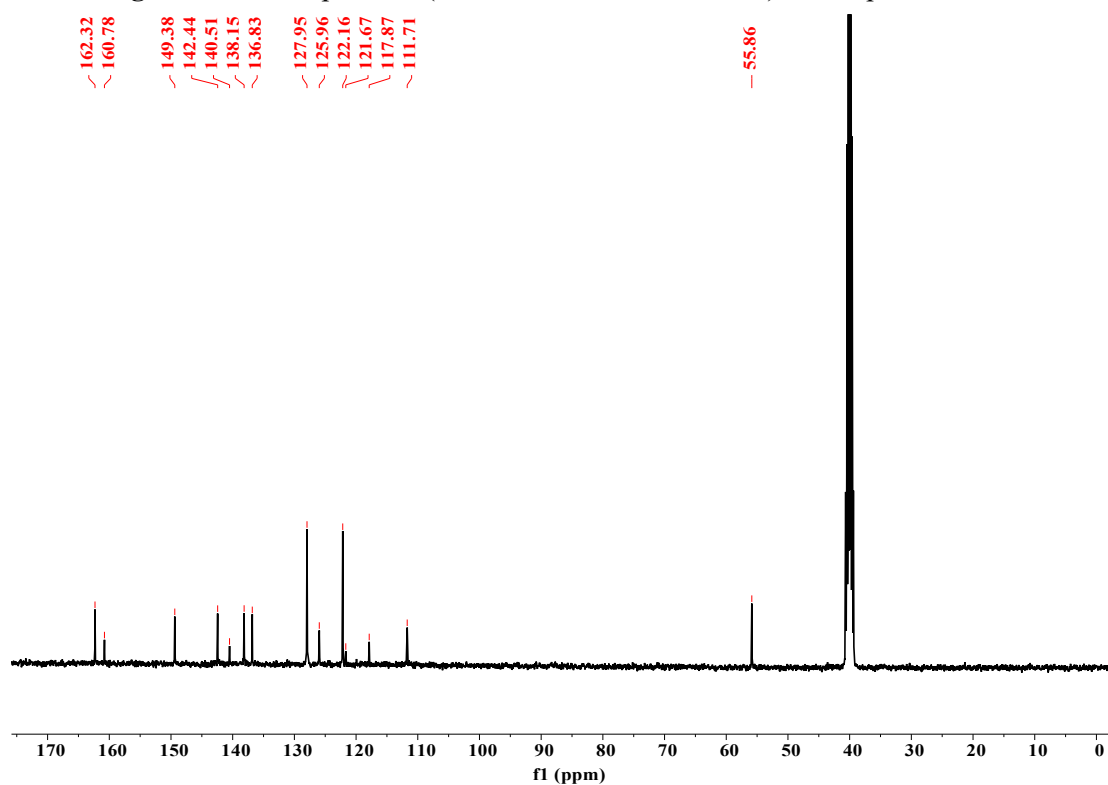


Fig. S4 ¹³C NMR spectrum (101 MHz, DMSO-*d*₆, 298 K) of compound MAA.

2. Quantitative research of the binding features of MAA

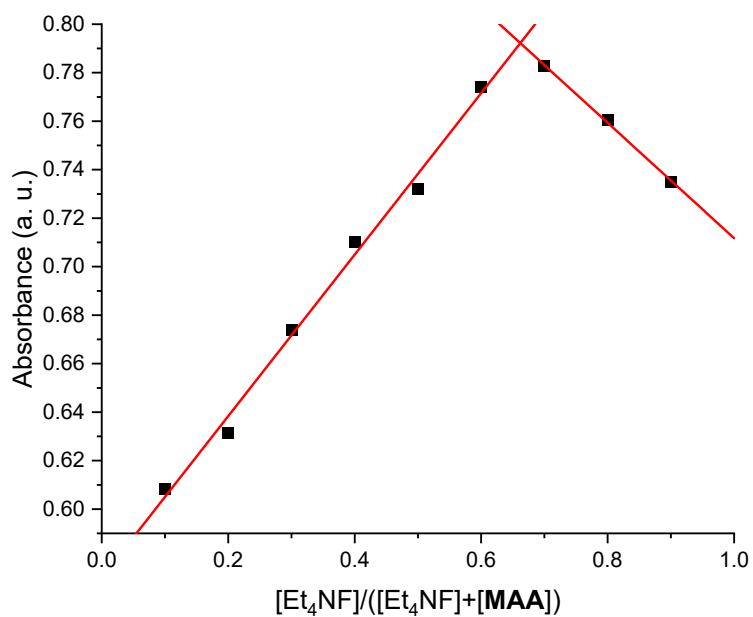


Fig. S5 Job's plot curve of UV-Vis variation detect the 1:2 complex ratio of MAA with F^-

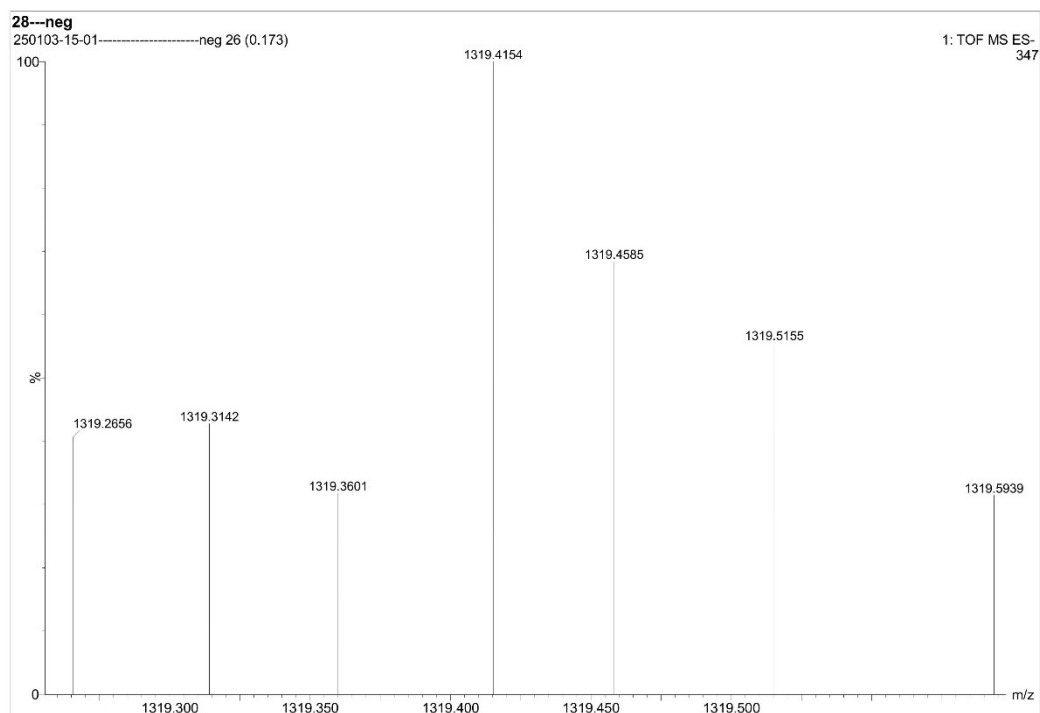


Fig. S6 Mass spectrum of MAA with F^- , the complex of $2F^-@MAA+NH_4^+$ was detected:

$C_{78}H_{61}F_2N_{10}O_9$, m/z , $[M + NH_4]^+$, Calculated: 1319.4596, Found: 1319.4585.

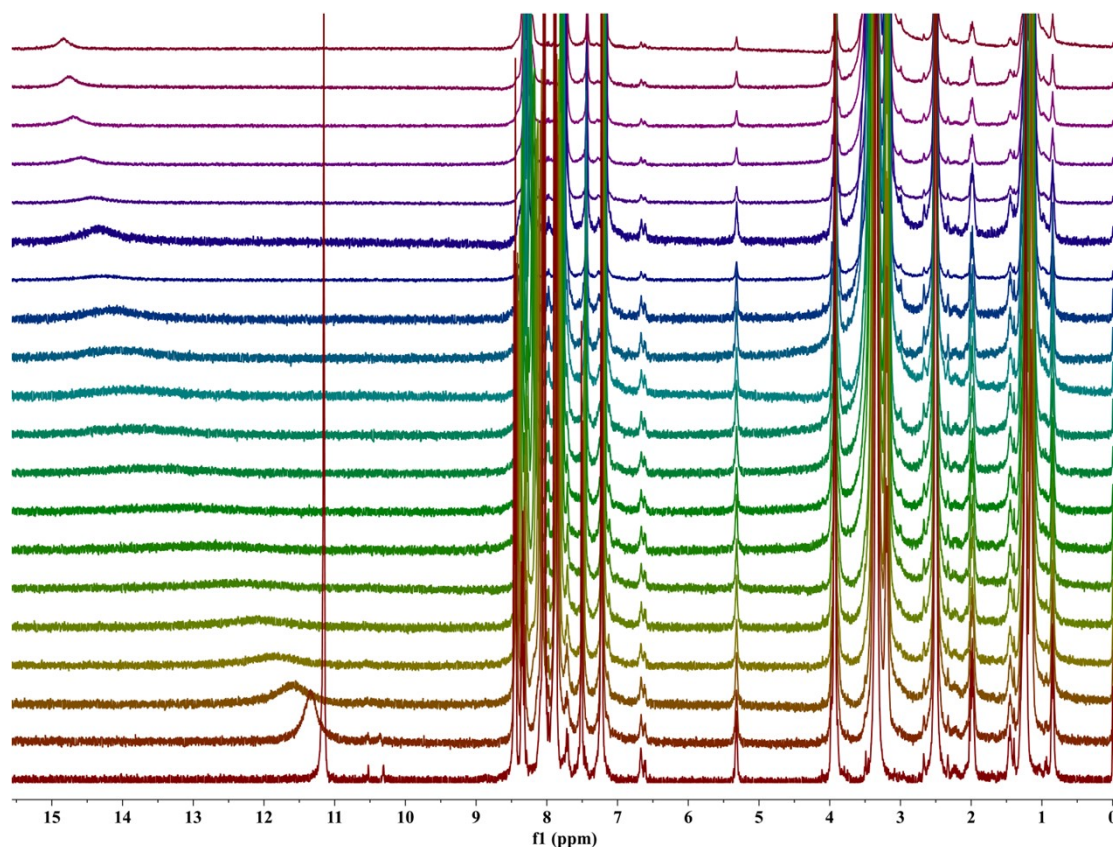


Fig. S7 ^1H NMR titration of **MAA** with fluoride ion (from bottom to top, the addition of 0 equiv. to 5.0 equiv. of F^- initially added 0.2 equiv. of F^- to each spectrum in turn, and the addition of 3 equiv. added 0.5 equiv. to each spectrum in turn to increase the amount of F^-).

3. Non-linear fitness of ^1H NMR titration data

The binding constants of **MAA** to fluoride ion were calculated by the non-linear fitting method on the BindFit website (<http://supramolecular.org>):

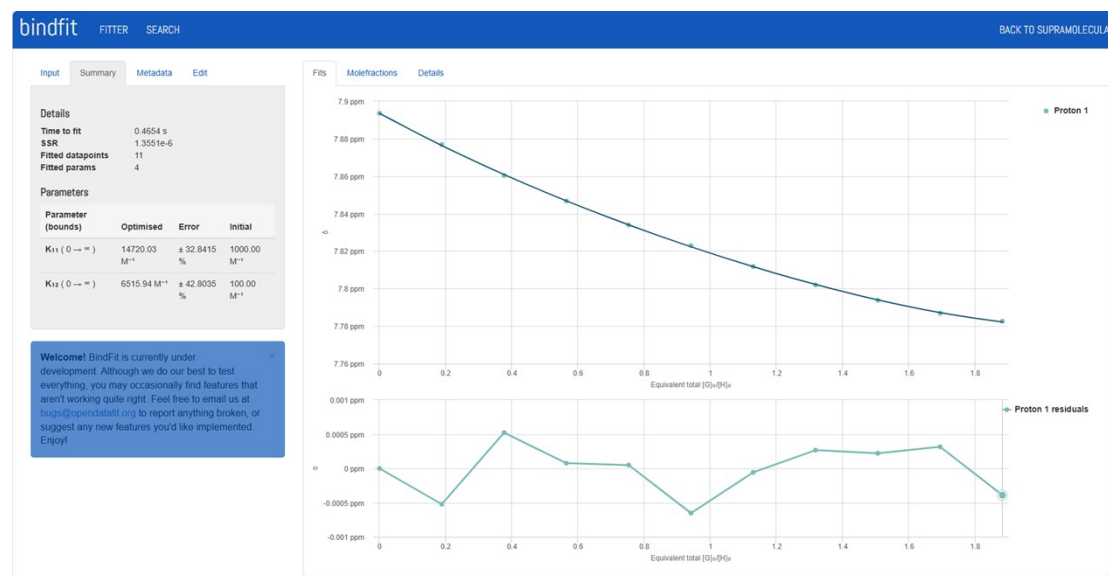


Fig. S8 Non-linear fit of ^1H NMR titration of **MAA** with Et_4NF (H_c signal was selected to calculate).

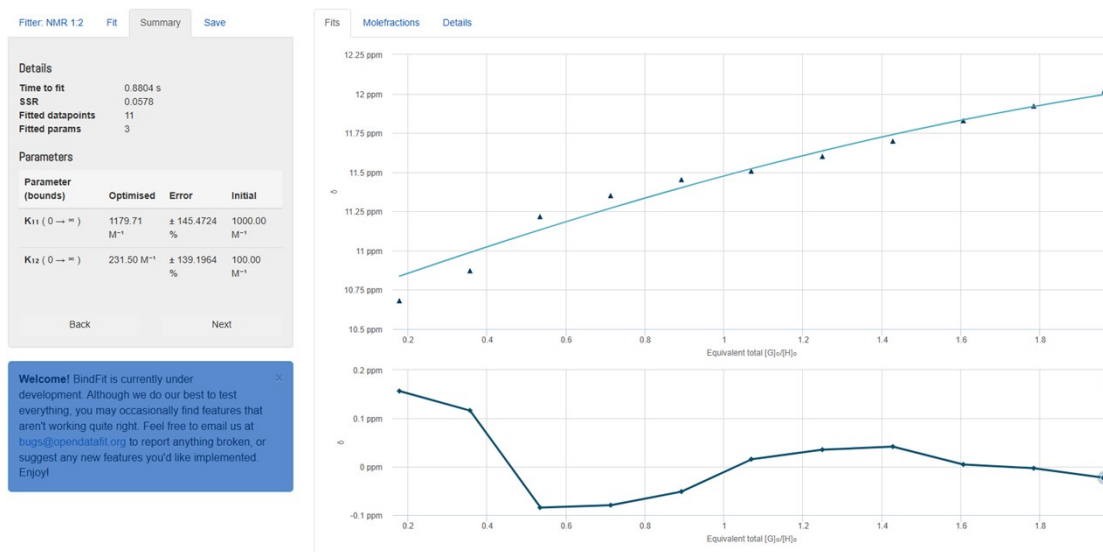


Fig. S9 Non-linear fit of ^1H NMR titration of **MAA** with $n\text{-Bu}_4\text{NF}$ (amide proton signal was selected).

4. ^{19}F NMR spectra studies

(a)

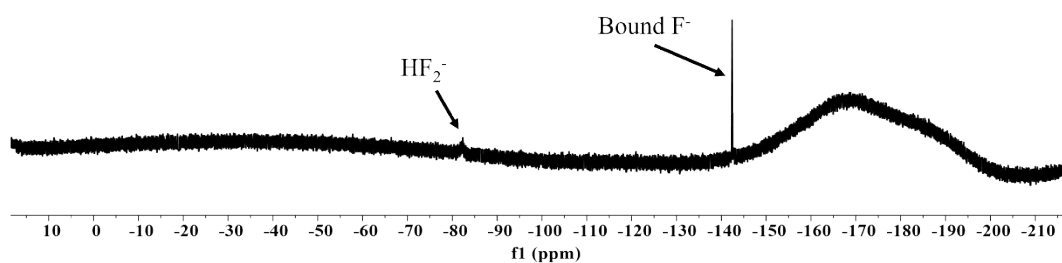
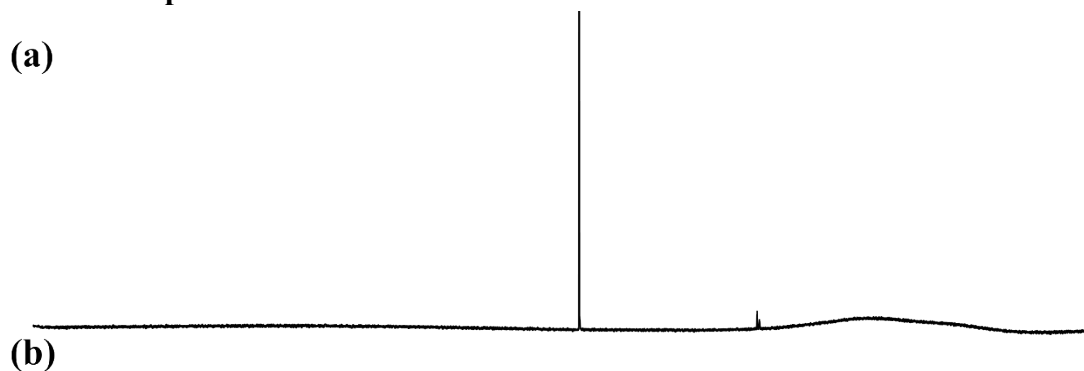


Fig. S10 ^{19}F NMR spectra of (a) Et_4NF and (b) **MAA** + 5.0 equiv. Et_4NF

5. ROESY study

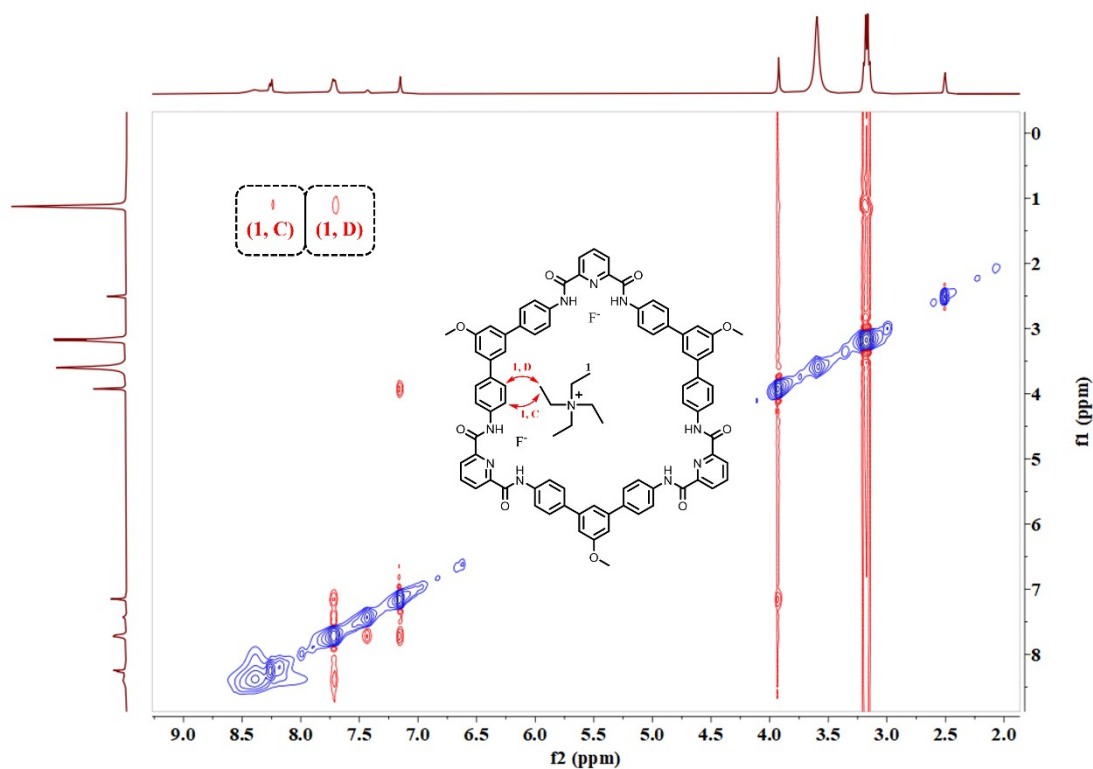


Fig. S11 ROESY spectrum of **MAA**, F^- and Et_4N^+ .

6. Detection limit

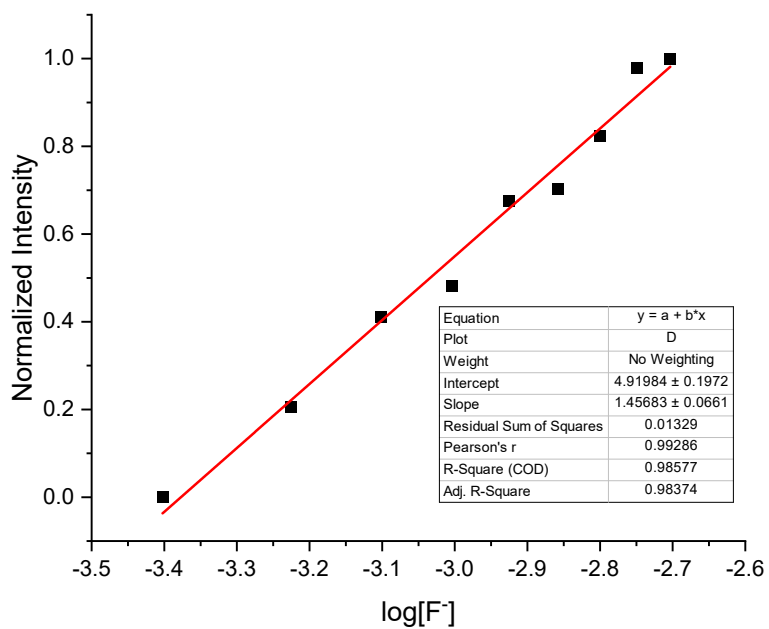


Fig. S12 Detection limit fit of **MAA** to fluoride ions in the presence of Et_4N^+ .

The linear fit equation is $y = 1.4568x + 4.9198$, the standard deviation (σ) of the data was

evaluated to be 0.3418, therefore, according to formula $D = 3\sigma/S$, which S is the slope of the linear fit line, the detection limit (D) was evaluated to be about 0.70×10^{-4} M.

7. DFT calculations

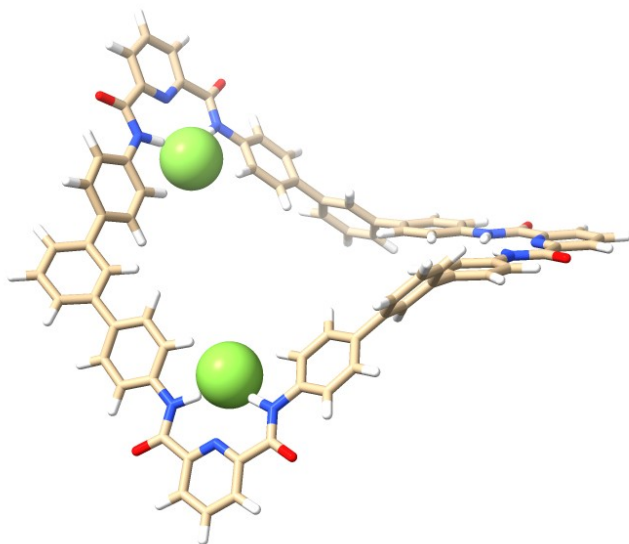


Fig. S13 The optimized structure of **MAA** with $2F^-$.

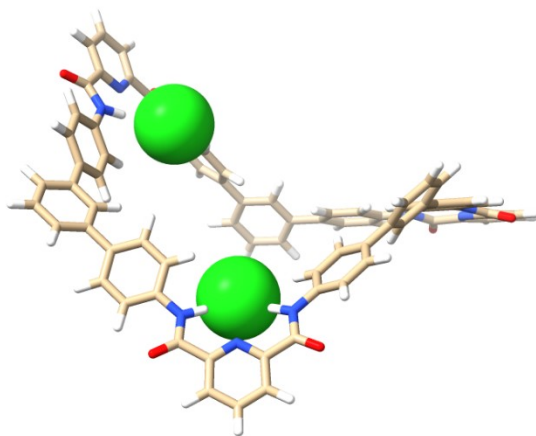


Fig. S14 The optimized structure of **MAA** with $2Cl^-$.

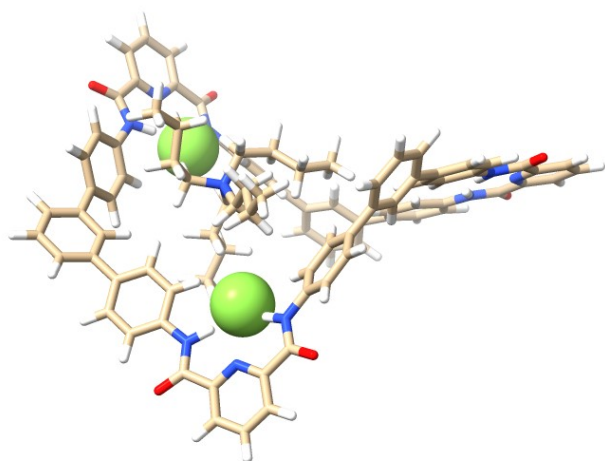


Fig. S15 The optimized structure of MAA with 2F^- and $\text{n-Bu}_4\text{N}^+$.

The coordination of the optimized structures:

MAA

C	-5.14730000	8.02010000	2.81640000
C	-5.40860000	9.11030000	3.63820000
C	-4.56590000	10.20950000	3.56260000
C	-3.50110000	10.18080000	2.67430000
C	-3.31590000	9.04000000	1.90190000
H	-6.25710000	9.08360000	4.30830000
H	-4.73940000	11.07870000	4.18520000
H	-2.81840000	11.01330000	2.57060000
C	-2.15490000	8.98620000	0.93530000
O	-1.48060000	9.97890000	0.71060000
N	-1.95760000	7.76410000	0.38810000
H	-2.57120000	7.03870000	0.73490000
C	-6.08020000	6.83030000	2.85600000
O	-6.99670000	6.78330000	3.66180000
N	-5.79770000	5.88960000	1.92470000
H	-4.99950000	6.11020000	1.34260000
N	-4.11940000	7.98110000	1.97150000
C	-0.93520000	7.38110000	-0.50340000
C	-0.35920000	8.27280000	-1.40760000
C	-0.51450000	6.05060000	-0.48900000
C	0.63220000	7.82990000	-2.27240000
H	-0.67690000	9.30510000	-1.42760000
C	0.47720000	5.62190000	-1.35730000
H	-0.96460000	5.34980000	0.20590000
C	1.07210000	6.50520000	-2.26160000
H	1.08220000	8.53830000	-2.95940000
H	0.78550000	4.58240000	-1.33670000
C	-6.50070000	4.71180000	1.61720000

C	-6.04440000	3.95680000	0.53270000
C	-7.62210000	4.27670000	2.32540000
C	-6.70560000	2.80090000	0.15320000
H	-5.17520000	4.28670000	-0.02670000
C	-8.27540000	3.11670000	1.92990000
H	-7.97780000	4.84080000	3.17380000
C	-7.84190000	2.36190000	0.83950000
H	-6.34570000	2.24770000	-0.70730000
H	-9.13940000	2.79000000	2.49830000
C	2.14650000	6.05310000	-3.18040000
C	3.19480000	5.26320000	-2.70570000
C	2.14100000	6.42720000	-4.52640000
C	4.23280000	4.84820000	-3.54240000
H	3.22510000	5.00470000	-1.65230000
C	3.16240000	6.01230000	-5.37150000
H	1.32770000	7.03010000	-4.91530000
C	4.20200000	5.22900000	-4.88690000
H	3.14280000	6.29310000	-6.41860000
H	4.98640000	4.89990000	-5.55950000
C	5.35870000	4.04510000	-3.00400000
C	6.67200000	4.29510000	-3.40300000
C	5.14370000	3.02620000	-2.07070000
C	7.74320000	3.57020000	-2.89680000
H	6.87480000	5.09040000	-4.11190000
C	6.20010000	2.29450000	-1.55610000
H	4.13500000	2.79020000	-1.74980000
C	7.51150000	2.56110000	-1.96090000
H	8.75060000	3.79160000	-3.21410000
H	6.00770000	1.50650000	-0.83540000
C	-8.57890000	1.14550000	0.41440000
C	-9.97660000	1.13320000	0.40880000
C	-7.89630000	0.00000000	0.00000000
C	-10.66700000	0.00000000	0.00000000
H	-10.52520000	2.01980000	0.70700000
C	-8.57890000	-1.14550000	-0.41440000
H	-6.81110000	0.00000000	0.00000000
C	-9.97660000	-1.13320000	-0.40890000
H	-11.75110000	0.00000000	0.00000000
H	-10.52520000	-2.01970000	-0.70700000
C	-7.84190000	-2.36190000	-0.83950000
C	-6.70570000	-2.80090000	-0.15320000
C	-8.27540000	-3.11670000	-1.92990000
C	-6.04440000	-3.95680000	-0.53270000
H	-6.34570000	-2.24770000	0.70730000

C	-7.62210000	-4.27670000	-2.32540000
H	-9.13940000	-2.79000000	-2.49830000
C	-6.50070000	-4.71180000	-1.61720000
H	-5.17520000	-4.28670000	0.02670000
H	-7.97780000	-4.84080000	-3.17380000
C	10.65570000	-0.88210000	0.72840000
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C	12.74860000	0.00000000	0.00000000
C	12.04480000	0.92020000	-0.76280000
C	10.65570000	0.88200000	-0.72840000
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H	13.83170000	0.00000000	0.00000000
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C	9.87280000	1.88540000	-1.54620000
O	10.44790000	2.69270000	-2.25960000
N	8.53280000	1.78320000	-1.38910000
H	8.24670000	1.05600000	-0.74630000
C	9.87280000	-1.88550000	1.54620000
O	10.44790000	-2.69270000	2.25960000
N	8.53280000	-1.78320000	1.38910000
H	8.24670000	-1.05600000	0.74630000
C	-3.31590000	-9.04000000	-1.90190000
C	-3.50110000	-10.18080000	-2.67430000
C	-4.56600000	-10.20950000	-3.56260000
C	-5.40860000	-9.11030000	-3.63820000
C	-5.14730000	-8.02010000	-2.81640000
H	-2.81840000	-11.01330000	-2.57060000
H	-4.73940000	-11.07870000	-4.18520000
H	-6.25710000	-9.08360000	-4.30830000
C	-6.08020000	-6.83030000	-2.85600000
O	-6.99670000	-6.78330000	-3.66180000
N	-5.79770000	-5.88960000	-1.92470000
H	-4.99960000	-6.11020000	-1.34260000
C	-2.15500000	-8.98620000	-0.93530000
O	-1.48060000	-9.97890000	-0.71060000
N	-1.95770000	-7.76410000	-0.38800000
H	-2.57120000	-7.03870000	-0.73490000
C	7.51150000	-2.56110000	1.96090000
C	6.20010000	-2.29450000	1.55610000
C	7.74320000	-3.57020000	2.89680000
C	5.14370000	-3.02620000	2.07070000
H	6.00770000	-1.50650000	0.83540000
C	6.67200000	-4.29510000	3.40300000
H	8.75060000	-3.79160000	3.21410000

C	5.35870000	-4.04510000	3.00400000
H	4.13500000	-2.79020000	1.74980000
H	6.87480000	-5.09040000	4.11190000
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C	4.20190000	-5.22900000	4.88690000
C	3.19480000	-5.26320000	2.70570000
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H	4.98640000	-4.89990000	5.55950000
C	2.14650000	-6.05310000	3.18040000
H	3.22510000	-5.00470000	1.65230000
C	2.14100000	-6.42720000	4.52640000
H	3.14280000	-6.29300000	6.41860000
H	1.32770000	-7.03010000	4.91530000
C	1.07210000	-6.50520000	2.26160000
C	0.47720000	-5.62190000	1.35730000
C	0.63210000	-7.82990000	2.27240000
C	-0.51450000	-6.05060000	0.48910000
H	0.78550000	-4.58240000	1.33670000
C	-0.35920000	-8.27280000	1.40760000
H	1.08220000	-8.53830000	2.95940000
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H	-0.96460000	-5.34980000	-0.20590000
H	-0.67700000	-9.30510000	1.42760000
N	9.97490000	0.00000000	0.00000000
N	-4.11940000	-7.98110000	-1.97150000
MAA + 2F-			
C	-5.40560000	8.27320000	2.62420000
C	-5.75240000	9.34480000	3.44390000
C	-4.95450000	10.48080000	3.40260000
C	-3.84940000	10.51170000	2.56170000
C	-3.58630000	9.38370000	1.78810000
H	-6.62490000	9.26200000	4.07930000
H	-5.19100000	11.33760000	4.02580000
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O	-1.70350000	10.37480000	0.75410000
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C	-6.25420000	7.01850000	2.61690000
O	-7.28500000	7.00280000	3.28810000
N	-5.77780000	6.02760000	1.83900000
H	-4.85030000	6.14840000	1.32520000
N	-4.35360000	8.30720000	1.82370000
C	-1.03580000	7.83240000	-0.49440000

C	-0.17250000	8.77570000	-1.06000000
C	-0.80140000	6.47020000	-0.72940000
C	0.89780000	8.35200000	-1.83800000
H	-0.33510000	9.82660000	-0.87490000
C	0.28460000	6.06760000	-1.48920000
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C	1.15420000	7.00050000	-2.06200000
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H	0.44900000	5.00850000	-1.66140000
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C	-5.86690000	3.99540000	0.57840000
C	-7.59220000	4.38180000	2.21670000
C	-6.48320000	2.80960000	0.21440000
H	-4.94780000	4.33100000	0.10530000
C	-8.18880000	3.18600000	1.84100000
H	-8.02190000	4.98650000	3.00030000
C	-7.66940000	2.38450000	0.82380000
H	-6.04650000	2.21700000	-0.58320000
H	-9.08130000	2.86580000	2.36940000
C	2.30920000	6.58880000	-2.90040000
C	3.27010000	5.69090000	-2.42920000
C	2.47060000	7.13540000	-4.17610000
C	4.39000000	5.34710000	-3.19230000
H	3.16970000	5.29410000	-1.42390000
C	3.56350000	6.78410000	-4.95670000
H	1.72160000	7.82240000	-4.55580000
C	4.51570000	5.89870000	-4.47150000
H	3.66850000	7.19500000	-5.95610000
H	5.36090000	5.61670000	-5.09030000
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C	6.79650000	4.77110000	-2.87610000
C	5.17060000	3.30200000	-1.92720000
C	7.82560000	3.97040000	-2.39900000
H	7.05160000	5.67950000	-3.41340000
C	6.18120000	2.48600000	-1.44570000
H	4.13750000	3.02050000	-1.74920000
C	7.52650000	2.81010000	-1.67690000
H	8.85590000	4.23960000	-2.57270000
H	5.96710000	1.57720000	-0.88890000
C	-8.38440000	1.15370000	0.39970000
C	-9.78340000	1.13970000	0.38000000
C	-7.70530000	-0.00250000	0.00210000
C	-10.47250000	-0.00370000	0.00420000
H	-10.32970000	2.03830000	0.64450000

C	-8.38400000	-1.15930000	-0.39440000
H	-6.62020000	-0.00200000	0.00130000
C	-9.78300000	-1.14650000	-0.37260000
H	-11.55830000	-0.00420000	0.00510000
H	-10.32880000	-2.04560000	-0.63630000
C	-7.66860000	-2.38940000	-0.81980000
C	-6.48100000	-2.81340000	-0.21220000
C	-8.18870000	-3.19120000	-1.83620000
C	-5.86410000	-3.99860000	-0.57730000
H	-6.04360000	-2.22060000	0.58480000
C	-7.59160000	-4.38640000	-2.21310000
H	-9.08240000	-2.87180000	-2.36310000
C	-6.42650000	-4.81580000	-1.56920000
H	-4.94400000	-4.33340000	-0.10570000
H	-8.02200000	-4.99130000	-2.99610000
C	10.63310000	-0.97470000	0.59480000
C	12.02510000	-1.02080000	0.62480000
C	12.72410000	0.00530000	0.00280000
C	12.02440000	1.03040000	-0.62010000
C	10.63240000	0.98230000	-0.59190000
H	12.51420000	-1.84600000	1.12620000
H	13.80970000	0.00620000	0.00350000
H	12.51290000	1.85640000	-1.12090000
C	9.82630000	2.07920000	-1.25580000
O	10.43110000	2.99260000	-1.81590000
N	8.49170000	1.93130000	-1.15590000
H	8.08540000	1.08810000	-0.64620000
C	9.82780000	-2.07260000	1.25780000
O	10.43310000	-2.98560000	1.81790000
N	8.49310000	-1.92610000	1.15720000
H	8.08610000	-1.08300000	0.64770000
C	-3.58050000	-9.38470000	-1.79130000
C	-3.84230000	-10.51180000	-2.56660000
C	-4.94740000	-10.48100000	-3.40750000
C	-5.74660000	-9.34580000	-3.44710000
C	-5.40110000	-8.27500000	-2.62570000
H	-3.18260000	-11.36700000	-2.49420000
H	-5.18290000	-11.33710000	-4.03190000
H	-6.61920000	-9.26310000	-4.08240000
C	-6.25110000	-7.02130000	-2.61670000
O	-7.28240000	-7.00610000	-3.28710000
N	-5.77500000	-6.03050000	-1.83850000
H	-4.84680000	-6.15070000	-1.32570000
C	-2.36970000	-9.35310000	-0.88180000

O	-1.69710000	-10.37530000	-0.75800000
N	-2.14080000	-8.15750000	-0.30710000
H	-2.80290000	-7.34130000	-0.48340000
C	7.52840000	-2.80600000	1.67760000
C	6.18290000	-2.48270000	1.44640000
C	7.82840000	-3.96650000	2.39890000
C	5.17290000	-3.29970000	1.92730000
H	5.96820000	-1.57370000	0.89020000
C	6.79980000	-4.76830000	2.87530000
H	8.85880000	-4.23510000	2.57250000
C	5.45770000	-4.45870000	2.65800000
H	4.13960000	-3.01880000	1.74950000
H	7.05550000	-5.67680000	3.41210000
C	4.39360000	-5.34620000	3.19110000
C	4.51980000	-5.89860000	4.47000000
C	3.27400000	-5.69020000	2.42780000
C	3.56820000	-6.78490000	4.95460000
H	5.36480000	-5.61640000	5.08890000
C	2.31370000	-6.58910000	2.89850000
H	3.17340000	-5.29280000	1.42280000
C	2.47550000	-7.13640000	4.17380000
H	3.67350000	-7.19640000	5.95370000
H	1.72700000	-7.82410000	4.55310000
C	1.15890000	-7.00090000	2.05980000
C	0.28880000	-6.06820000	1.48760000
C	0.90330000	-8.35240000	1.83510000
C	-0.79700000	-6.47100000	0.72750000
H	0.45260000	-5.00910000	1.66040000
C	-0.16680000	-8.77630000	1.05680000
H	1.57280000	-9.09520000	2.25880000
C	-1.03060000	-7.83320000	0.49190000
H	-1.50050000	-5.75500000	0.31170000
H	-0.32880000	-9.82720000	0.87110000
N	9.97000000	0.00330000	0.00090000
N	-4.34910000	-8.30900000	-1.82520000
F	-3.54230000	-5.95370000	-0.48330000
F	-3.54660000	5.95210000	0.48150000
MAA + 2F⁻			
C	-5.77900000	7.91900000	2.43180000
C	-6.07300000	8.99340000	3.26470000
C	-5.17830000	10.05200000	3.31620000
C	-4.04260000	10.00830000	2.52210000
C	-3.83720000	8.88910000	1.72050000
H	-6.98360000	8.98480000	3.84840000

H	-5.36760000	10.90210000	3.96030000
H	-3.32300000	10.81570000	2.50960000
C	-2.62350000	8.85780000	0.82090000
O	-2.02780000	9.89670000	0.56680000
N	-2.28490000	7.63460000	0.35220000
H	-2.77250000	6.82930000	0.74970000
C	-6.76570000	6.77710000	2.34270000
O	-7.90500000	6.91400000	2.77090000
N	-6.27870000	5.66110000	1.75980000
H	-5.29160000	5.66940000	1.49910000
N	-4.67990000	7.86060000	1.68290000
C	-1.20610000	7.35300000	-0.51440000
C	-0.73990000	8.26940000	-1.45860000
C	-0.61420000	6.09040000	-0.44230000
C	0.30960000	7.92290000	-2.29900000
H	-1.18560000	9.25040000	-1.52950000
C	0.42920000	5.75680000	-1.29130000
H	-0.99110000	5.37040000	0.27560000
C	0.91730000	6.66760000	-2.23200000
H	0.67030000	8.65710000	-3.01140000
H	0.86160000	4.76410000	-1.22640000
C	-6.98500000	4.47560000	1.47630000
C	-6.50970000	3.67130000	0.43790000
C	-8.10860000	4.06470000	2.19420000
C	-7.14870000	2.48420000	0.12050000
H	-5.63420000	3.98410000	-0.11930000
C	-8.74170000	2.87380000	1.86290000
H	-8.48000000	4.66790000	3.00910000
C	-8.28140000	2.06270000	0.82400000
H	-6.77100000	1.88960000	-0.70400000
H	-9.60120000	2.56320000	2.44700000
C	2.04650000	6.31210000	-3.12750000
C	3.13280000	5.58350000	-2.63880000
C	2.05360000	6.70520000	-4.46870000
C	4.21290000	5.24050000	-3.45450000
H	3.15540000	5.30920000	-1.58930000
C	3.12310000	6.37320000	-5.29070000
H	1.21230000	7.25580000	-4.87520000
C	4.19620000	5.64540000	-4.79210000
H	3.11300000	6.67090000	-6.33330000
H	5.01560000	5.37450000	-5.44890000
C	5.35640000	4.47250000	-2.90240000
C	6.67080000	4.77990000	-3.25360000
C	5.15210000	3.41970000	-2.00460000

C	7.75190000	4.07770000	-2.73380000
H	6.86610000	5.60330000	-3.93220000
C	6.21690000	2.70640000	-1.48270000
H	4.14320000	3.13910000	-1.72180000
C	7.53070000	3.02910000	-1.83820000
H	8.75880000	4.34520000	-3.01420000
H	6.04060000	1.89730000	-0.78310000
C	-8.97340000	0.79500000	0.48010000
C	-10.36790000	0.70770000	0.52270000
C	-8.24500000	-0.33350000	0.09770000
C	-11.00710000	-0.48130000	0.19650000
H	-10.95630000	1.57720000	0.79380000
C	-8.87470000	-1.53350000	-0.23870000
H	-7.16220000	-0.27630000	0.05910000
C	-10.27000000	-1.59630000	-0.18090000
H	-12.08910000	-0.53920000	0.23560000
H	-10.77980000	-2.52420000	-0.41540000
C	-8.07860000	-2.71790000	-0.64770000
C	-6.86580000	-3.02970000	-0.02540000
C	-8.51730000	-3.55610000	-1.67400000
C	-6.12880000	-4.13780000	-0.40890000
H	-6.49980000	-2.41170000	0.78710000
C	-7.78650000	-4.66780000	-2.07250000
H	-9.44060000	-3.32830000	-2.19570000
C	-6.58180000	-4.97030000	-1.43590000
H	-5.19190000	-4.36580000	0.08610000
H	-8.14540000	-5.29300000	-2.87590000
C	10.78960000	-0.64660000	0.46480000
C	12.18070000	-0.63330000	0.47650000
C	12.83610000	0.38650000	-0.19730000
C	12.08390000	1.33770000	-0.87010000
C	10.69700000	1.23890000	-0.82290000
H	12.71930000	-1.41030000	1.00200000
H	13.91820000	0.43530000	-0.20370000
H	12.54480000	2.14300000	-1.42600000
C	9.86920000	2.24760000	-1.58680000
O	10.39810000	2.95670000	-2.43350000
N	8.55940000	2.26500000	-1.25510000
H	8.28320000	1.66600000	-0.47620000
C	10.06570000	-1.77690000	1.16110000
O	10.67800000	-2.78300000	1.49650000
N	8.74440000	-1.56580000	1.34370000
H	8.38800000	-0.64930000	1.07050000
C	-3.05300000	-9.07180000	-1.92730000

C	-3.16020000	-10.15130000	-2.79940000
C	-4.29000000	-10.24580000	-3.59730000
C	-5.27540000	-9.27710000	-3.47990000
C	-5.07570000	-8.23600000	-2.57930000
H	-2.37070000	-10.88970000	-2.83700000
H	-4.40450000	-11.06640000	-4.29520000
H	-6.18500000	-9.31240000	-4.06410000
C	-6.16230000	-7.19720000	-2.42110000
O	-7.28920000	-7.42010000	-2.84590000
N	-5.77420000	-6.06980000	-1.78700000
H	-4.78610000	-5.99860000	-1.53990000
C	-1.84170000	-8.98970000	-1.02780000
O	-1.15040000	-9.98360000	-0.84630000
N	-1.61490000	-7.77480000	-0.47670000
H	-2.17620000	-6.99460000	-0.82290000
C	7.79670000	-2.46360000	1.87210000
C	6.44970000	-2.20790000	1.59930000
C	8.13300000	-3.57070000	2.65290000
C	5.46230000	-3.04530000	2.08980000
H	6.18280000	-1.33630000	1.01280000
C	7.13080000	-4.40260000	3.13740000
H	9.16840000	-3.78480000	2.86970000
C	5.78350000	-4.16300000	2.86620000
H	4.42370000	-2.81700000	1.87620000
H	7.41320000	-5.26810000	3.72730000
C	4.72480000	-5.06640000	3.38210000
C	4.78560000	-5.57430000	4.68250000
C	3.65240000	-5.43620000	2.56820000
C	3.79320000	-6.42740000	5.14840000
H	5.60140000	-5.28660000	5.33670000
C	2.64900000	-6.29430000	3.02300000
H	3.61930000	-5.07880000	1.54410000
C	2.73080000	-6.78640000	4.32860000
H	3.84070000	-6.80440000	6.16390000
H	1.95280000	-7.43850000	4.71020000
C	1.53250000	-6.68710000	2.12700000
C	0.93840000	-5.76270000	1.26340000
C	1.04610000	-7.99580000	2.11390000
C	-0.08750000	-6.13440000	0.40870000
H	1.27350000	-4.73110000	1.26360000
C	0.01530000	-8.38130000	1.26750000
H	1.49020000	-8.74060000	2.76550000
C	-0.55430000	-7.45050000	0.39720000
H	-0.54560000	-5.40590000	-0.25120000

H	-0.33440000	-9.40290000	1.27540000
N	10.06200000	0.27420000	-0.16250000
N	-3.98390000	-8.12690000	-1.82550000
Cl	-2.70300000	-4.78640000	-1.68030000
Cl	-3.13830000	4.62090000	1.66310000
MAA + 2F⁻ + Et₄N⁺			
C	-2.86198500	8.68327800	3.23252200
C	-2.86082800	9.54163500	4.32815400
C	-1.70915200	10.27368200	4.58416200
C	-0.61035600	10.12550500	3.74811900
C	-0.71325000	9.23907900	2.68026800
H	-3.74077300	9.62336900	4.95228400
H	-1.66708600	10.95061400	5.42914100
H	0.30841300	10.67347000	3.90933200
C	0.45950600	9.02773200	1.75144400
O	1.42523200	9.78444500	1.80470900
N	0.33497500	7.96636200	0.92597800
H	-0.48388100	7.32204100	1.03363200
C	-4.09248400	7.86944500	2.90703600
O	-5.15311200	8.12182100	3.47230100
N	-3.89691600	6.90043700	1.98617400
H	-2.92636800	6.72718300	1.63668600
N	-1.81553000	8.54589100	2.43051800
C	1.31089900	7.53959200	0.00410800
C	2.21862900	8.40446300	-0.61136900
C	1.33763600	6.18096600	-0.32675500
C	3.14516300	7.90571300	-1.51813000
H	2.20913500	9.45770000	-0.37300900
C	2.27341300	5.69566700	-1.22643500
H	0.60013500	5.52565800	0.12332100
C	3.20081500	6.54748300	-1.83360300
H	3.85425300	8.59001500	-1.97220600
H	2.27539500	4.63824700	-1.47003500
C	-4.87837400	6.04946900	1.44602700
C	-4.43191300	5.02237500	0.60348400
C	-6.25185800	6.18617100	1.67070200
C	-5.33526200	4.16417200	-0.00011000
H	-3.36478600	4.93460000	0.42518700
C	-7.14402000	5.31762100	1.05373400
H	-6.61755100	6.96133100	2.32550800
C	-6.71269900	4.29599800	0.20809500
H	-4.96180700	3.39225500	-0.66525100
H	-8.20375200	5.43664400	1.25371100
C	4.22480700	6.02553500	-2.77274500

C	4.95145300	4.87718700	-2.45342600
C	4.50339500	6.68451200	-3.97294400
C	5.94805000	4.38166000	-3.29736500
H	4.76803700	4.38617500	-1.50320600
C	5.48405200	6.19625400	-4.82752800
H	3.94117800	7.57168500	-4.24371200
C	6.20293400	5.05463200	-4.49587800
H	5.68330000	6.70424700	-5.76462500
H	6.95782000	4.67695900	-5.17684200
C	6.73891200	3.18861200	-2.90594600
C	8.11318600	3.13028800	-3.13579300
C	6.14135200	2.09406700	-2.27148100
C	8.87857000	2.03729200	-2.74542000
H	8.61333500	3.96837100	-3.60982900
C	6.88668500	0.99674300	-1.87678300
H	5.07107200	2.09374600	-2.09271600
C	8.26992100	0.95532600	-2.10139700
H	9.94165200	2.02943800	-2.92703200
H	6.42315800	0.14688100	-1.38585500
C	-7.68437700	3.38889900	-0.45137700
C	-8.88931300	3.87975600	-0.96336900
C	-7.41025000	2.02664300	-0.58432600
C	-9.78837400	3.02511800	-1.58845500
H	-9.11514100	4.93790400	-0.89050400
C	-8.30484500	1.15735200	-1.21106100
H	-6.47748700	1.63350400	-0.19305600
C	-9.50179200	1.67176000	-1.71518300
H	-10.71931700	3.41776100	-1.98204700
H	-10.21644600	1.00939900	-2.19135900
C	-7.97589600	-0.28316200	-1.33898900
C	-7.38247900	-0.98038400	-0.28398400
C	-8.21923700	-0.97326900	-2.52873200
C	-7.02907700	-2.31329400	-0.41981800
H	-7.20110500	-0.47840400	0.66043000
C	-7.85792400	-2.30528900	-2.67812700
H	-8.66255200	-0.45163800	-3.37012000
C	-7.25008200	-2.98457500	-1.62213800
H	-6.55712400	-2.84231900	0.39981700
H	-8.02921300	-2.81184200	-3.61760000
C	10.24620500	-3.45909500	0.30537400
C	11.51623300	-4.00781200	0.15364900
C	12.41875700	-3.35169300	-0.67237900
C	12.02799300	-2.18241100	-1.31058800
C	10.73555500	-1.71453100	-1.09097300

H	11.77454000	-4.92154700	0.67192200
H	13.41598800	-3.74911100	-0.81906800
H	12.69558000	-1.63636100	-1.96348900
C	10.27209800	-0.44112700	-1.76187500
O	11.08724600	0.25696600	-2.35928700
N	8.95265500	-0.18347100	-1.63449100
H	8.34684900	-0.88552800	-1.15060200
C	9.22909500	-4.14784800	1.18678700
O	9.58009600	-5.08809700	1.89471800
N	7.97744100	-3.64908600	1.09837900
H	7.78787500	-2.88105800	0.41408900
C	-5.27924100	-7.97847600	-1.22655300
C	-5.70626600	-9.11302300	-1.90985400
C	-6.76916700	-8.98344600	-2.79379800
C	-7.36621200	-7.74067900	-2.95968700
C	-6.86563800	-6.66981900	-2.22613400
H	-5.21095000	-10.06069700	-1.74572900
H	-7.12801200	-9.84214500	-3.34852800
H	-8.19815400	-7.59100300	-3.63487400
C	-7.48791500	-5.29980000	-2.35149100
O	-8.53906500	-5.15303500	-2.96777700
N	-6.80493200	-4.31876000	-1.72577900
H	-5.90661800	-4.53268000	-1.24168000
C	-4.12044400	-8.06195900	-0.26228800
O	-3.65898600	-9.15521900	0.05020400
N	-3.66738300	-6.86690700	0.17482900
H	-4.06281900	-5.98453000	-0.21753900
C	6.84255800	-4.10634900	1.79414400
C	5.60845800	-3.56468800	1.40975500
C	6.87284800	-5.03962100	2.83514300
C	4.44070300	-3.95759500	2.03944900
H	5.60137300	-2.82605500	0.61428900
C	5.68943700	-5.42077900	3.45773900
H	7.81078500	-5.47304400	3.14511100
C	4.45419600	-4.89894900	3.07467400
H	3.50134700	-3.51184900	1.72903300
H	5.73620000	-6.16318800	4.24765600
C	3.19651700	-5.33863900	3.72782800
C	3.13629600	-5.56846800	5.10533600
C	2.04598900	-5.55235000	2.96617600
C	1.95513200	-6.00353100	5.69368100
H	4.01145000	-5.39178700	5.72103400
C	0.85235300	-5.98747800	3.54457600
H	2.09142900	-5.41751200	1.89053100

C	0.81828500	-6.21371700	4.92290400
H	1.91668800	-6.16747000	6.76488000
H	-0.10271400	-6.53856300	5.39471500
C	-0.34224600	-6.22095300	2.69593300
C	-0.67939200	-5.33008300	1.67322000
C	-1.15185800	-7.34356100	2.87825700
C	-1.77016600	-5.56417700	0.85275100
H	-0.07978700	-4.43759200	1.52598800
C	-2.25059300	-7.58657500	2.06404400
H	-0.91123000	-8.05631200	3.65989600
C	-2.56287200	-6.69882600	1.03349400
H	-2.04112500	-4.87340500	0.06393600
H	-2.85484700	-8.46844700	2.22103200
N	9.87480400	-2.33836400	-0.29835000
N	-5.84998100	-6.79218800	-1.38237100
F	-4.33875900	-4.33868800	-0.57302200
F	-1.54953700	6.04810500	0.93026400
N	-2.58828800	-1.33643100	-0.66498800
C	-1.91080300	-2.28286800	-1.63157600
H	-2.54755100	-3.17025700	-1.64790700
H	-1.95533600	-1.81113900	-2.61011800
C	-0.47371200	-2.64568800	-1.29410300
H	-0.39869300	-3.33305900	-0.45297400
H	-0.05039000	-3.15096000	-2.16389400
H	0.14987800	-1.77557600	-1.08346500
C	-2.57389800	-1.99313800	0.70715900
H	-1.52623800	-2.16550300	0.94713800
H	-3.07931400	-2.95126500	0.56383100
C	-3.22127700	-1.20339900	1.83110600
H	-3.05675300	-1.77183800	2.74878600
H	-2.77275400	-0.21915200	1.97326700
H	-4.29875500	-1.09160700	1.70938100
C	-4.04632500	-1.21641900	-1.06786600
H	-4.42150400	-2.24086200	-1.01821200
H	-4.52645900	-0.63522800	-0.28407400
C	-4.35869000	-0.58028900	-2.40838800
H	-3.85359900	-1.06031200	-3.24737100
H	-5.43282400	-0.70469300	-2.56201100
H	-4.15122900	0.48999100	-2.42406000
C	-1.90102400	0.01156000	-0.58483200
H	-1.10021400	-0.09489500	0.14760700
H	-2.63756100	0.69798600	-0.16745800
C	-1.32962200	0.57153200	-1.87805900
H	-2.06775000	0.66831200	-2.67101900

H	-0.95408000	1.57129300	-1.65102800
H	-0.49059200	-0.01443800	-2.25294900
MAA + 2F⁻ + Bu₄N⁺			
C	4.04696600	8.25829700	-3.27494100
C	4.10456800	9.23333400	-4.26598900
C	3.10540500	10.19697800	-4.29383800
C	2.09447300	10.15513500	-3.34262700
C	2.12611200	9.13569100	-2.39627500
C	1.04079000	9.02979800	-1.35061400
O	0.25788300	9.96086600	-1.18330100
N	1.02439100	7.85720600	-0.68246400
C	5.11756900	7.19593700	-3.18609600
O	6.15959600	7.32624800	-3.82224900
N	4.81039500	6.16246600	-2.37289100
N	3.08481200	8.22059900	-2.36405800
C	0.06985900	7.49664400	0.28939400
C	-0.53004600	8.41585300	1.15232400
C	-0.25500600	6.14249200	0.40729800
C	-1.45652300	7.98224900	2.09134800
C	-1.18698500	5.72448500	1.34286700
C	-1.81310100	6.63691100	2.19649000
C	5.66027100	5.10857600	-1.99360000
C	5.15698500	4.20528600	-1.04721500
C	6.95980200	4.92608800	-2.47580400
C	5.94406700	3.16956700	-0.57716700
C	7.73647400	3.88074400	-1.99013900
C	7.25690200	2.99256500	-1.02826100
C	-2.84423300	6.19108800	3.16573800
C	-3.82890400	5.28680200	2.76698400
C	-2.87474300	6.68053900	4.47408400
C	-4.83716400	4.86571500	3.63599800
C	-3.86812500	6.26499700	5.35245100
C	-4.84379100	5.36497100	4.94124100
C	-5.88629800	3.93450400	3.15435300
C	-7.22418000	4.09542400	3.51207000
C	-5.56897800	2.88197900	2.28904900
C	-8.22227100	3.26135800	3.01882500
C	-6.54703200	2.04363700	1.78764300
C	-7.89244200	2.22835900	2.13594300
C	8.11258500	1.91215600	-0.48041200
C	9.46600100	2.13522300	-0.20850700
C	7.57217600	0.66062000	-0.18403900
C	10.24652400	1.13129300	0.35086500
C	8.34181700	-0.35024600	0.39081200

C	9.69019400	-0.10427600	0.65773000
C	7.70890100	-1.64375600	0.74113800
C	6.86195200	-2.29968200	-0.15502600
C	7.88817400	-2.20181600	2.00733400
C	6.20201400	-3.46085500	0.21071000
C	7.21981700	-3.35633300	2.38994200
C	6.36013300	-3.99113100	1.49285600
C	-10.82045200	-1.37740600	-0.63868800
C	-12.20607600	-1.50871100	-0.64897300
C	-12.95075700	-0.66483500	0.16336200
C	-12.29509300	0.27443100	0.94726900
C	-10.90584000	0.32928100	0.88342900
C	-10.15849900	1.35419900	1.70916000
O	-10.78654000	2.10776300	2.44813900
N	-8.81947800	1.35079100	1.54193600
C	-9.97638000	-2.28422900	-1.50840300
O	-10.52562900	-3.13913000	-2.19841900
N	-8.64716100	-2.06230200	-1.43857700
C	3.24698300	-8.35901400	1.84644700
C	3.34020400	-9.39753900	2.76743600
C	4.35746700	-9.34627700	3.71095700
C	5.24106300	-8.27545100	3.69868800
C	5.06390100	-7.29086000	2.73212700
C	6.00825200	-6.11552500	2.65536500
O	7.05145400	-6.12096100	3.30106400
N	5.60358300	-5.13141500	1.82479600
C	2.14963700	-8.35362300	0.80986900
O	1.45362400	-9.35012100	0.64509600
N	2.02212200	-7.18808900	0.13863000
C	-7.63491600	-2.77982200	-2.10449200
C	-6.31448500	-2.40050700	-1.82481900
C	-7.85746900	-3.82793000	-3.00304200
C	-5.25288000	-3.06581200	-2.40893700
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C	-2.15748400	-6.34973200	-4.88154600
C	-1.00528500	-6.24665100	-2.64771500
C	-0.47199100	-5.28740300	-1.78313900
C	-0.47958900	-7.53884600	-2.59665600

C	0.52376100	-5.61917100	-0.88089900
C	0.51917900	-7.88195000	-1.69428900
C	1.01741000	-6.92213800	-0.81247600
N	-10.19418300	-0.48029500	0.11080900
N	4.09203700	-7.33776600	1.83152500
H	4.91250500	9.22634800	-4.98533600
H	3.11344900	10.97218100	-5.05067600
H	1.29605300	10.88490800	-3.32458200
H	1.66936300	7.08470400	-0.97536600
H	3.86323600	6.13601500	-1.93399300
H	-0.28457100	9.46529600	1.07961500
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H	-1.92902300	8.71383100	2.73826200
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H	5.53866300	2.50411800	0.17808700
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H	-2.11184900	7.37478700	4.80908400
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H	9.90407300	3.10629100	-0.41046000
H	6.52362000	0.47167500	-0.39017900
H	11.29415500	1.31758000	0.55896100
H	10.30437100	-0.88394400	1.09499600
H	6.71746000	-1.89742800	-1.15228000
H	8.52645300	-1.70070200	2.72716700
H	5.53083300	-3.95408700	-0.48282600
H	7.34775600	-3.75084900	3.38707100
H	-12.67156200	-2.25433100	-1.27915100
H	-14.03154200	-0.73702800	0.18370700
H	-12.83153300	0.95495900	1.59451700
H	-8.39212800	0.65551400	0.88866100
H	-8.29210200	-1.30263200	-0.81384400
H	2.62955500	-10.21262400	2.73628000
H	4.45977800	-10.13232600	4.44939400
H	6.05067200	-8.19341400	4.41157300
H	4.68212700	-5.21047700	1.34644300
H	2.58471600	-6.36053800	0.43240100

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H	-8.86484400	-4.13669800	-3.23350300
H	-4.24213700	-2.74519100	-2.17933200
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H	-3.21348200	-4.87140400	-2.02837000
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H	-1.32253500	-6.91436800	-5.28204200
H	-0.83824800	-4.26642300	-1.82029100
H	-0.87598600	-8.30360100	-3.25607400
H	0.94703400	-4.87587200	-0.21848200
H	0.89655400	-8.89391900	-1.66396600
F	3.18755400	-4.76650900	0.60174000
F	2.43338900	5.63491200	-1.16835900
N	2.14980300	-1.41754000	0.50599200
C	1.32949500	-2.08279500	1.60287300
C	-0.11921600	-2.46320500	1.30681500
C	-1.13240000	-1.36172000	0.99704900
C	1.87990700	-2.17010600	-0.78306000
C	2.61631200	-1.70809200	-2.03169000
C	2.10169100	-2.51133200	-3.22953700
C	3.62667000	-1.63207800	0.80788500
C	4.27141000	-0.96887000	2.01625800
C	3.97088600	-1.54054800	3.40107600
C	1.85505100	0.05490100	0.30833600
C	1.52889800	0.87434000	1.55050000
C	1.57466100	2.36809000	1.22044200
C	2.83576100	-2.15939500	-4.51906900
C	-2.52053300	-1.94438900	0.74311100
C	1.24875600	3.23590800	2.43191500
C	4.96634600	-1.02861600	4.43840300
H	1.87861400	-2.99814600	1.82733700
H	1.37708000	-1.42990300	2.46885700
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H	-1.17918300	-0.65916700	1.83440500
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H	2.14472600	-3.20707400	-0.56043300
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H	1.02832100	-2.32995200	-3.35354600
H	2.21240300	-3.58111600	-3.01967000
H	3.74219900	-2.71816000	0.84979500

H	4.14350500	-1.26717300	-0.07639400
H	5.33995900	-1.12245500	1.83126000
H	4.13820900	0.11665100	1.99914900
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H	2.95926700	-1.28538000	3.72751300
H	1.02993300	0.12402300	-0.40031800
H	2.73749000	0.46572000	-0.18452300
H	2.23097900	0.67071100	2.36097900
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H	0.87082600	2.58522300	0.40922100
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H	2.45060700	-2.73923200	-5.36114200
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H	-2.87436500	-2.50653600	1.61224700
H	-2.50518200	-2.62730900	-0.11156500
H	1.30336300	4.29720000	2.18146400
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