

Probing the Hydroxyl in [2,2,2]-Cryptand/KF/Choline Chloride Non-Covalent Host-Guest Complex in Solution by ^{19}F -NMR Spectroscopy: Structural Correlation and Thermodynamic Reversal of Host-Guest Configurations in Solution and in the Gas Phase

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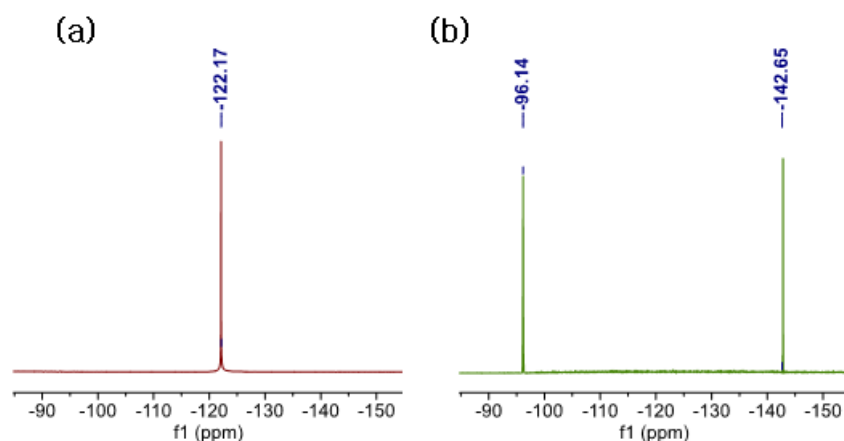


Figure S1. ^{19}F -NMR spectrum of KF/[2,2,2]-cryptand (a) in D_2O and (b) in $\text{DMSO}-d_6$. Ref. [].

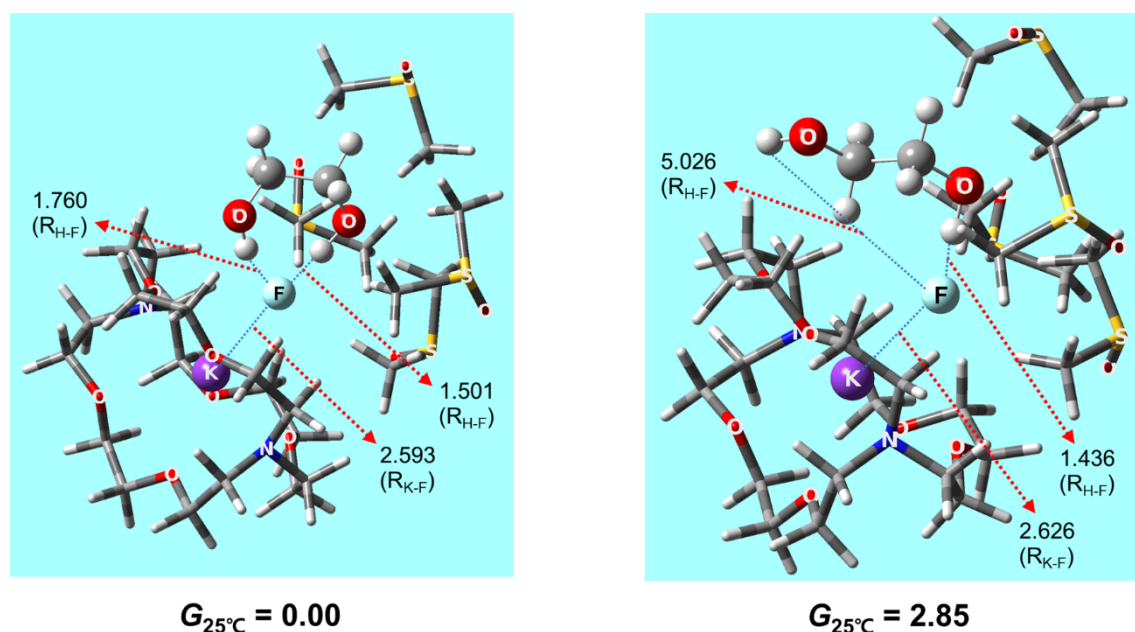


Figure S2. Calculated structures of [2,2,2]/KF/EG- d_6 (1:1:1) complex in $\text{DMSO}-d_6$. Relative Gibbs free energy in kcal/mol, distance in Å

500 MHz, EG-d₆, 25 °C

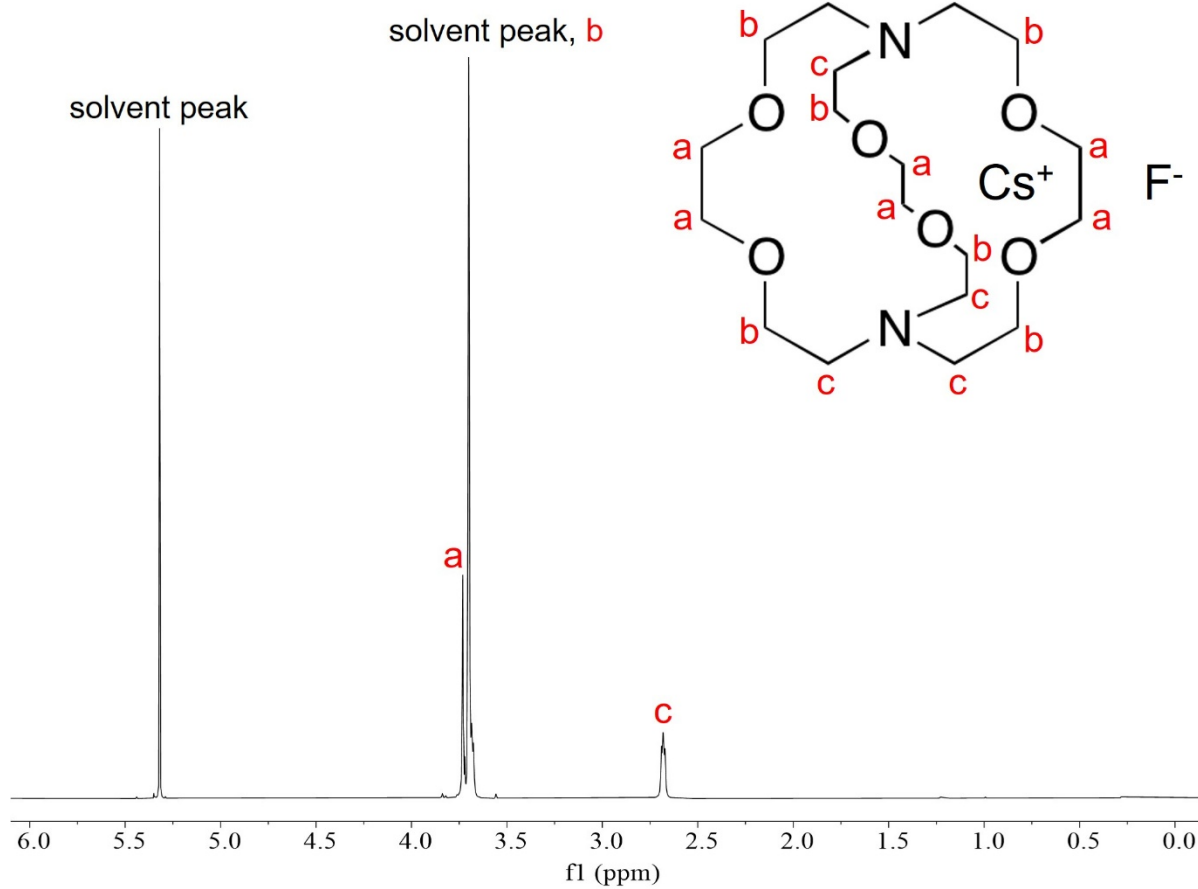


Figure S3. ¹H-NMR spectrum of Kf/[2,2,2]-cryptand in EG-d₆.

500 MHz, DMSO-d₆, 25 °C

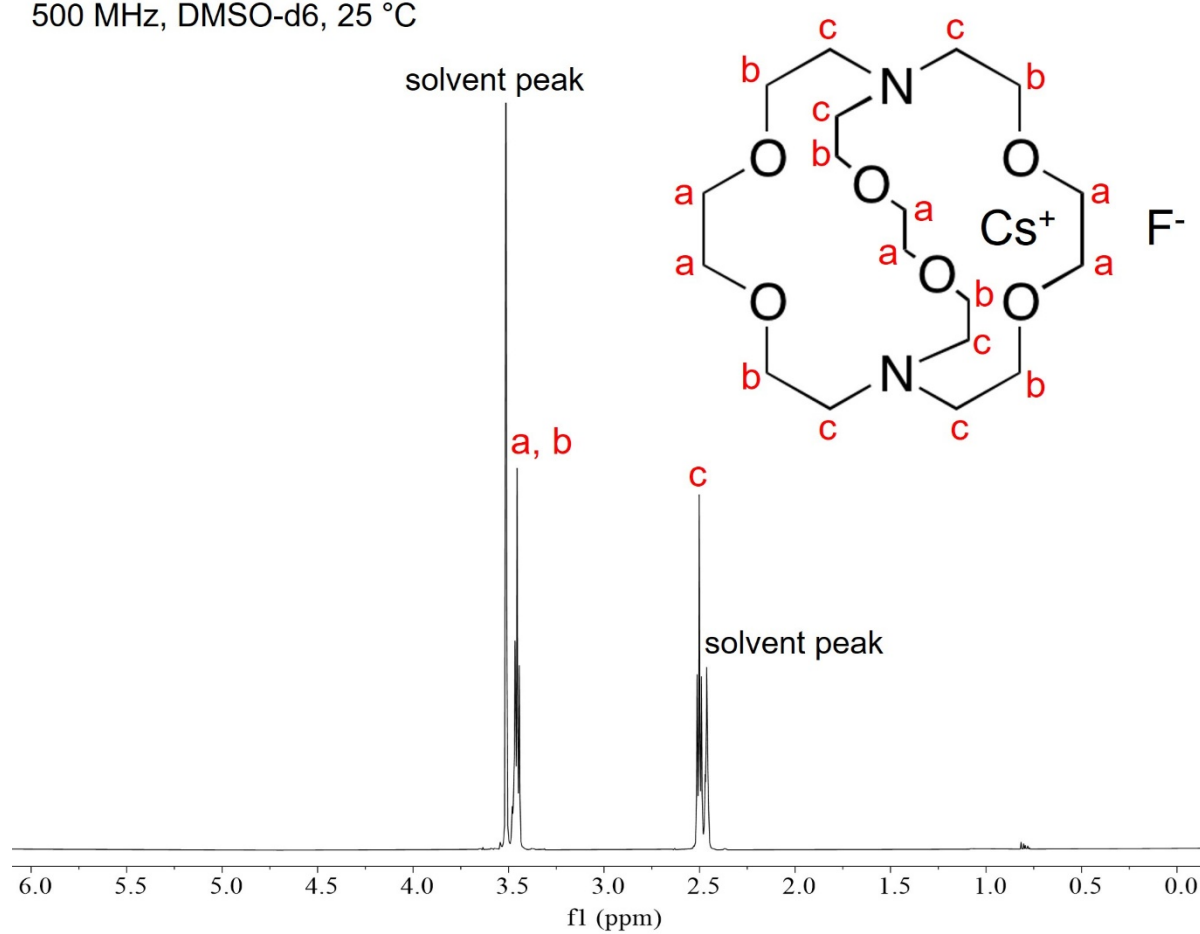


Figure S4. ¹H-NMR spectrum of Kf/[2,2,2]-cryptand in DMSO-*d*₆

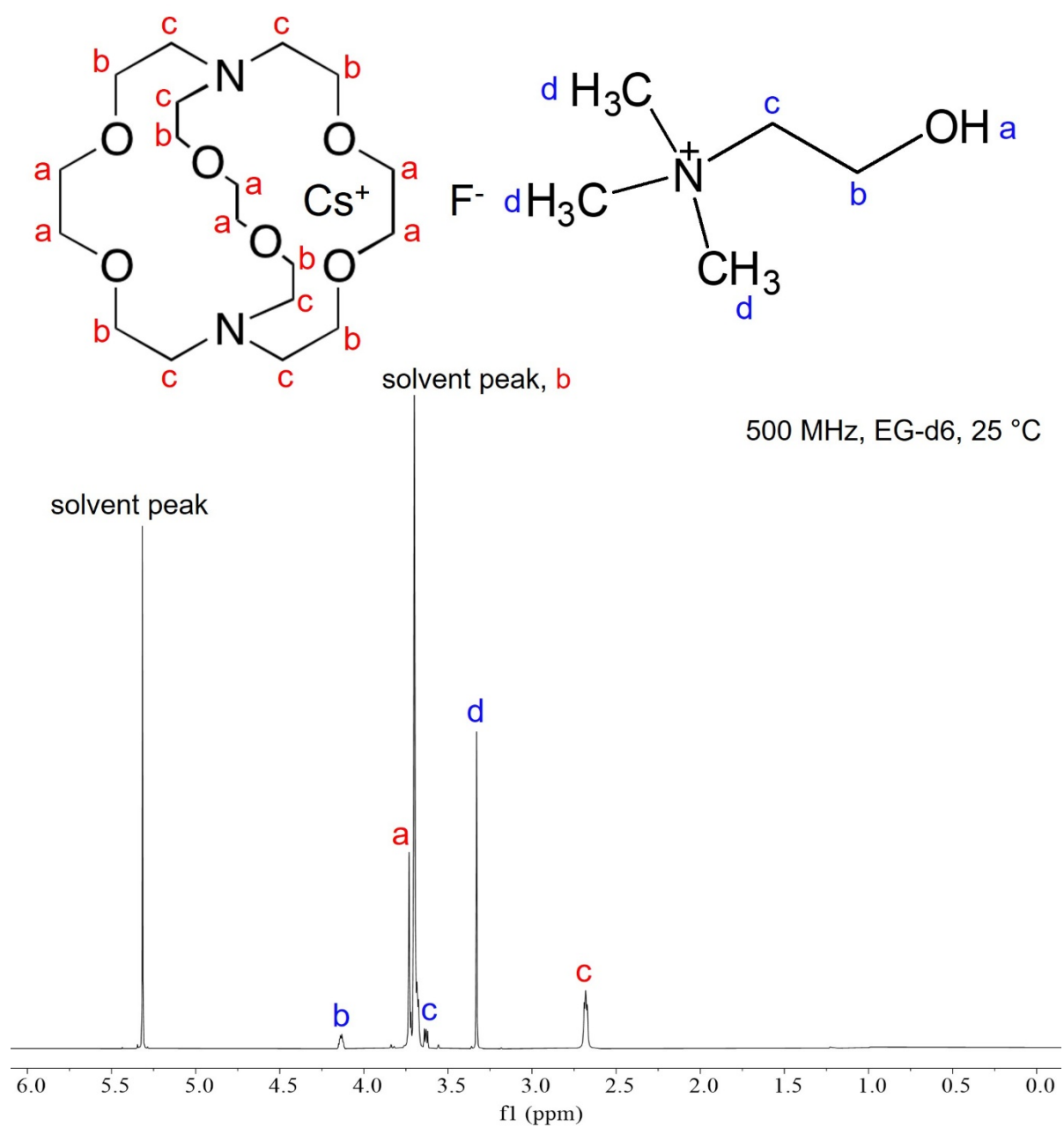


Figure S5. ^1H -NMR spectrum of $\text{KF}/[2,2,2]\text{-cryptand}/\text{KF}/\text{choline chloride}$ in EG-d_6 .

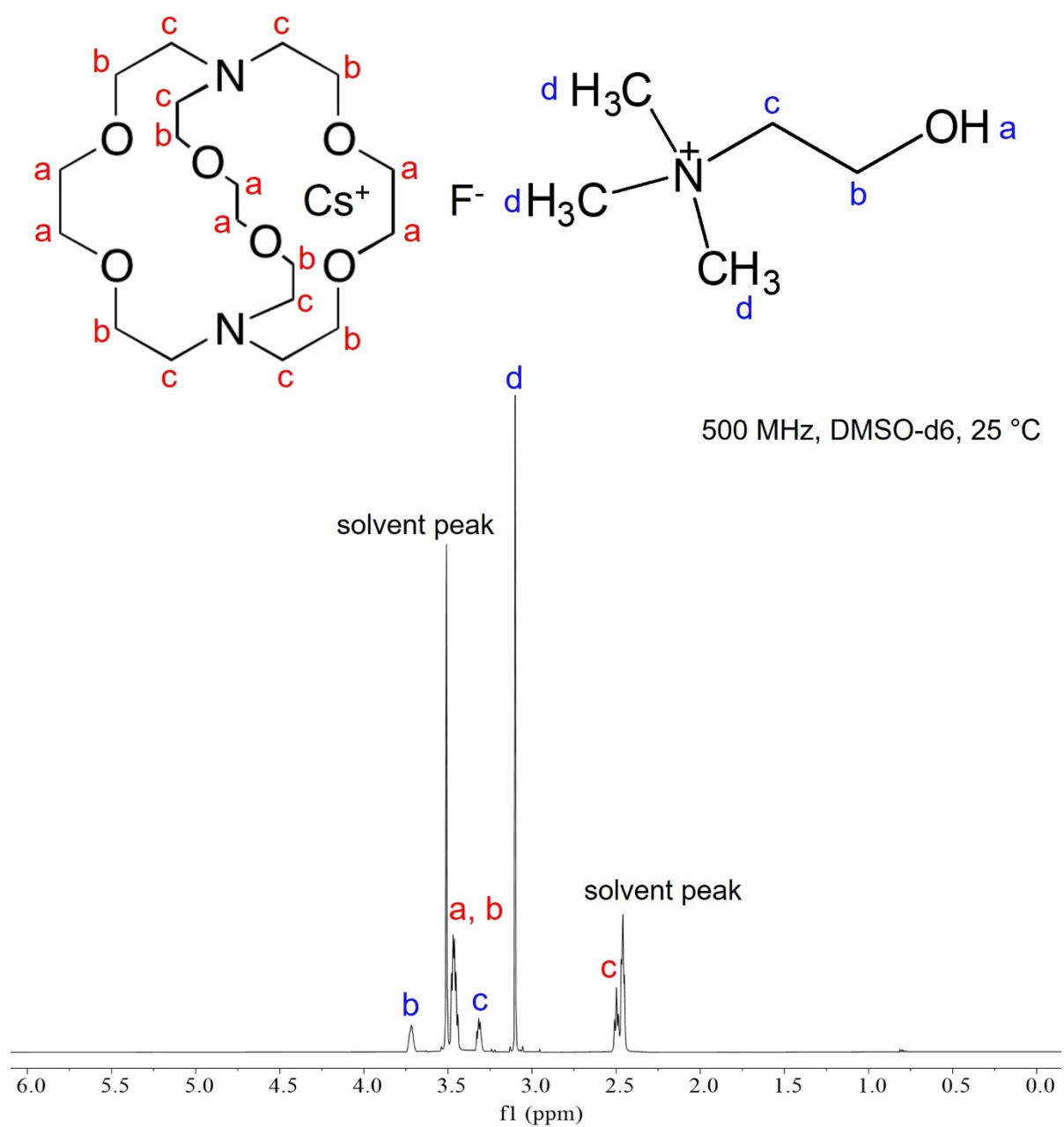


Figure S6. ¹H-NMR spectrum of KF/[2,2,2]-cryptand/KF/choline chloride in DMSO-*d*₆.

500 MHz, CD₃OD, 25 °C

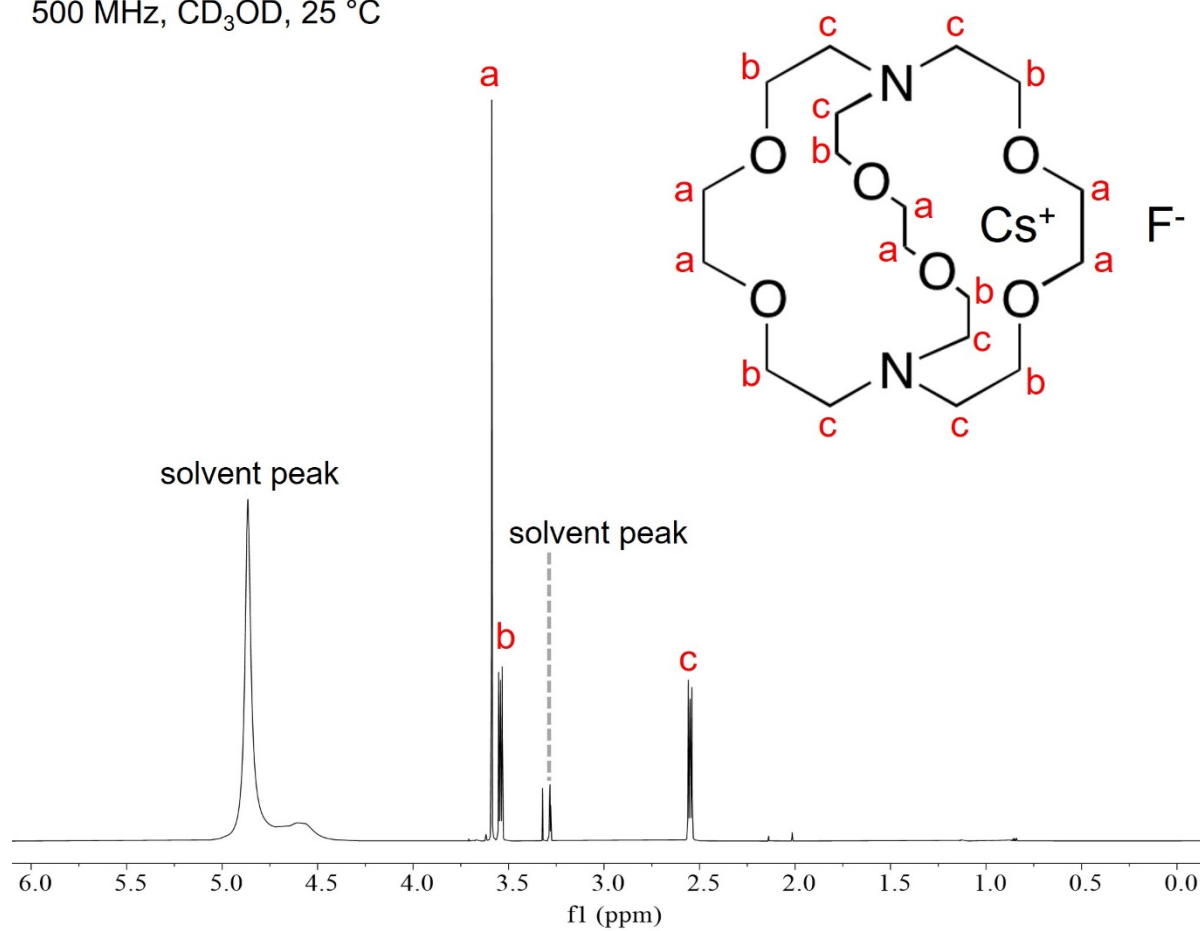


Figure S7. ¹H-NMR spectrum of KF/[2,2,2] in CD₃OD.

Cartesian coordinates

Fig 1.(a) [2,2,2]/KF/(CH₃)₄N⁺Cl⁻ in EG-d₆

C	3.9908360000	3.0633190000	1.9346730000
C	3.2760460000	3.4823050000	0.6615520000
O	4.1442400000	1.6554670000	1.9660060000
N	3.7841960000	2.8597750000	-0.5619560000
C	3.0299170000	3.3392390000	-1.7222010000
C	4.4060980000	1.1687020000	3.2701130000
C	2.6790960000	2.2717320000	-2.7457180000
O	1.9800090000	1.2230370000	-2.0986230000
C	1.2802020000	0.3790050000	-2.9975830000
C	4.7062330000	-0.3084560000	3.1902180000
C	1.1259500000	-0.9800470000	-2.3636510000
O	2.4122470000	-1.5917540000	-2.3363200000
O	3.6449770000	-0.9360090000	2.4976320000
C	2.3831360000	-2.9832330000	-2.0618530000
C	3.4769180000	-2.3144950000	2.7746880000
C	2.1308550000	-3.3130330000	-0.5998840000
N	3.1568950000	-2.8275010000	0.3293690000
C	2.6070610000	-2.9080790000	1.6869950000
H	3.3785640000	3.3949490000	2.7824520000
H	4.9723800000	3.5434360000	2.0325060000
H	2.0401820000	2.7359640000	-3.5093430000
H	3.5594090000	1.8582330000	-3.2491560000
H	1.5965260000	-3.4601140000	-2.6605000000
H	3.3393240000	-3.3792980000	-2.4086100000
H	2.9629760000	-2.4400750000	3.7368610000
H	4.4425000000	-2.8220830000	2.8570950000

H	1.9972650000	-4.4066520000	-0.5164570000
H	1.1807840000	-2.8543190000	-0.3121870000
H	1.6690680000	-2.3459900000	1.6834010000
H	2.3872920000	-3.9553290000	1.9616110000
H	2.0851060000	3.7584570000	-1.3658500000
H	3.5628650000	4.1547080000	-2.2361490000
H	3.3222140000	4.5850430000	0.6146370000
H	2.2212970000	3.2041980000	0.7495730000
H	5.2648550000	1.6890140000	3.7135930000
H	3.5276250000	1.3390350000	3.9057060000
H	4.7989240000	-0.7008160000	4.2100930000
H	5.6513980000	-0.4845120000	2.6601290000
H	0.2947620000	0.8047230000	-3.2244430000
H	1.8414650000	0.2750290000	-3.9344180000
K	3.2307670000	0.0062960000	-0.0254260000
C	5.2253240000	3.0183690000	-0.7135660000
C	4.4174950000	-3.5567510000	0.1745950000
C	5.8104850000	2.1419610000	-1.8063390000
H	5.7035430000	2.7156900000	0.2190810000
H	5.5059520000	4.0676920000	-0.9143710000
H	4.4818570000	-3.9254520000	-0.8505630000
H	4.4453570000	-4.4494960000	0.8220340000
C	5.6861340000	-2.7463730000	0.4551720000
O	5.7376250000	-1.4781860000	-0.1711210000
H	6.5425250000	-3.3542810000	0.1301290000
H	5.8160700000	-2.5411760000	1.5156710000
O	5.3839480000	0.8113850000	-1.5761710000
H	6.9036580000	2.2052040000	-1.7457920000
H	5.5165570000	2.4710180000	-2.8103860000

C	6.2542690000	-0.1819720000	-2.0809620000
C	5.7508960000	-1.5172820000	-1.5890940000
H	0.4354640000	-1.5884950000	-2.9589660000
H	0.7304760000	-0.8689700000	-1.3476390000
H	7.2728590000	-0.0084480000	-1.7108880000
H	6.2720960000	-0.1723260000	-3.1785550000
H	4.7422180000	-1.6988620000	-1.9756720000
H	6.4176440000	-2.3121850000	-1.9470300000
F	0.7852940000	-0.2823470000	0.8515240000
C	-1.1531080000	-4.0012720000	1.4441140000
H	-1.4826960000	-4.6390330000	0.6247910000
H	-0.1189020000	-3.6975990000	1.2964000000
H	-1.2596910000	-4.5197870000	2.3959960000
C	-1.5181870000	-1.8456660000	2.5256830000
C	-3.4191050000	-3.1657870000	1.7567910000
H	-2.2263640000	-1.0218120000	2.6010790000
H	-1.4650750000	-2.3884480000	3.4688550000
H	-0.5393460000	-1.4687110000	2.2252930000
H	-3.4537160000	-3.6377330000	2.7382490000
H	-4.0207550000	-2.2585070000	1.7431510000
H	-3.7529300000	-3.8613760000	0.9871900000
C	-1.9351170000	-2.0893460000	0.1460230000
H	-2.5679840000	-1.2038390000	0.2015020000
H	-0.8983420000	-1.7980610000	-0.0213310000
N	-2.0068420000	-2.7823440000	1.4686490000
Cl	-4.3877080000	0.4150470000	1.5665860000
C	-6.3479490000	2.5847260000	-0.7462230000
C	-7.2514410000	1.4567280000	-1.1949510000
H	-5.7799310000	2.2757050000	0.1360240000

H	-6.9538570000	3.4608970000	-0.4910430000
H	-7.8753410000	1.1077170000	-0.3722680000
H	-7.8979570000	1.7961190000	-2.0121800000
O	-5.4538770000	2.8911950000	-1.8147660000
H	-4.5603830000	2.8986780000	-1.4323810000
O	-6.4703340000	0.3475640000	-1.6396460000
H	-5.8268290000	0.7182250000	-2.2595670000
C	-0.7168470000	2.2278910000	-0.4091680000
C	-1.9000690000	2.8550390000	-1.1083590000
H	-0.5696790000	2.7057760000	0.5678730000
H	0.1804680000	2.3958660000	-1.0165170000
H	-1.7783760000	3.9366580000	-1.1848470000
H	-2.0030440000	2.4384800000	-2.1175280000
O	-0.9883820000	0.8514820000	-0.2463080000
H	-0.1885690000	0.3600340000	0.2619600000
O	-3.1070800000	2.6250690000	-0.3749590000
H	-3.1475500000	1.6890350000	-0.1119100000
C	-6.7077220000	-2.6697180000	-0.2168530000
C	-7.1072600000	-2.2225100000	1.1742080000
H	-7.5033560000	-2.4217620000	-0.9291040000
H	-6.5514130000	-3.7506780000	-0.2314120000
H	-8.0501080000	-2.7016620000	1.4501490000
H	-6.3434930000	-2.5276160000	1.8990030000
O	-5.4879520000	-2.0554140000	-0.6187440000
H	-5.6808420000	-1.1130670000	-0.7755800000
O	-7.3088150000	-0.8160650000	1.2289290000
H	-6.4390640000	-0.3891170000	1.3165590000
C	-3.3253680000	-0.1696490000	-2.4428090000
C	-3.9640500000	-1.2612130000	-3.2780260000

H	-3.7342680000	-0.1890060000	-1.4226350000
H	-3.5759380000	0.8066170000	-2.8851900000
H	-5.0309040000	-1.0483220000	-3.4155930000
H	-3.4920610000	-1.2723360000	-4.2641120000
O	-1.9232540000	-0.3761290000	-2.4225310000
H	-1.5490060000	0.0762380000	-1.6305190000
O	-3.7800390000	-2.5534200000	-2.7166620000
H	-4.3526680000	-2.5851630000	-1.9301280000
H	-2.2876010000	-2.7683350000	-0.6287790000
C	-2.2649160000	3.9006000000	2.9513810000
C	-2.0512120000	2.5570430000	3.6172750000
H	-1.3607120000	4.1797790000	2.3957270000
H	-2.4333800000	4.6549840000	3.7248410000
H	-1.2458340000	2.6447050000	4.3510690000
H	-2.9670860000	2.2615210000	4.1432440000
O	-3.4032160000	3.9160800000	2.1026710000
H	-3.2084080000	3.4086650000	1.2967920000
O	-1.6645390000	1.5490390000	2.6911370000
H	-2.4630350000	1.2515760000	2.2226080000

Fig 1.(b) [2,2,2]/KF/EG-d₆ in DMSO-d₆

C	-2.3215240000	3.0300690000	-2.0679450000
C	-2.1360850000	3.3418880000	-0.5917230000
O	-2.5462650000	1.6482270000	-2.2549410000
N	-3.1114090000	2.7175680000	0.3010860000
C	-2.8798100000	3.1322900000	1.6843570000
C	-2.2686330000	1.2212360000	-3.5764780000
C	-2.9277330000	1.9991200000	2.6982830000

O	-2.0282040000	0.9922710000	2.2851210000
C	-1.6577890000	0.1026120000	3.3208360000
C	-2.6863980000	-0.2258660000	-3.7179150000
C	-1.1457860000	-1.1690430000	2.6932530000
O	-2.2699420000	-1.8718670000	2.1821720000
O	-2.1191190000	-0.9684470000	-2.6614770000
C	-2.0348840000	-3.2330610000	1.8815940000
C	-1.6296570000	-2.2460380000	-2.9971650000
C	-1.3229760000	-3.4551040000	0.5564900000
N	-2.0245350000	-2.9100210000	-0.6070210000
C	-1.0807700000	-2.8644200000	-1.7282150000
H	-1.4045510000	3.3414670000	-2.5864020000
H	-3.1526210000	3.6029480000	-2.5003880000
H	-2.6246650000	2.4045340000	3.6745090000
H	-3.9295380000	1.5692670000	2.8056900000
H	-1.4335010000	-3.6954000000	2.6759880000
H	-3.0137210000	-3.7167610000	1.8949830000
H	-0.8085860000	-2.1538700000	-3.7172620000
H	-2.4116060000	-2.8665110000	-3.4524950000
H	-1.1336470000	-4.5386680000	0.4478350000
H	-0.3453040000	-2.9684430000	0.6080680000
H	-0.2359980000	-2.2474190000	-1.4074490000
H	-0.7060420000	-3.8748310000	-1.9723210000
H	-1.8796490000	3.5698020000	1.7453640000
H	-3.5900380000	3.9158920000	1.9917440000
H	-2.1292430000	4.4428680000	-0.4970350000
H	-1.1481750000	2.9818200000	-0.2824330000
H	-2.8223070000	1.8302450000	-4.3044300000
H	-1.1943280000	1.3129270000	-3.7696730000

H	-2.3409540000	-0.5923750000	-4.6918470000
H	-3.7798710000	-0.3172600000	-3.6800340000
H	-0.8728270000	0.5460800000	3.9431570000
H	-2.5268790000	-0.1370960000	3.9469270000
K	-2.3893810000	-0.0803390000	-0.1632380000
C	-4.4949730000	2.8687510000	-0.1255940000
C	-3.2519110000	-3.6487920000	-0.9026590000
C	-5.4417860000	1.9508380000	0.6338260000
H	-4.5581000000	2.5900420000	-1.1780800000
H	-4.8548150000	3.9080170000	-0.0196420000
H	-3.6345240000	-4.0671070000	0.0296960000
H	-3.0538680000	-4.5081750000	-1.5664940000
C	-4.3809840000	-2.8280460000	-1.5369600000
O	-4.6707710000	-1.6028940000	-0.9002250000
H	-5.2776810000	-3.4656650000	-1.5469140000
H	-4.1567480000	-2.5597460000	-2.5669930000
O	-4.9203480000	0.6393770000	0.5796690000
H	-6.4245360000	1.9922020000	0.1474450000
H	-5.5773200000	2.2691670000	1.6756840000
C	-5.8712690000	-0.3922970000	0.7305210000
C	-5.1807640000	-1.7012730000	0.4156020000
H	-0.6297880000	-1.7736690000	3.4492730000
H	-0.4352820000	-0.9232790000	1.8934280000
H	-6.7046080000	-0.2388780000	0.0325880000
H	-6.2711930000	-0.4179360000	1.7534870000
H	-4.3686240000	-1.8774540000	1.1319350000
H	-5.9085400000	-2.5202270000	0.4936310000
F	0.1850740000	0.0154630000	-0.4608530000
C	2.8129840000	0.4729790000	-2.3300360000

C	1.9535330000	-0.5615710000	-3.0316060000
H	2.6006700000	1.4518270000	-2.7868640000
H	3.8755910000	0.2519090000	-2.4948510000
H	2.3177340000	-0.6886050000	-4.0554980000
H	2.0551330000	-1.5285040000	-2.5156710000
O	2.5947000000	0.5169620000	-0.9331270000
H	1.6272530000	0.3370970000	-0.7264100000
O	0.5969010000	-0.1760110000	-3.1204090000
H	0.2274250000	-0.1386050000	-2.2136640000
S	2.0714010000	1.5093140000	3.2958810000
O	1.5335880000	0.1781080000	3.8224140000
C	0.8818800000	2.1105040000	2.0871660000
C	3.3840420000	1.1014030000	2.1337220000
H	-0.0174500000	2.3919170000	2.6333480000
H	0.6530200000	1.3181860000	1.3671160000
H	1.3369880000	2.9824190000	1.6104510000
H	3.6917300000	2.0327680000	1.6518770000
H	2.9884670000	0.3972800000	1.4011870000
H	4.2046100000	0.6646640000	2.7041060000
S	2.5272670000	-3.4746730000	1.7016460000
O	3.6779490000	-4.3109460000	1.1516800000
C	2.2362240000	-2.1934180000	0.4750430000
C	3.2354710000	-2.4066560000	2.9650320000
H	1.9382580000	-2.6963730000	-0.4467240000
H	3.1626190000	-1.6447540000	0.3207780000
H	1.4423870000	-1.5162830000	0.7943830000
H	2.5155160000	-1.6283190000	3.2398830000
H	4.1476290000	-1.9691670000	2.5527950000
H	3.4746460000	-3.0302420000	3.8270620000

S	3.2096600000	4.4182440000	-0.4924090000
O	3.1136800000	4.2189500000	1.0171410000
C	1.7051400000	3.7046710000	-1.1936070000
C	4.3699350000	3.1673960000	-1.0767700000
H	0.8746310000	4.3120190000	-0.8318250000
H	1.6143400000	2.6676980000	-0.8638150000
H	1.7627750000	3.7717250000	-2.2816210000
H	4.4216630000	3.2071310000	-2.1663140000
H	4.0153830000	2.1959390000	-0.7310370000
H	5.3424330000	3.4157660000	-0.6508620000
S	6.4173470000	-1.1583950000	-1.2131070000
O	6.3188890000	-0.2846680000	-2.4548890000
C	5.1958060000	-2.4698750000	-1.4249800000
C	5.5653950000	-0.2652740000	0.1018010000
H	5.5745030000	-3.1395040000	-2.1977380000
H	4.2604500000	-2.0117940000	-1.7533400000
H	5.0516200000	-3.0169160000	-0.4887970000
H	5.5418270000	-0.8969110000	0.9923970000
H	4.5583040000	-0.0138300000	-0.2383140000
H	6.1443250000	0.6369170000	0.3047000000

Fig 3.(a) [2,2,2]/KF/ChCl in EG-d₆

C	5.2313340000	1.9276550000	2.0109140000
C	3.9735480000	2.6961230000	1.6441810000
O	5.1251300000	0.5783980000	1.5881250000
N	3.5091760000	2.5191390000	0.2664120000
C	2.2793290000	3.2889720000	0.0651290000
C	5.9369490000	-0.2945000000	2.3548780000

C	1.2478540000	2.6490770000	-0.8516290000
O	0.9932120000	1.3383960000	-0.3886760000
C	-0.1555780000	0.7449480000	-0.9673780000
C	5.8999610000	-1.6729040000	1.7401220000
C	-0.0752600000	-0.7479720000	-0.7523350000
O	0.7785040000	-1.2919860000	-1.7526980000
O	4.5467030000	-2.0527460000	1.5885720000
C	0.6906910000	-2.7026330000	-1.8618130000
C	4.3096330000	-3.4476730000	1.5334540000
C	1.2414000000	-3.4572060000	-0.6610520000
N	2.6484660000	-3.1812090000	-0.3492280000
C	2.9059790000	-3.6713170000	1.0107140000
H	5.3311240000	1.9737860000	3.1022650000
H	6.1342020000	2.3784520000	1.5821150000
H	0.3317990000	3.2561400000	-0.7968870000
H	1.5601650000	2.6126920000	-1.9003510000
H	-0.3598290000	-2.9956900000	-1.9898510000
H	1.2180900000	-2.9622710000	-2.7816410000
H	4.3731560000	-3.8742110000	2.5432160000
H	5.0638980000	-3.9542200000	0.9228460000
H	1.0756670000	-4.5342820000	-0.8421730000
H	0.6439650000	-3.1950450000	0.2178030000
H	2.2206060000	-3.1338090000	1.6721920000
H	2.6931130000	-4.7525380000	1.0839190000
H	1.7965770000	3.3967790000	1.0406020000
H	2.4943190000	4.3071910000	-0.2993510000
H	4.1651460000	3.7586660000	1.8801990000
H	3.1668430000	2.3573940000	2.3007800000
H	6.9751050000	0.0606910000	2.3791280000

H	5.5567460000	-0.3330320000	3.3837050000
H	6.4321190000	-2.3647210000	2.4044620000
H	6.4004960000	-1.6731560000	0.7630940000
H	-1.0624810000	1.1564840000	-0.5058090000
H	-0.1904800000	0.9547180000	-2.0457610000
K	2.9763070000	-0.3798520000	0.1677890000
C	4.5531600000	2.8219000000	-0.7053870000
C	3.5393410000	-3.7588070000	-1.3575190000
C	4.2398100000	2.3543620000	-2.1167930000
H	5.4608040000	2.2977220000	-0.4019610000
H	4.7838640000	3.9019780000	-0.7367710000
H	3.0013190000	-3.8066770000	-2.3057580000
H	3.8076430000	-4.7995820000	-1.1075810000
C	4.8447840000	-2.9965350000	-1.6050440000
O	4.7041700000	-1.5982050000	-1.7764120000
H	5.3121270000	-3.4323100000	-2.4997890000
H	5.5483080000	-3.1118210000	-0.7836240000
O	3.8633020000	0.9888730000	-2.0660750000
H	5.1497840000	2.4741290000	-2.7168070000
H	3.4540610000	2.9506360000	-2.5931320000
C	4.2323540000	0.2345850000	-3.2047790000
C	3.9465350000	-1.2190790000	-2.9149300000
H	-1.0702580000	-1.2034290000	-0.8318890000
H	0.3344620000	-0.9426380000	0.2452440000
H	5.3026370000	0.3679160000	-3.4079060000
H	3.6649710000	0.5512860000	-4.0895540000
H	2.8778240000	-1.3597210000	-2.7240780000
H	4.2359680000	-1.8217400000	-3.7856850000
F	1.3780980000	-0.8857160000	2.1388400000

C	-0.6871390000	0.0261820000	4.3624890000
H	-1.2783230000	-0.7142710000	4.8966520000
H	0.2499010000	-0.3974580000	3.9983030000
H	-0.5063450000	0.8861860000	5.0060650000
C	-0.6109460000	1.5311480000	2.4718130000
C	-2.7524950000	1.0838630000	3.5651000000
H	-1.1836170000	1.9239910000	1.6300330000
H	-0.3892540000	2.3206920000	3.1885240000
H	0.3000970000	1.0284560000	2.1417040000
H	-2.5574110000	1.9768860000	4.1601880000
H	-3.3037170000	1.3445770000	2.6602610000
H	-3.3042010000	0.3556170000	4.1581860000
C	-1.6178520000	-0.6287020000	2.1842820000
H	-2.0193160000	-0.1840600000	1.2697260000
H	-0.6047290000	-1.0005850000	2.0117560000
C	-2.5137870000	-1.7704010000	2.6264250000
H	-2.2000590000	-2.1816480000	3.5903580000
H	-3.5630950000	-1.4734360000	2.6883570000
O	-2.3294250000	-2.7404260000	1.6006090000
H	-2.9795070000	-3.4581120000	1.6923810000
N	-1.4441350000	0.4959960000	3.1636260000
Cl	-3.6053950000	2.1980970000	0.0261530000
C	-4.1967640000	-3.7076190000	-1.1831760000
C	-4.1950490000	-4.9863120000	-0.3832570000
H	-5.0227890000	-3.0731540000	-0.8455040000
H	-4.3558330000	-3.9470050000	-2.2360110000
H	-5.0851480000	-5.5688480000	-0.6377360000
H	-3.3010740000	-5.5745940000	-0.6105570000
O	-2.9619100000	-3.0062340000	-1.1046860000

H	-2.8273270000	-2.6761570000	-0.1980520000
O	-4.2196040000	-4.6509780000	1.0095880000
H	-4.3000940000	-5.4579800000	1.5311630000
C	-1.1582880000	4.8894640000	1.3822080000
C	-2.2260990000	4.7031240000	2.4482360000
H	-0.3493690000	4.1622330000	1.5367140000
H	-0.7289660000	5.8904980000	1.4645830000
H	-3.0212600000	5.4364280000	2.2973210000
H	-2.6667890000	3.7032960000	2.3609120000
O	-1.7052000000	4.7708280000	0.0774250000
H	-2.2063060000	3.9389120000	0.0290700000
O	-1.7090270000	4.9216660000	3.7544850000
H	-0.9783820000	4.3114000000	3.9000550000
C	-6.5123630000	-1.6897120000	1.2640930000
C	-5.7134520000	-0.4308050000	1.0273680000
H	-6.7676270000	-2.1536520000	0.3045140000
H	-7.4453020000	-1.4138390000	1.7623940000
H	-6.3230320000	0.2833870000	0.4615850000
H	-5.4487060000	0.0229340000	1.9903720000
O	-5.8323320000	-2.6094200000	2.1051740000
H	-5.2839190000	-3.2015990000	1.5675350000
O	-4.5277740000	-0.7561200000	0.3011470000
H	-4.0412720000	0.0814430000	0.1867700000
C	-2.8107980000	-0.0873200000	-2.7444670000
C	-4.2807180000	0.0533550000	-3.0839800000
H	-2.6842610000	0.0338510000	-1.6625390000
H	-2.2466290000	0.7070140000	-3.2395640000
H	-4.6197970000	1.0556820000	-2.7877120000
H	-4.4246760000	-0.0553000000	-4.1622340000

O	-2.2642770000	-1.3258070000	-3.1731210000
H	-2.5288790000	-1.9904280000	-2.5118700000
O	-5.0650450000	-0.9593830000	-2.4653880000
H	-4.9104540000	-0.9140890000	-1.5048220000
C	-1.5625300000	3.4812130000	-2.9502050000
C	-2.9215910000	3.5243280000	-3.6317870000
H	-1.6155070000	2.8095350000	-2.0854530000
H	-1.3000120000	4.4768630000	-2.5875060000
H	-2.9238100000	4.2852010000	-4.4153510000
H	-3.1307750000	2.5560210000	-4.1050920000
O	-0.5316740000	3.0800920000	-3.8431780000
H	-0.6608080000	2.1496570000	-4.0591900000
O	-3.9389610000	3.8723830000	-2.7046450000
H	-3.8990760000	3.2537210000	-1.9565420000

Fig 3.(b) [2,2,2]/KF/ChCl in DMSO-d₆

C	-2.4043200000	2.2700340000	-2.5830760000
C	-2.0666720000	2.8374650000	-1.2134980000
O	-2.7678700000	0.9117290000	-2.4715760000
N	-2.9930030000	2.4643760000	-0.1456220000
C	-2.5478480000	3.0455880000	1.1222540000
C	-2.8879010000	0.2705030000	-3.7220570000
C	-2.7137130000	2.1452690000	2.3343550000
O	-1.9908460000	0.9456230000	2.1307760000
C	-1.8575510000	0.1811450000	3.3175260000
C	-3.3679540000	-1.1425840000	-3.4918060000
C	-1.6507900000	-1.2672950000	2.9571750000
O	-2.8898470000	-1.7853970000	2.4907590000

O	-2.5066690000	-1.7586700000	-2.5549800000
C	-2.9206690000	-3.1978490000	2.3894050000
C	-2.4896050000	-3.1737690000	-2.5940480000
C	-2.2817620000	-3.7416540000	1.1211190000
N	-2.9479860000	-3.3427600000	-0.1247460000
C	-2.0578410000	-3.6885000000	-1.2367230000
H	-1.5113190000	2.3771530000	-3.2167800000
H	-3.2156250000	2.8298700000	-3.0687930000
H	-2.3135390000	2.6804350000	3.2071940000
H	-3.7604960000	1.8982550000	2.5387010000
H	-2.4033150000	-3.6425770000	3.2497280000
H	-3.9715750000	-3.4838990000	2.4662900000
H	-1.7608790000	-3.5144160000	-3.3426790000
H	-3.4633240000	-3.5724370000	-2.8922780000
H	-2.2348100000	-4.8419900000	1.2136050000
H	-1.2581740000	-3.3629640000	1.0649140000
H	-1.0872060000	-3.2418990000	-1.0099630000
H	-1.9340830000	-4.7838790000	-1.3143170000
H	-1.4821350000	3.2792600000	1.0337190000
H	-3.0643490000	3.9986530000	1.3253180000
H	-1.9904190000	3.9344730000	-1.3261000000
H	-1.0896130000	2.4545460000	-0.9185970000
H	-3.6101100000	0.7959810000	-4.3625440000
H	-1.9167010000	0.2611120000	-4.2333080000
H	-3.3591050000	-1.6765300000	-4.4499940000
H	-4.3930520000	-1.1364470000	-3.0992710000
H	-1.0045950000	0.5478550000	3.9044360000
H	-2.7671350000	0.2668200000	3.9254370000
K	-2.6720460000	-0.4651810000	-0.1320900000

C	-4.3767050000	2.7755410000	-0.4743850000
C	-4.2816620000	-3.9303780000	-0.2532060000
C	-5.3788340000	2.1345280000	0.4696640000
H	-4.5835370000	2.3779140000	-1.4690320000
H	-4.5598710000	3.8653670000	-0.4952010000
H	-4.6711380000	-4.1333270000	0.7454610000
H	-4.2433190000	-4.9036510000	-0.7713760000
C	-5.3094560000	-3.0578860000	-0.9831040000
O	-5.3358950000	-1.7050140000	-0.5824310000
H	-6.2985320000	-3.5137200000	-0.8276300000
H	-5.1312500000	-3.0333860000	-2.0562210000
O	-5.0771130000	0.7573640000	0.5661800000
H	-6.3820420000	2.2754550000	0.0480300000
H	-5.3736980000	2.6018880000	1.4623790000
C	-6.1801510000	-0.0590870000	0.8944710000
C	-5.7476490000	-1.4986570000	0.7568790000
H	-1.3352580000	-1.8145080000	3.8557450000
H	-0.8837080000	-1.3616410000	2.1794910000
H	-7.0138070000	0.1441150000	0.2095710000
H	-6.5196470000	0.1279450000	1.9225710000
H	-4.9234060000	-1.7026750000	1.4487610000
H	-6.5940570000	-2.1530830000	1.0057420000
F	-0.1898920000	-1.5083390000	0.1622010000
C	1.9328540000	-2.6159650000	-2.1059880000
H	1.0325620000	-2.5249910000	-1.4984970000
H	1.6928040000	-2.8315050000	-3.1469030000
H	2.5815670000	-3.3908070000	-1.6990780000
C	4.0268640000	-1.4791980000	-2.6438090000
C	2.8427320000	-0.9405060000	-0.6012310000

H	4.5184760000	-0.5050730000	-2.6141000000
H	4.5995000000	-2.2077570000	-2.0667750000
H	3.9081470000	-1.8148670000	-3.6739000000
H	3.3939610000	-1.7400750000	-0.1014090000
H	3.4044630000	-0.0051320000	-0.5690840000
H	1.8594700000	-0.8310160000	-0.1544230000
C	1.9473450000	-0.2428210000	-2.8146310000
H	2.4848810000	0.6829680000	-2.5931730000
H	2.0865640000	-0.4956180000	-3.8679130000
C	0.4565780000	-0.0762140000	-2.5426730000
H	0.1237900000	0.6471250000	-3.2985250000
H	-0.0917260000	-1.0046930000	-2.7424970000
O	0.1618350000	0.4289530000	-1.2731560000
H	-0.0054030000	-0.3613350000	-0.6514710000
N	2.6698880000	-1.3223190000	-2.0387000000
Cl	4.9661490000	2.0536440000	-1.0598630000
S	3.4398930000	-1.7307630000	3.3337590000
O	3.9977880000	-2.7403140000	2.3342590000
C	1.6857500000	-1.5594530000	2.9633450000
C	3.9654180000	-0.0997400000	2.7747880000
H	1.1963390000	-2.4665490000	3.3201200000
H	1.5515650000	-1.4663790000	1.8840610000
H	1.3086840000	-0.6749030000	3.4852520000
H	3.3759950000	0.6438740000	3.3171050000
H	3.7973990000	-0.0255840000	1.6989330000
H	5.0276420000	0.0037660000	2.9979440000
S	0.8986240000	2.4834490000	2.8329570000
O	1.3310750000	1.5184450000	3.9432830000
C	0.9887430000	1.5795020000	1.2824550000

C	2.3146110000	3.5583170000	2.5348520000
H	0.2644180000	0.7669140000	1.3192180000
H	2.0052860000	1.2089710000	1.1428230000
H	0.7213530000	2.2830350000	0.4949070000
H	2.0804250000	4.1648040000	1.6572220000
H	3.1971420000	2.9364150000	2.3689100000
H	2.4480970000	4.1844030000	3.4171030000
S	0.8226540000	4.8031000000	-1.3976930000
O	0.5586450000	4.5805560000	0.0890700000
C	1.5261520000	3.2668180000	-2.0237370000
C	2.3289980000	5.7886970000	-1.4855750000
H	0.7811620000	2.4825620000	-1.8862520000
H	2.4300510000	3.0275610000	-1.4565540000
H	1.7573840000	3.3966580000	-3.0834410000
H	2.6406710000	5.8708100000	-2.5280130000
H	3.0993280000	5.3023030000	-0.8848350000
H	2.0993660000	6.7766530000	-1.0869630000
S	7.2627060000	-2.4316830000	-0.4836080000
O	6.2965210000	-3.2995400000	-1.2791620000
C	6.2641880000	-1.2691520000	0.4645360000
C	7.9435670000	-1.2414760000	-1.6544330000
H	5.5955410000	-1.8639820000	1.0927730000
H	5.7015140000	-0.6245380000	-0.2145870000
H	6.9356850000	-0.6699990000	1.0838840000
H	8.5248160000	-0.4952990000	-1.1101470000
H	7.1184470000	-0.7733200000	-2.1943810000
H	8.5892140000	-1.7859140000	-2.3431780000

Fig 4.(a) [2,2,2]/KF/Ch⁺

C	-2.7131150000	-2.0546920000	2.6212490000
C	-2.5271760000	-2.9118270000	1.3782910000
O	-2.1534430000	-0.7783400000	2.4022780000
N	-2.8497520000	-2.2312220000	0.1242000000
C	-2.6676240000	-3.1386300000	-1.0087980000
C	-2.0325480000	-0.0164380000	3.5840130000
C	-2.0643040000	-2.4986010000	-2.2498170000
O	-0.8107020000	-1.9454640000	-1.9106030000
C	-0.0481510000	-1.5831440000	-3.0449320000
C	-1.6018850000	1.3835160000	3.2068220000
C	0.9835870000	-0.5603370000	-2.6371560000
O	0.3158470000	0.6853190000	-2.4800160000
O	-0.4322700000	1.2809100000	2.4239590000
C	1.1726190000	1.8071520000	-2.4112630000
C	0.4781040000	2.3537380000	2.5111620000
C	1.7339030000	2.0598900000	-1.0199450000
N	0.7378200000	2.3550680000	0.0112340000
C	1.4024730000	2.2679290000	1.3121450000
H	-2.2107650000	-2.5554610000	3.4590370000
H	-3.7730230000	-1.9546100000	2.8898870000
H	-1.9397330000	-3.2852780000	-3.0075320000
H	-2.6971840000	-1.7140860000	-2.6753010000
H	2.0211000000	1.6742760000	-3.0946840000
H	0.5906290000	2.6546780000	-2.7802000000
H	1.0793150000	2.2661280000	3.4263210000
H	-0.0406590000	3.3170520000	2.5608030000
H	2.4888570000	2.8670820000	-1.0964720000
H	2.2393020000	1.1468120000	-0.7003260000

H	1.8803770000	1.2851570000	1.3412230000
H	2.1737730000	3.0548300000	1.4154610000
H	-1.9759580000	-3.9270380000	-0.7022340000
H	-3.6137130000	-3.6333180000	-1.2831230000
H	-3.1267490000	-3.8286540000	1.5201690000
H	-1.4771640000	-3.2116990000	1.3177690000
H	-2.9916690000	0.0265510000	4.1177500000
H	-1.2835750000	-0.4741680000	4.2430580000
H	-1.4192030000	1.9570940000	4.1237800000
H	-2.3898760000	1.8773390000	2.6237990000
H	0.4409570000	-2.4716970000	-3.4650930000
H	-0.6946070000	-1.1426020000	-3.8143310000
K	-0.7796270000	-0.1072860000	0.1177330000
C	-4.1597290000	-1.5935730000	0.1556990000
C	0.0290070000	3.6124910000	-0.2050940000
C	-4.4069840000	-0.6671920000	-1.0235920000
H	-4.2067630000	-0.9707920000	1.0490560000
H	-4.9789040000	-2.3338640000	0.2032180000
H	0.0419380000	3.8402470000	-1.2721770000
H	0.5368400000	4.4579760000	0.2907010000
C	-1.4369160000	3.6038240000	0.2526300000
O	-2.1673070000	2.4654460000	-0.1360010000
H	-1.9172730000	4.5132160000	-0.1368990000
H	-1.5209160000	3.6355250000	1.3368430000
O	-3.3055250000	0.2074540000	-1.1361890000
H	-5.3253440000	-0.1020900000	-0.8227440000
H	-4.5635800000	-1.2169210000	-1.9603990000
C	-3.6066070000	1.4584670000	-1.7148240000
C	-2.4032370000	2.3530200000	-1.5272660000

H	1.7443920000	-0.4739800000	-3.4236500000
H	1.4463540000	-0.8603500000	-1.6892850000
H	-4.4731980000	1.9038710000	-1.2103900000
H	-3.8334450000	1.3553680000	-2.7845190000
H	-1.5355630000	1.9154310000	-2.0336080000
H	-2.6180040000	3.3384150000	-1.9627830000
F	1.6870090000	-0.7484440000	0.4153520000
C	4.0944890000	-0.8849670000	1.9678540000
H	4.7388410000	-0.0218060000	2.1276790000
H	3.0565960000	-0.6105120000	1.7486230000
H	4.1601860000	-1.5516190000	2.8273540000
C	3.7273640000	-2.8678450000	0.6243970000
C	6.0062810000	-2.0330970000	0.9468360000
H	4.0377180000	-3.3968480000	-0.2762410000
H	3.8826650000	-3.4963600000	1.5006570000
H	2.6955130000	-2.5126820000	0.5499560000
H	6.0906600000	-2.6381040000	1.8484830000
H	6.3261950000	-2.6102420000	0.0805000000
H	6.6194040000	-1.1400410000	1.0476690000
C	4.3919600000	-0.8318530000	-0.4930380000
H	4.8896130000	-1.3732870000	-1.2995490000
H	3.3110140000	-0.7975260000	-0.6394950000
C	4.9249600000	0.5916670000	-0.4416550000
H	4.3380710000	1.1890280000	0.2656630000
H	5.9827210000	0.6325170000	-0.1522700000
O	4.7433180000	1.0486530000	-1.7656610000
H	4.9570290000	1.9838250000	-1.8062980000
N	4.5817140000	-1.6411580000	0.7666520000

Fig 4.(b) [2,2,2]/KF/Ch⁺

C	0.2519020000	2.8318680000	-2.2617970000
C	0.1727620000	3.3997990000	-0.8528080000
O	-0.0268560000	1.4477750000	-2.2265280000
N	-0.9897280000	2.9361650000	-0.0919020000
C	-0.9535160000	3.5000300000	1.2575100000
C	0.1791340000	0.8108100000	-3.4661070000
C	-1.4682720000	2.5863470000	2.3579960000
O	-0.6915620000	1.4070400000	2.3851490000
C	-0.9060100000	0.6517520000	3.5618140000
C	-0.2919850000	-0.6198750000	-3.3446810000
C	-0.4957040000	-0.7784370000	3.3194900000
O	-1.4691600000	-1.3579700000	2.4595800000
O	0.3740200000	-1.2094690000	-2.2443550000
C	-1.4031120000	-2.7670350000	2.3692780000
C	0.4526130000	-2.6244430000	-2.2681740000
C	-0.3932980000	-3.2614400000	1.3450780000
N	-0.6921550000	-2.8721060000	-0.0409310000
C	0.5031360000	-3.1402150000	-0.8440620000
H	1.2661150000	3.0052220000	-2.6481050000
H	-0.4451850000	3.3292600000	-2.9489770000
H	-1.3680600000	3.1252090000	3.3107720000
H	-2.5212670000	2.3155800000	2.2333360000
H	-1.1416930000	-3.1937160000	3.3459480000
H	-2.4169670000	-3.1035940000	2.1409230000
H	1.3704230000	-2.9319770000	-2.7863270000
H	-0.3851250000	-3.0529540000	-2.8251110000
H	-0.3133070000	-4.3592240000	1.4400600000

H	0.5765650000	-2.8222590000	1.5892100000
H	1.3324280000	-2.6410750000	-0.3371060000
H	0.7135230000	-4.2245790000	-0.8850570000
H	0.0901740000	3.7113270000	1.5013190000
H	-1.4980360000	4.4579790000	1.3066040000
H	0.1943490000	4.5011650000	-0.9404600000
H	1.0577440000	3.0762590000	-0.3025170000
H	-0.3841820000	1.3156480000	-4.2623700000
H	1.2468450000	0.8381310000	-3.7278660000
H	-0.0616030000	-1.1504140000	-4.2765940000
H	-1.3757410000	-0.6418090000	-3.1727390000
H	-0.3266950000	1.0780510000	4.3909050000
H	-1.9694970000	0.6683150000	3.8322530000
K	-0.6078330000	0.0194200000	0.0461460000
C	-2.2375290000	3.1905790000	-0.8009490000
C	-1.8955520000	-3.5232430000	-0.5567420000
C	-3.4476030000	2.5028150000	-0.1906080000
H	-2.1351690000	2.7858410000	-1.8084480000
H	-2.4494300000	4.2720940000	-0.8844570000
H	-2.5390550000	-3.7801090000	0.2857970000
H	-1.6581870000	-4.4791130000	-1.0543260000
C	-2.7235770000	-2.6745590000	-1.5330490000
O	-2.9012780000	-1.3315590000	-1.1447780000
H	-3.7004530000	-3.1622920000	-1.6611520000
H	-2.2618250000	-2.6256070000	-2.5173280000
O	-3.1304610000	1.1410780000	0.0058190000
H	-4.2826300000	2.6014500000	-0.8950950000
H	-3.7627240000	2.9669290000	0.7518200000
C	-4.2402170000	0.2697340000	-0.0263780000

C	-3.7162880000	-1.1473880000	-0.0004450000
H	-0.4884040000	-1.3119110000	4.2788720000
H	0.4963960000	-0.8238670000	2.8562880000
H	-4.8145880000	0.4312070000	-0.9471670000
H	-4.8983540000	0.4376810000	0.8365060000
H	-3.1377280000	-1.3079190000	0.9160610000
H	-4.5653700000	-1.8436770000	-0.0187560000
F	1.6531980000	-0.9397070000	1.0712030000
C	4.4016940000	-0.1647090000	1.7722360000
H	3.7921590000	0.7098880000	1.9722220000
H	3.7622990000	-1.0437560000	1.8210050000
H	5.2476700000	-0.2264020000	2.4559530000
C	6.0270450000	-1.0700460000	0.2098550000
C	5.5307820000	1.3179290000	0.1960940000
H	6.4603420000	-0.9785030000	-0.7846720000
H	6.7925920000	-0.9071660000	0.9667800000
H	5.5825460000	-2.0561300000	0.3362020000
H	6.3378960000	1.4486310000	0.9159100000
H	5.9149190000	1.4119560000	-0.8194000000
H	4.7404530000	2.0430170000	0.3789770000
C	3.8883220000	-0.3216460000	-0.6776390000
H	4.4220390000	-0.5212540000	-1.6098050000
H	3.3632100000	-1.2133460000	-0.3357930000
C	2.8805530000	0.8074910000	-0.8782250000
H	3.3535440000	1.6584680000	-1.3816900000
H	2.1286450000	0.3935610000	-1.5640300000
O	2.3170570000	1.2462130000	0.3202500000
H	1.9551980000	0.3777300000	0.7567780000
N	4.9543830000	-0.0456450000	0.3742700000

Fig S2 [2,2,2]/KF/EG-d₆ in DMSO-d₆

C	1.5261020000	3.1039020000	2.1054320000
C	1.4275320000	3.4129120000	0.6214390000
O	1.9117930000	1.7586290000	2.3043250000
N	2.5581890000	2.9671900000	-0.1897440000
C	2.3720560000	3.3672750000	-1.5849650000
C	1.5864100000	1.2831180000	3.5963470000
C	2.6612740000	2.2732190000	-2.6027110000
O	1.9113790000	1.1305210000	-2.2566210000
C	1.7273380000	0.2204280000	-3.3236300000
C	2.1856850000	-0.0924530000	3.7802930000
C	1.3767260000	-1.1265040000	-2.7409880000
O	2.5526380000	-1.6411230000	-2.1277590000
O	1.7824860000	-0.9052860000	2.6967120000
C	2.5369780000	-3.0298310000	-1.8643110000
C	1.6232250000	-2.2751060000	2.9884730000
C	1.7954900000	-3.4082910000	-0.5925300000
N	2.3173810000	-2.7983940000	0.6322420000
C	1.3217000000	-2.9916750000	1.6885720000
H	0.5338470000	3.2823180000	2.5417810000
H	2.2330550000	3.7714010000	2.6155090000
H	2.3596540000	2.6446710000	-3.5929290000
H	3.7245820000	2.0114260000	-2.6492010000
H	2.0704620000	-3.5670860000	-2.7009710000
H	3.5830240000	-3.3413190000	-1.8245320000
H	0.7723200000	-2.4283170000	3.6688450000
H	2.5056070000	-2.6836930000	3.4923550000

H	1.7819230000	-4.5115400000	-0.5237250000
H	0.7564480000	-3.0898450000	-0.6986710000
H	0.3689920000	-2.6060550000	1.3122500000
H	1.1847200000	-4.0642880000	1.9136810000
H	1.3256530000	3.6541830000	-1.7185120000
H	2.9794940000	4.2523540000	-1.8309350000
H	1.2548280000	4.5012440000	0.5343730000
H	0.5420990000	2.9062700000	0.2251870000
H	1.9864500000	1.9534910000	4.3692800000
H	0.4959850000	1.2283400000	3.7087550000
H	1.8316780000	-0.5019670000	4.7349590000
H	3.2813370000	-0.0390340000	3.8115250000
H	0.9134680000	0.5572550000	-3.9757570000
H	2.6531090000	0.1238440000	-3.9060260000
K	2.2158110000	0.0844040000	0.1943280000
C	3.8608400000	3.3275970000	0.3483840000
C	3.6379330000	-3.3198040000	0.9887720000
C	4.9927300000	2.5824130000	-0.3414270000
H	3.8854140000	3.0423510000	1.4011290000
H	4.0587560000	4.4123950000	0.2789620000
H	4.1470630000	-3.6285680000	0.0743770000
H	3.5541630000	-4.2242240000	1.6153610000
C	4.5561930000	-2.3350330000	1.7183150000
O	4.6789630000	-1.0676660000	1.1118900000
H	5.5451080000	-2.8106430000	1.7973080000
H	4.2107060000	-2.1290190000	2.7292480000
O	4.6781790000	1.2056770000	-0.3308050000
H	5.9197580000	2.7674490000	0.2157660000
H	5.1505330000	2.9334490000	-1.3696060000

C	5.7882840000	0.3402820000	-0.4218390000
C	5.2914300000	-1.0640760000	-0.1640770000
H	1.0446600000	-1.7984590000	-3.5430180000
H	0.5669850000	-1.0080340000	-2.0074120000
H	6.5381170000	0.6106020000	0.3331150000
H	6.2557520000	0.3948910000	-1.4146290000
H	4.5703530000	-1.3528280000	-0.9387260000
H	6.1412250000	-1.7592200000	-0.1911850000
F	-0.3893250000	0.1205860000	-0.1323700000
C	-2.3944460000	0.2694100000	2.3917300000
C	-1.4612440000	-0.7598990000	3.0028260000
H	-1.9749170000	1.2692920000	2.5865360000
H	-3.3842010000	0.2221230000	2.8592260000
H	-1.8946250000	-1.7644890000	2.9031920000
H	-0.5102460000	-0.7299680000	2.4609900000
O	-2.5594270000	0.0344500000	1.0146470000
H	-1.6489740000	0.0806350000	0.5549230000
O	-1.2772090000	-0.4217890000	4.3752690000
H	-0.6400060000	-1.0369140000	4.7516310000
S	-2.1805860000	1.3327920000	-3.5182140000
O	-1.3882350000	0.2170020000	-4.1998210000
C	-1.0000030000	2.2765070000	-2.5364720000
C	-3.0467980000	0.5737200000	-2.1343060000
H	-0.3079680000	2.7455660000	-3.2378420000
H	-0.4717690000	1.5993040000	-1.8587570000
H	-1.5750550000	3.0356150000	-2.0011890000
H	-3.5515550000	1.3803540000	-1.5968040000
H	-2.3085230000	0.0775610000	-1.5024990000
H	-3.7675190000	-0.1324080000	-2.5483070000

S	-1.6176990000	-3.7505340000	-1.9176510000
O	-2.6210180000	-4.8872860000	-1.7807980000
C	-1.9798860000	-2.6060030000	-0.5740160000
C	-2.2063170000	-2.7101990000	-3.2631390000
H	-1.8396390000	-3.1612280000	0.3556610000
H	-3.0200260000	-2.2876100000	-0.6640250000
H	-1.3011210000	-1.7486790000	-0.6044630000
H	-1.6489360000	-1.7699160000	-3.3042610000
H	-3.2710270000	-2.5260060000	-3.1031090000
H	-2.0594660000	-3.2661470000	-4.1901410000
S	-3.7555240000	3.8943370000	0.2604010000
O	-3.8095200000	3.5593830000	-1.2284300000
C	-2.0835360000	3.4822780000	0.7985930000
C	-4.6069650000	2.5543170000	1.1130600000
H	-1.4115550000	4.1879880000	0.3100230000
H	-1.8615050000	2.4538090000	0.5012080000
H	-2.0260650000	3.6058120000	1.8813670000
H	-4.5611370000	2.7380230000	2.1878030000
H	-4.1257230000	1.6085680000	0.8635080000
H	-5.6457440000	2.5733840000	0.7848450000
S	-6.0420630000	-1.2190780000	1.4477790000
O	-5.8149080000	-0.0258230000	2.3633720000
C	-4.7025830000	-2.3829210000	1.7835770000
C	-5.4592070000	-0.7298120000	-0.1890270000
H	-4.8004290000	-2.6989660000	2.8225390000
H	-3.7585130000	-1.8648760000	1.6116070000
H	-4.8064310000	-3.2450650000	1.1215320000
H	-5.5397290000	-1.5882580000	-0.8596160000
H	-4.4263580000	-0.3969750000	-0.0766990000

H	-6.1027240000	0.0767670000	-0.5423390000
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