

Supporting Information

Anion binding and fluoride ion induced conformational changes in bisurea receptors

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Synthesis and characterization

The methods of obtaining crystals **L1**, **L1·H₂O**, **L3**, **L3·TBAF** and **L5**.

Crystal **L1**: A suspension of the **L1** (30.6 mg, 0.1 mmol) in the methanol (2.5 mL) and water (2.5 mL), is refluxed and stirred 30 minutes. Then the mixture is filtered and keep the filtrate stand still. Crystals suitable for X-ray diffraction formed over a period of one week.

Crystal **L1·H₂O**: A solution of the **L1** (30.6 mg, 0.1 mmol) in the ethyl acetate (3 mL), added to a solution of TBAHSO₄ (34.0 mg, 0.1 mmol) in the ethyl acetate (2 mL), the mixture is refluxed and stirred 30 minutes. Then the mixture is filtered and keep the filtrate stand still. Crystals suitable for X-ray diffraction formed over a period of one week.

Crystal **L3**: A suspension of the **L3** (40.4 mg, 0.1 mmol) in the methanol (2.5 mL) and water (2.5 mL), is refluxed and stirred 30 minutes. Then the mixture is filtered and keep the filtrate stand still. Crystals suitable for X-ray diffraction formed over a period of one week.

Crystal **L3·TBAF**: A solution of the **L3** (40.4 mg, 0.1 mmol) in the THF (3 mL), added to a solution of TBAF (26.1 mg, 0.1 mmol) in the THF (1 mL), the mixture is refluxed and stirred 30 minutes. Then the mixture is filtered and keep the filtrate stand still. Crystals suitable for X-ray diffraction formed over a period of one week.

Crystal **L5**: A suspension of the **L5** (30.6 mg, 0.1 mmol) in the methanol (2.5 mL) and water (2.5 mL), is refluxed and stirred 30 minutes. Then the mixture is filtered and keep the filtrate stand still. Crystals suitable for X-ray diffraction formed over a period of one week.

The Compound characterization.

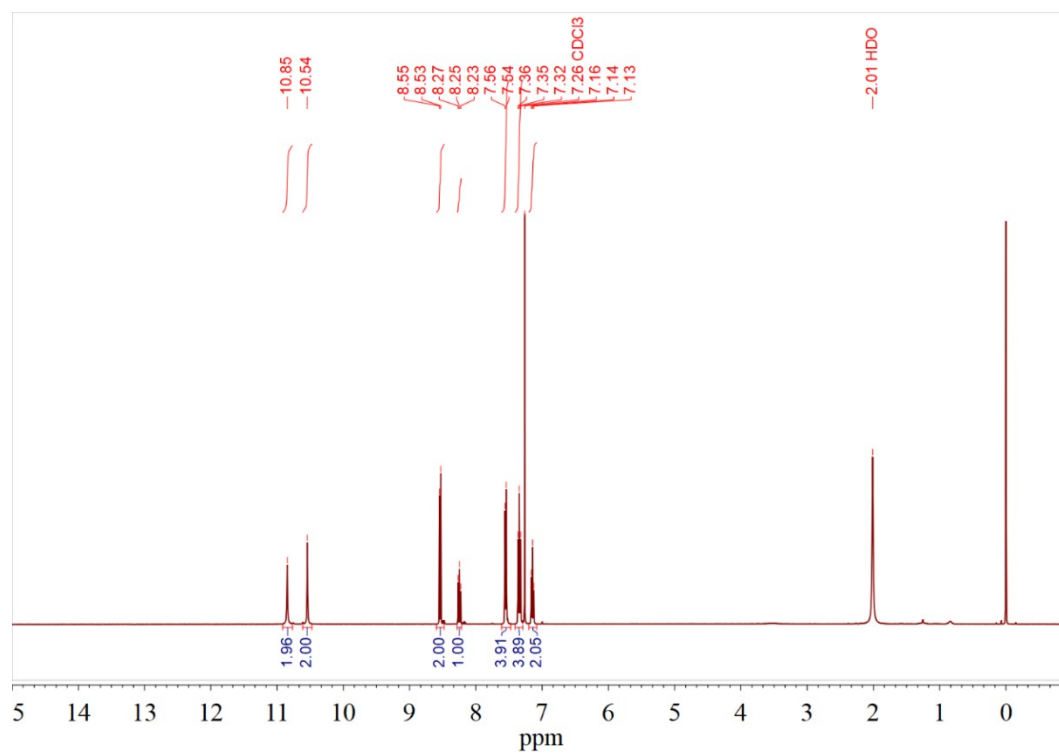


Fig. S1 The ¹H NMR spectra of L3

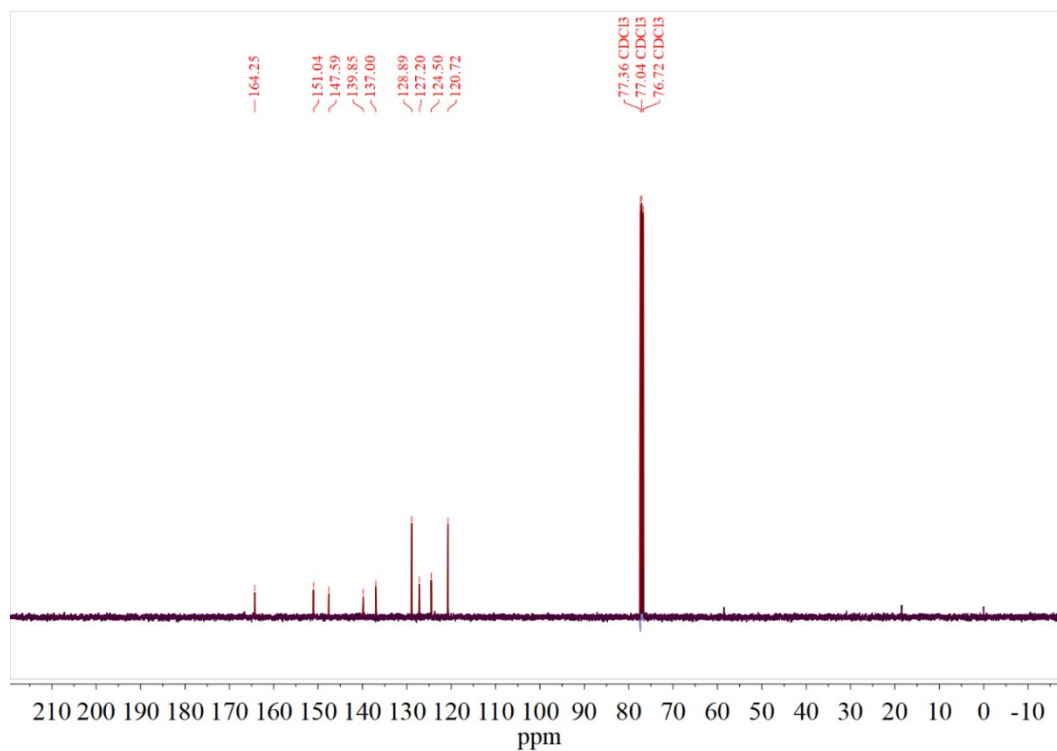


Fig. S2 The ¹³C NMR spectra of L3

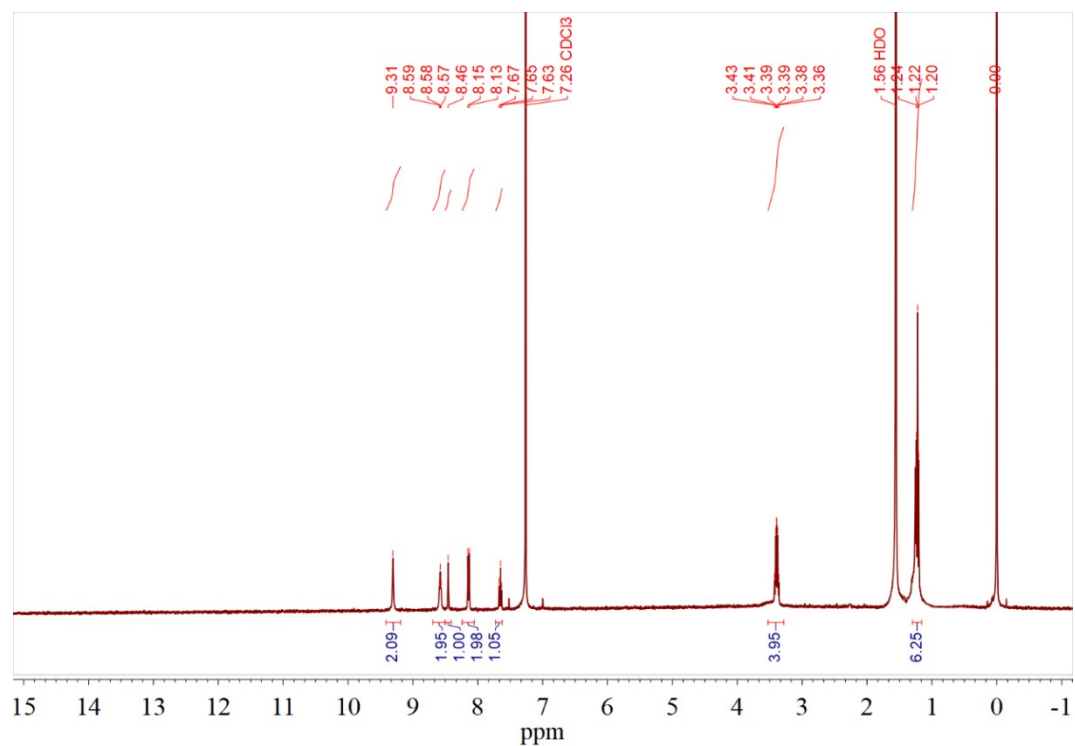


Fig. S3 The ¹H NMR spectra of L4

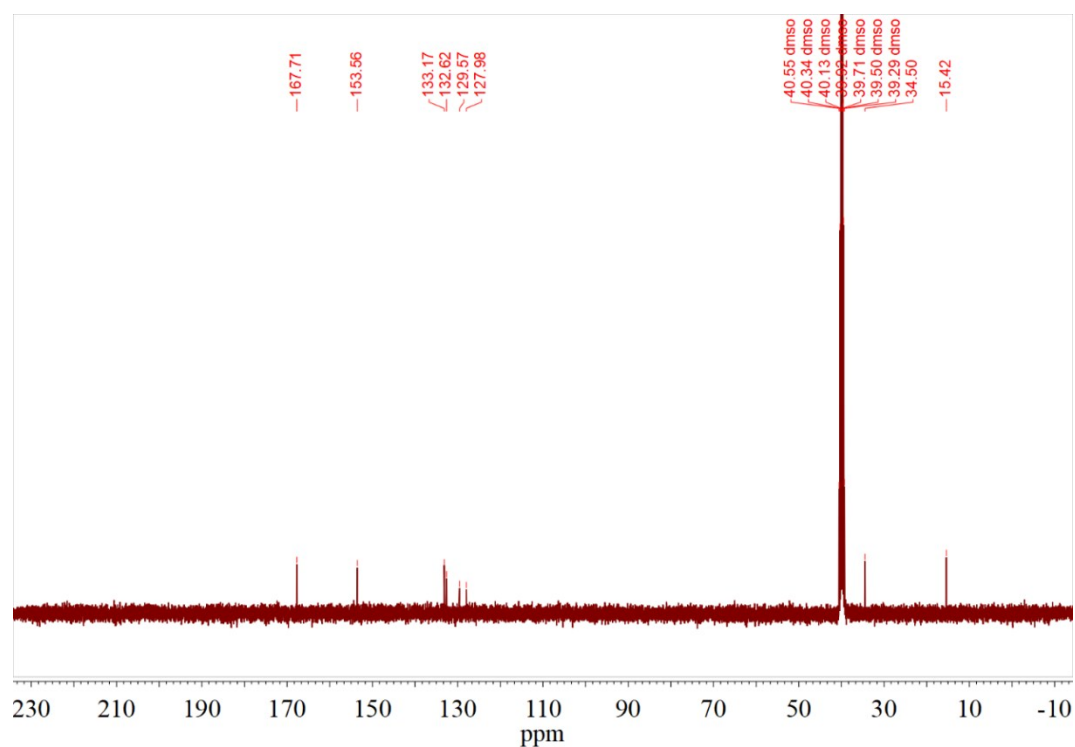


Fig. S4 The ¹³C NMR spectra of L4

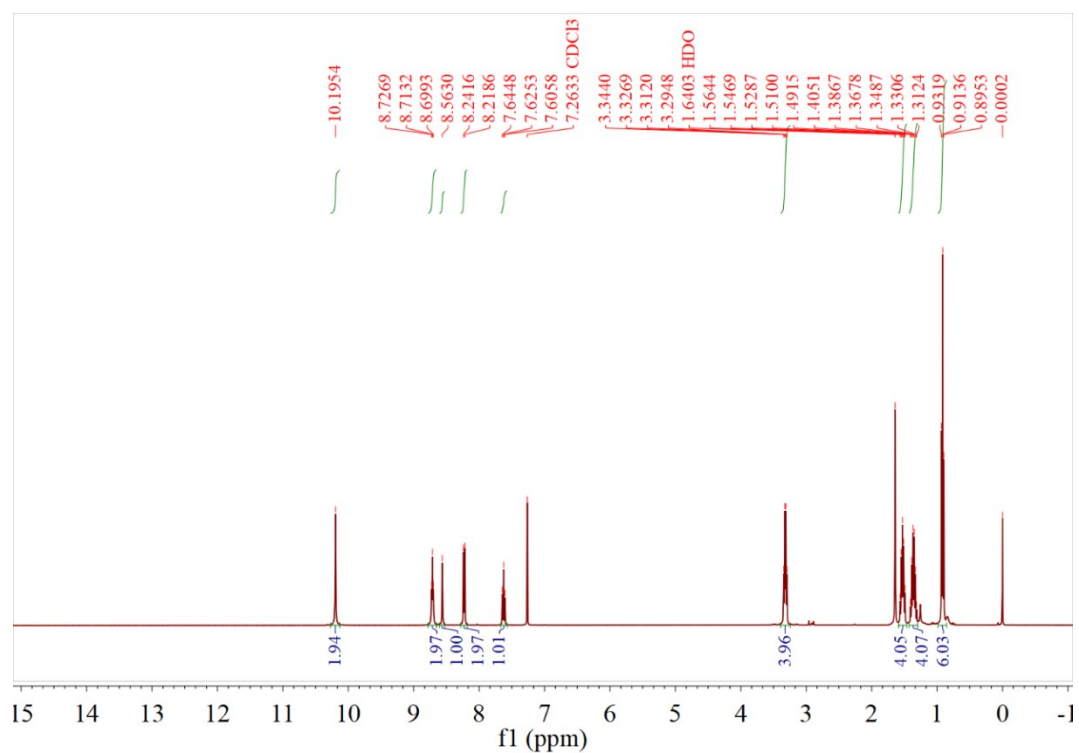


Fig. S5 The ^1H NMR spectra of **L5**

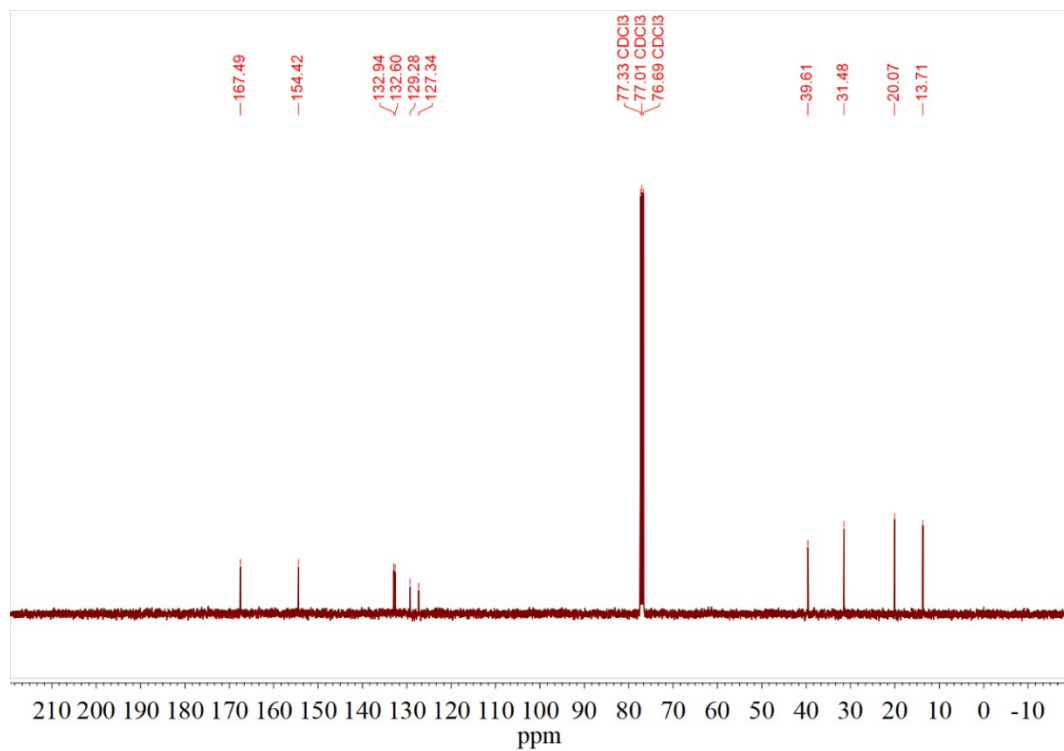


Fig. S6 The ^{13}C NMR spectra of **L5**

NMR titration

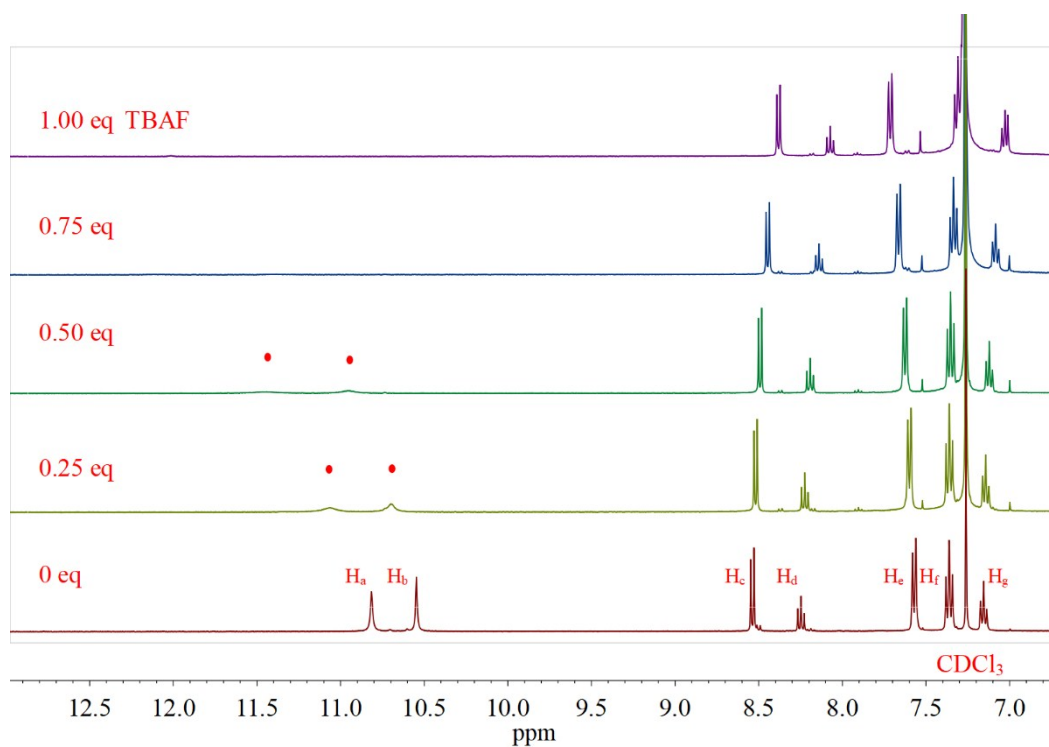


Fig. S7 Stacked ^1H NMR spectra for titration of **L3** (0.005M) with TBAF (0-1 equiv) in CDCl_3 at 298 K.

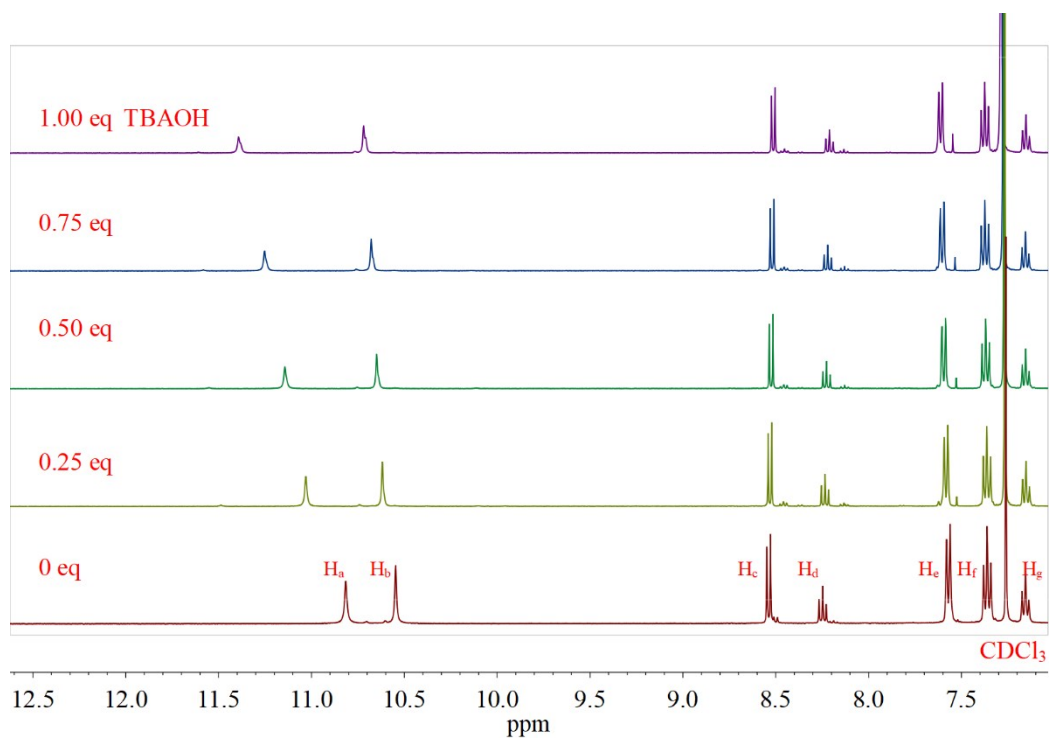


Fig. S8 Stacked ^1H NMR spectra for titration of **L3** (0.005M) with TBAOH (0-1 equiv) in CDCl_3 at 298 K.

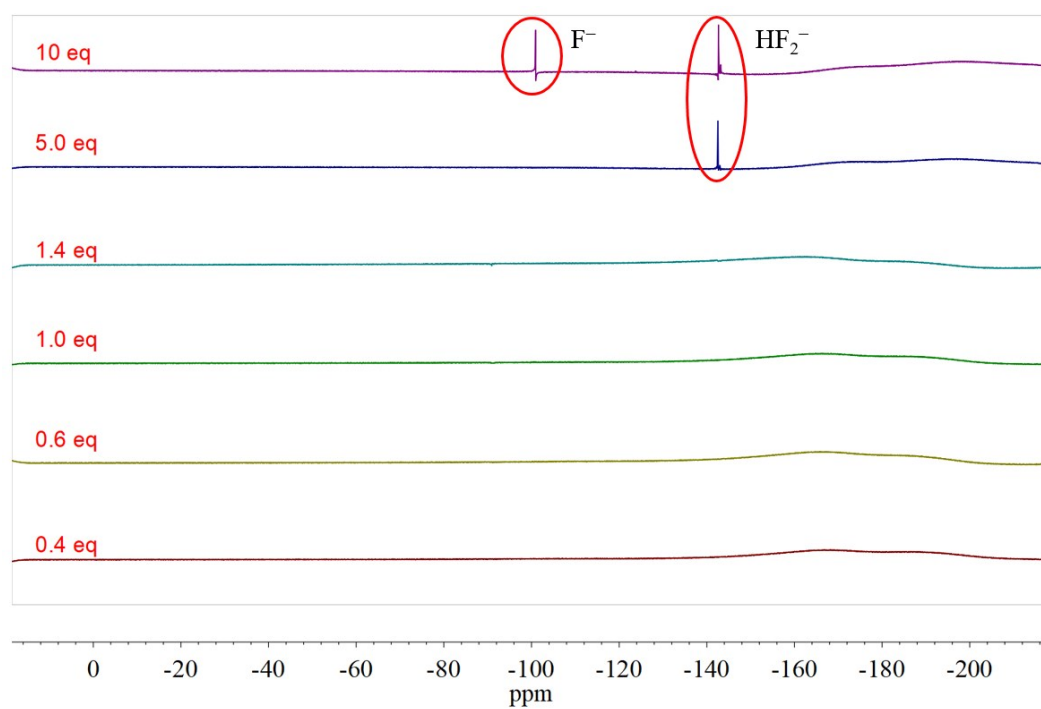


Fig. S9 Stacked ^{19}F NMR spectra for titration of **L3** (0.002M) with TBAF (0-10 equiv) in $\text{DMSO-}d_6$ at 298 K.

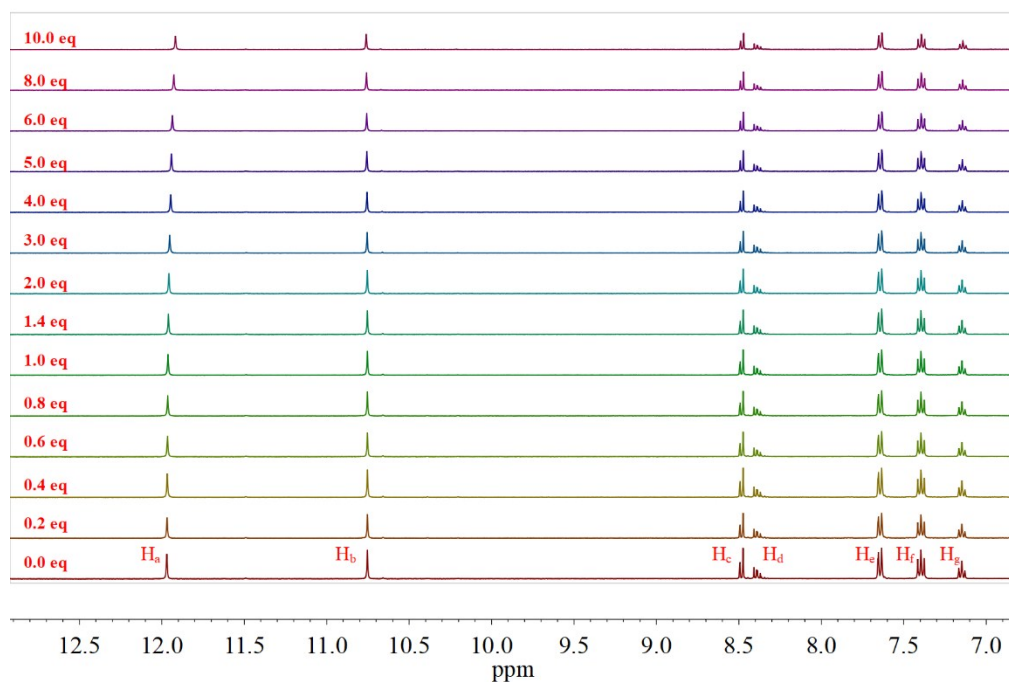


Fig. S10 Stacked ^1H NMR spectra for titration of **L3** (0.002M) with TBACl (0-10 equiv) in $\text{DMSO}-d_6$ at 298 K.

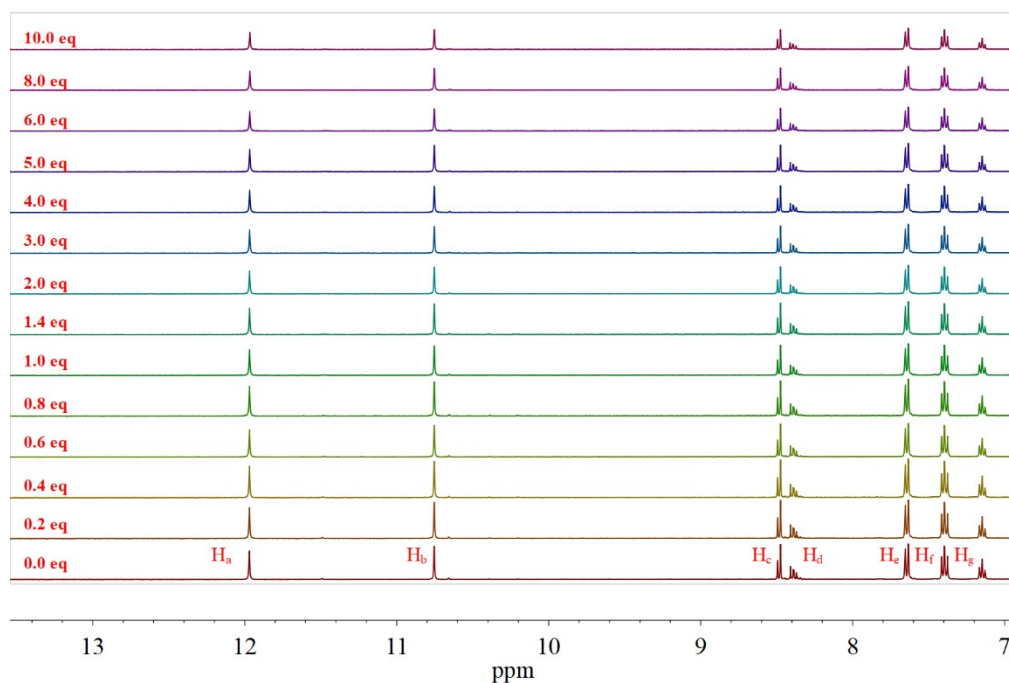


Fig. S11 Stacked ^1H NMR spectra for titration of **L3** (0.002M) with TBABr (0-10 equiv) in $\text{DMSO}-d_6$ at 298 K.

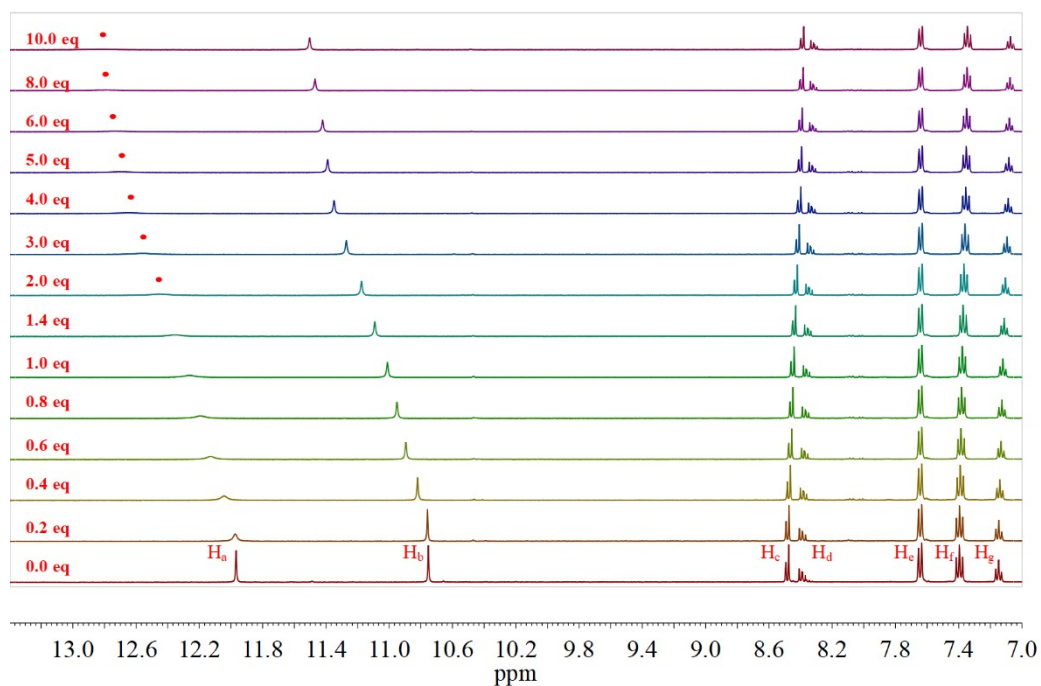


Fig. S12 Stacked ^1H NMR spectra for titration of **L3** (0.002M) with TBACH_3COO (0-10 equiv) in $\text{DMSO}-d_6$ at 298 K.

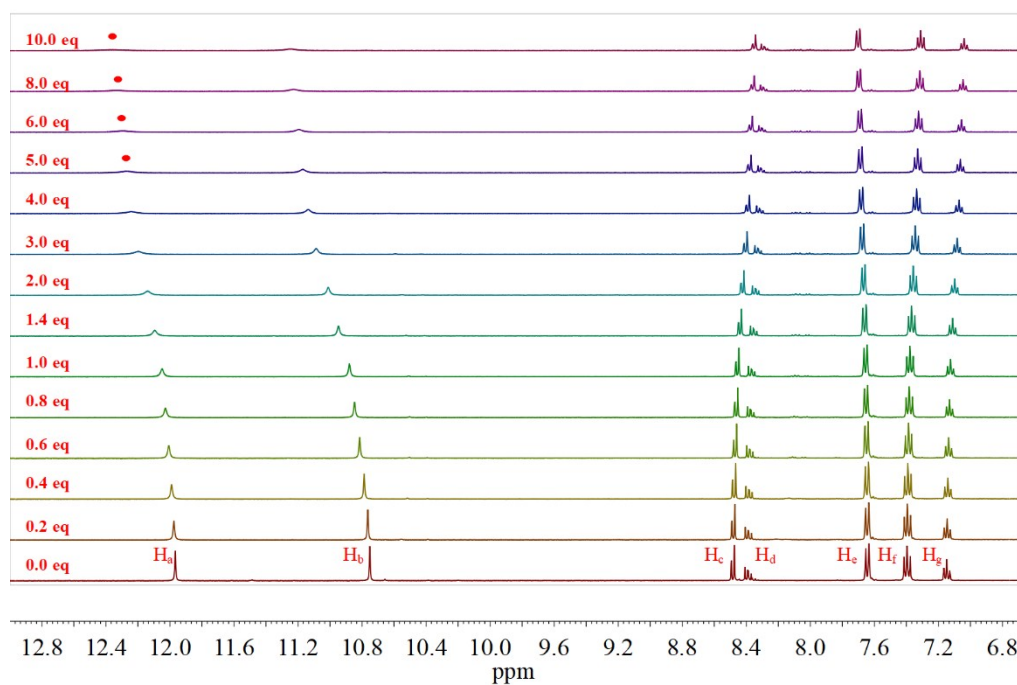


Fig. S13 Stacked ^1H NMR spectra for titration of **L3** (0.002M) with TBAH_2PO_4 (0-10 equiv) in $\text{DMSO}-d_6$ at 298 K.

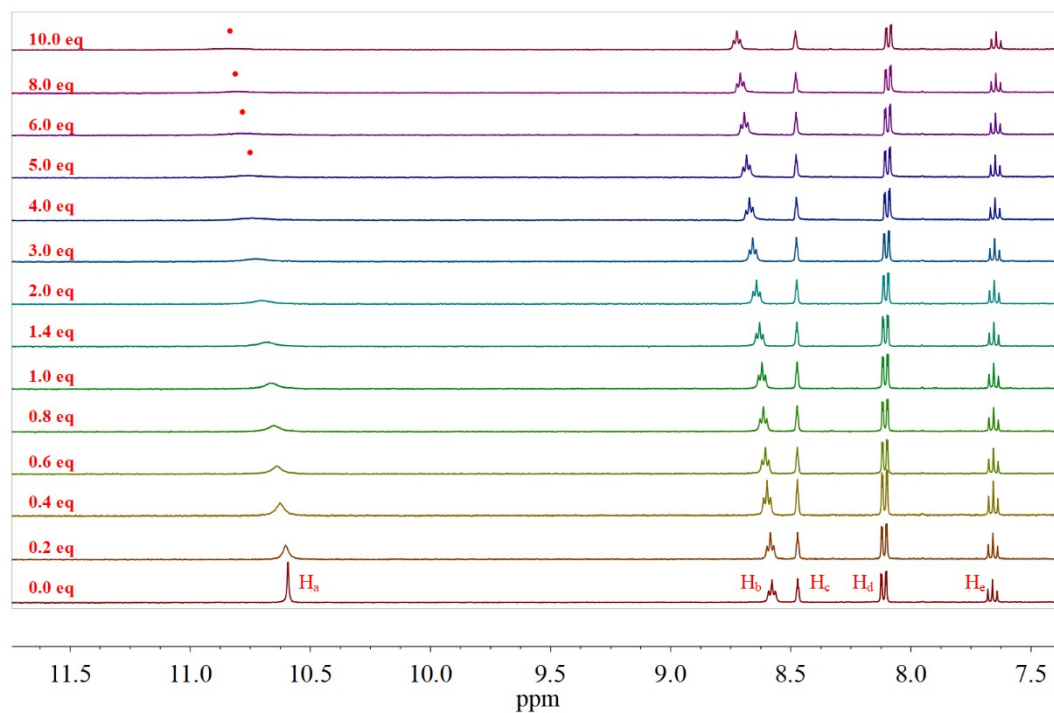


Fig. S14 Stacked ^1H NMR spectra for titration of **L4** (0.002M) with TBACH_3COO (0-10 equiv) in $\text{DMSO}-d_6$ at 298 K.

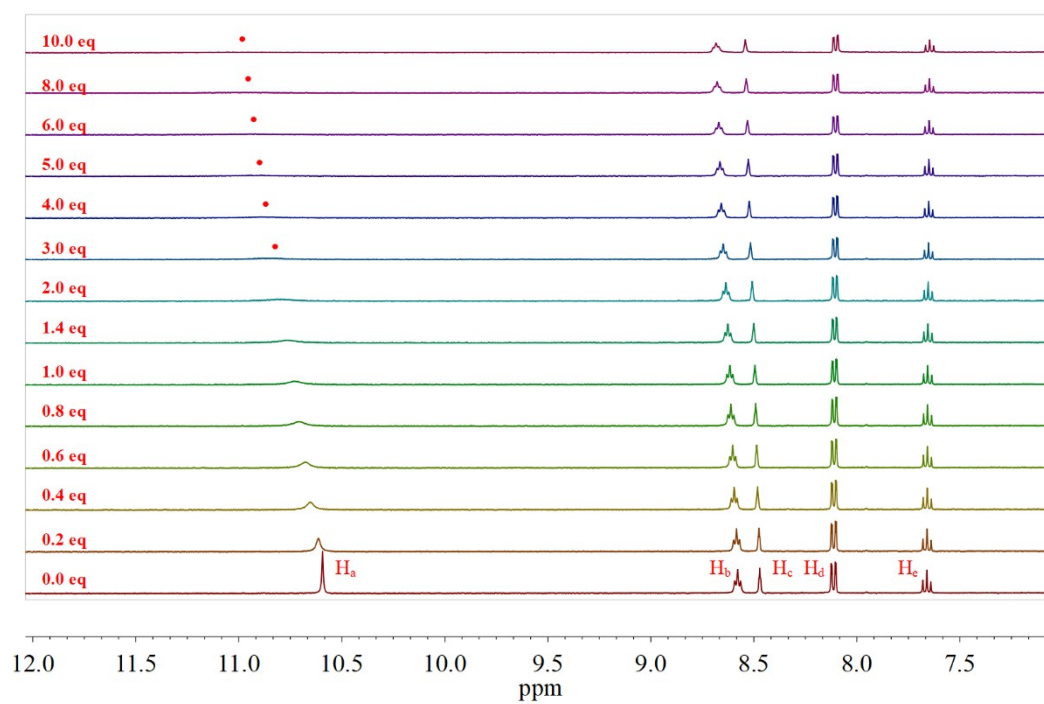


Fig. S15 Stacked ^1H NMR spectra for titration of **L4** (0.002M) with TBAH_2PO_4 (0-10 equiv) in $\text{DMSO}-d_6$ at 298 K.

Association constants

Table S1 Representative data obtained for NMR titration of **L3** with TBACl

L3, M	Cl⁻, M	G/H equivalent total	H_a, ppm	fitted line
0.002	0	0	11.9699	11.9699
0.002	0.0004	0.2	11.9681	11.96880568
0.002	0.0008	0.4	11.9667	11.96771142
0.002	0.0012	0.6	11.9654	11.96661721
0.002	0.0016	0.8	11.964	11.96552305
0.002	0.002	1	11.9626	11.96442894
0.002	0.0028	1.4	11.9604	11.96224089
0.002	0.004	2	11.9573	11.95895921
0.002	0.006	3	11.9519	11.9534908
0.002	0.008	4	11.9466	11.94802371
0.002	0.01	5	11.9413	11.94255796
0.002	0.012	6	11.9361	11.93709352
0.002	0.016	8	11.9271	11.92616862
0.002	0.02	10	11.9178	11.91524901

Table S2 Representative data obtained for NMR titration of **L3** with TBABr

L3, M	Br⁻, M	G/H equivalent total	H_a, ppm	fitted line
0.002	0	0	11.9698	11.9698
0.002	0.0004	0.2	11.9693	11.96971673
0.002	0.0008	0.4	11.969	11.96963346
0.002	0.0012	0.6	11.9688	11.9695502
0.002	0.0016	0.8	11.9686	11.96946694
0.002	0.002	1	11.9684	11.96938368
0.002	0.0028	1.4	11.9682	11.96921716
0.002	0.004	2	11.9681	11.96896741
0.002	0.006	3	11.9678	11.96855121
0.002	0.008	4	11.9676	11.96813507
0.002	0.01	5	11.9674	11.96771899
0.002	0.012	6	11.9672	11.96730298
0.002	0.016	8	11.9668	11.96647113
0.002	0.02	10	11.9666	11.96563952

Table S3 Representative data obtained for NMR titration of **L3** with TBACH₃COO

L3, M	CH₃COO⁻, M	G/H equivalent total	H_a, ppm	fitted line
0.002	0	0	11.9677	11.9677
0.002	0.0004	0.2	11.9733	12.03600443
0.002	0.0008	0.4	12.0461	12.09836714
0.002	0.0012	0.6	12.135	12.1552447
0.002	0.0016	0.8	12.1918	12.20709695
0.002	0.002	1	12.2616	12.25437323
0.002	0.0028	1.4	12.3462	12.33688632
0.002	0.004	2	12.4516	12.43611798
0.002	0.006	3	12.5654	12.55514463
0.002	0.008	4	12.6528	12.63691287
0.002	0.01	5	12.7195	12.69572535
0.002	0.012	6	12.721	12.73972304
0.002	0.016	8	12.7989	12.80072193
0.002	0.02	10	12.8268	12.8407549

Table S4 Representative data obtained for NMR titration of **L3** with TBAH₂PO₄

L3, M	H₂PO₄⁻, M	G/H equivalent total	H_a, ppm	fitted line
0.002	0	0	11.9667	11.9667
0.002	0.0004	0.2	11.975	11.98748896
0.002	0.0008	0.4	11.9892	12.00712679
0.002	0.0012	0.6	12.0076	12.02568995
0.002	0.0016	0.8	12.0281	12.04324998
0.002	0.002	1	12.0479	12.0598737
0.002	0.0028	1.4	12.0954	12.09055687
0.002	0.004	2	12.1416	12.13097968
0.002	0.006	3	12.1969	12.18635274
0.002	0.008	4	12.2369	12.23034799
0.002	0.01	5	12.2759	12.2659603
0.002	0.012	6	12.2926	12.29527389
0.002	0.016	8	12.3272	12.34049459
0.002	0.02	10	12.3756	12.37360547

Table S5 Representative data obtained for NMR titration of **L4** with TBACH₃COO

L4, M	CH₃COO⁻, M	G/H equivalent total	H_a, ppm	fitted line
0.002	0	0	10.593	10.593
0.002	0.0004	0.2	10.6036	10.60793252
0.002	0.0008	0.4	10.6254	10.62168639
0.002	0.0012	0.6	10.6376	10.63435374
0.002	0.0016	0.8	10.6508	10.64602372
0.002	0.002	1	10.6651	10.65678119
0.002	0.0028	1.4	10.6732	10.67587176
0.002	0.004	2	10.7123	10.69947106
0.002	0.006	3	10.7223	10.72893101
0.002	0.008	4	10.7406	10.75005466
0.002	0.01	5	10.7583	10.76576401
0.002	0.012	6	10.7711	10.77782494
0.002	0.016	8	10.7988	10.79501404
0.002	0.02	10	10.8162	10.80660532

Table S6 Representative data obtained for NMR titration of **L4** with TBAH₂PO₄

L4, M	H₂PO₄⁻, M	G/H equivalent total	H_a, ppm	fitted line
0.002	0	0	10.5932	10.5932
0.002	0.0004	0.2	10.6137	10.62454232
0.002	0.0008	0.4	10.6543	10.65301303
0.002	0.0012	0.6	10.6795	10.6788236
0.002	0.0016	0.8	10.7126	10.70219567
0.002	0.002	1	10.7346	10.72335144
0.002	0.0028	1.4	10.7637	10.75986419
0.002	0.004	2	10.7899	10.80295935
0.002	0.006	3	10.8462	10.85327048
0.002	0.008	4	10.8965	10.88686223
0.002	0.01	5	10.9097	10.91050922
0.002	0.012	6	10.9175	10.927915
0.002	0.016	8	10.9444	10.95164657
0.002	0.02	10	10.9805	10.96697356

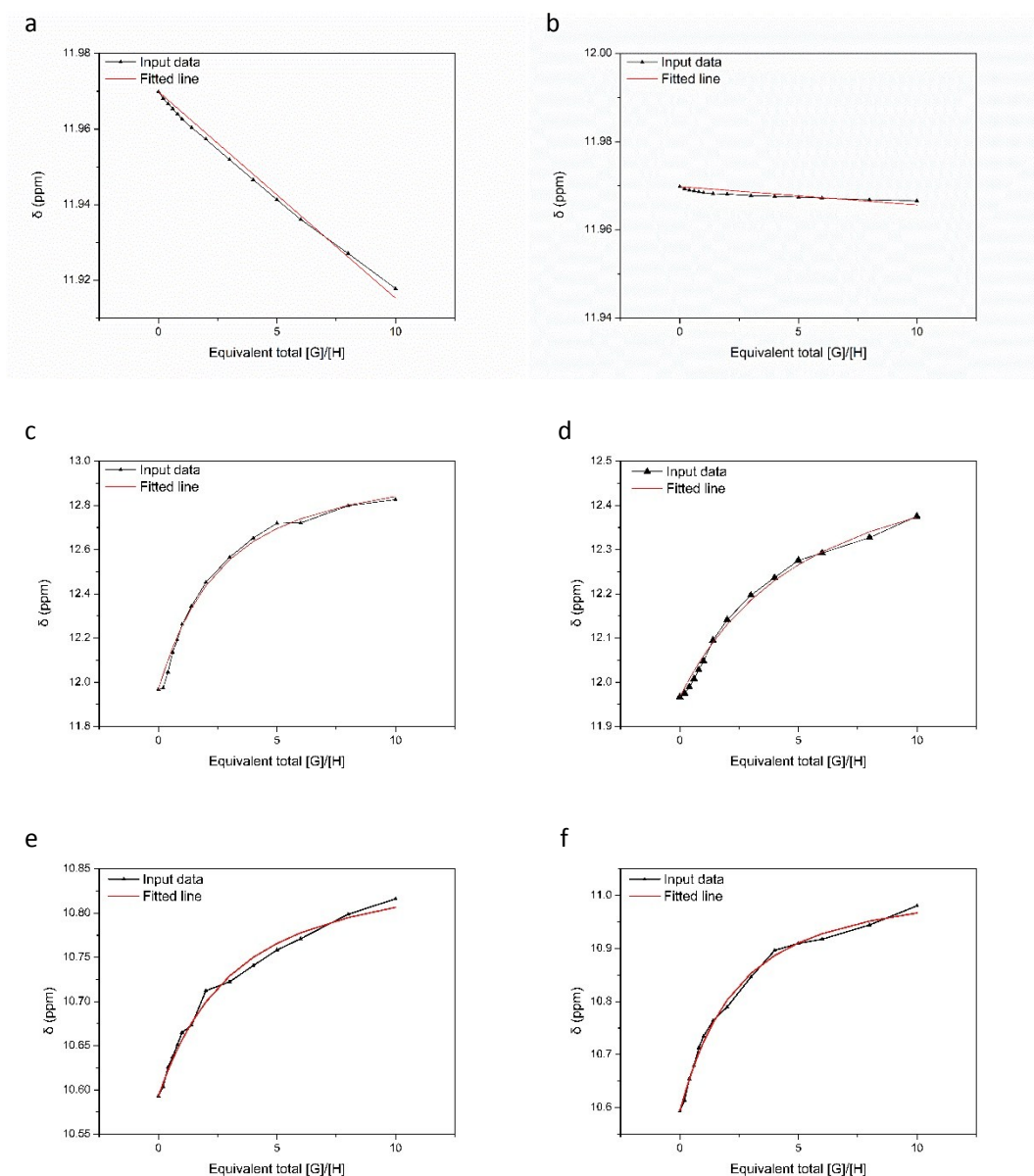


Fig. S16 The chemical shifts of H_a protons of the **L3-L4** were plotted against the guest concentration. The binding constants were determined using the Bindfit software: a. **L3** with TBACl, 1:1 H-G model; b. **L3** with TBABr, 1:1 H-G model; c. **L3** with TBACH₃COO, 1:1 H-G model; d. **L3** with TBAH₂PO₄, 1:1 H-G model; e. **L4** with TBACH₃COO, 1:1 H-G model; f. **L4** with TBAH₂PO₄, 1:1 H-G model.

We measured the binding constants for receptors to anions using the Thordarson method. This method was proposed by Hibbert and Thordarson in 2016 to calculate the binding constants for host-guest binding (*Chem. Commun.*, **2016**, 52, 12792-12805). They established the web-portal OpenDataFit which includes the site <http://supramolecular.org>. This website provides data deposition and storage, and offers the community a free (open) access web-tool to fit their data to a range of binding models.

Table S7. Association constants of anions with receptors **L3** and **L4**.^a

Anion	L3	L4
CH ₃ COO ⁻	253.89; ±9.81%	105.61; ±7.17%
H ₂ PO ₄ ⁻	200.89; ±9.93%	294.43; ±8.03%
Cl ⁻	0.06; ±0.02%	\
Br ⁻	0.04; ±0.01%	\

a: NMR titration, solvent: DMSO-*d*₆, 298 K, [L] = 2 × 10⁻³ M, anions added as TBA salts, where [TBAX] ~ 2 × 10⁻² M; Models: 1:1; M⁻¹, errors <10%.

Theoretical

studies

L1+Cl⁻: trans-trans

N	0.00010800	1.18169200	0.23939700
C	-1.13594300	1.86600400	0.20335200
C	-1.19418600	3.25640400	0.15705400
H	-2.16130400	3.74098600	0.14634700
C	0.00002300	3.96221200	0.13061500
H	-0.00002300	5.04502300	0.08666900
C	1.19428900	3.25649100	0.15698200
H	2.16139100	3.74110100	0.14618100
C	1.13610800	1.86609900	0.20331100
C	-2.43180100	1.09553700	0.23653600
O	-3.44228800	1.65194700	0.65195700
N	-2.34836300	-0.18054900	-0.20951900
C	-3.37982600	-1.14952300	-0.21374100
O	-3.15593700	-2.28475900	-0.56654800
N	-4.59852600	-0.71843400	0.20426800
H	-4.68602600	0.24119500	0.50996000
C	2.43199400	1.09568900	0.23637500
O	3.44283300	1.65243400	0.65043700
N	2.34815300	-0.18089200	-0.20830300
H	1.48868400	-0.46366000	-0.71832000
C	3.37956400	-1.14987800	-0.21267600
O	3.15528300	-2.28542700	-0.56428500
N	4.59865800	-0.71850400	0.20381700
H	4.68656600	0.24145800	0.50833600
C	5.69206800	-1.66459300	0.29113300
H	6.62203500	-1.09197200	0.30476300
C	-5.69181200	-1.66461400	0.29209500
H	-6.62187500	-1.09215200	0.30619300
H	-1.48926400	-0.46298500	-0.72054600
H	5.68619900	-2.27756700	-0.61278100
H	-5.68622800	-2.27750500	-0.61186300
C	5.59299500	-2.56751400	1.51912700
H	4.66470400	-3.13802000	1.46959200
H	6.43252800	-3.26651400	1.55762900
H	5.59112900	-1.97134700	2.43433900
C	-5.59196800	-2.56765600	1.51993600
H	-6.43132700	-3.26685000	1.55880600
H	-4.66358000	-3.13797100	1.46986700
H	-5.58973700	-1.97161900	2.43523200
Cl	-0.00072000	-0.46801800	-2.37477100

L1+Br⁻: trans-trans

N	-0.00000700	1.18703300	-0.50051200
C	1.13572500	1.87261200	-0.46908700
C	1.19393600	3.26250700	-0.42353800
H	2.16098400	3.74716300	-0.41230600
C	-0.00011500	3.96828100	-0.39505100
H	-0.00015700	5.05088200	-0.34818400
C	-1.19411100	3.26241600	-0.42356900
H	-2.16119500	3.74700000	-0.41236900
C	-1.13579300	1.87252400	-0.46911300
C	2.43069800	1.10257600	-0.50448500
O	3.44255600	1.65238000	-0.92251800
N	2.34456700	-0.17480200	-0.05929000
C	3.36794000	-1.15158900	-0.05370800
O	3.13353600	-2.28337900	0.30410000
N	4.58697100	-0.73104600	-0.47785100
H	4.68151200	0.22880400	-0.78090700
C	-2.43070700	1.10238500	-0.50455100
O	-3.44262600	1.65209600	-0.92255400
N	-2.34455900	-0.17491900	-0.05916600
H	-1.49047300	-0.44567800	0.45451800
C	-3.36798600	-1.15163100	-0.05350300
O	-3.13371900	-2.28339400	0.30447500
N	-4.58689900	-0.73100600	-0.47790800
H	-4.68125600	0.22879900	-0.78116300
C	-5.67444900	-1.68422800	-0.56544500
H	-6.60767600	-1.11725300	-0.58324600
C	5.67441200	-1.68439600	-0.56535200
H	6.60771400	-1.11753900	-0.58290600
H	1.49045700	-0.44562100	0.45432300
H	-5.66734500	-2.29439500	0.34029900
H	5.66707700	-2.29470800	0.34029400
C	-5.56565400	-2.58931500	-1.79086900
H	-4.63395500	-3.15388900	-1.73719000
H	-6.40050700	-3.29374600	-1.83034100
H	-5.56473700	-1.99537200	-2.70749500
C	5.56571300	-2.58927600	-1.79093900
H	6.40048000	-3.29381200	-1.83037300
H	4.63392900	-3.15373400	-1.73751700
H	5.56504000	-1.99518700	-2.70747000
Br	0.00011300	-0.21392400	2.39521000

L1+Cl⁻: cis-cis

O	-3.54775500	2.21760400	-0.05746100
O	-4.59873600	-0.37025500	0.21071400
O	4.46857400	-0.28258000	0.83883400
N	2.29977000	0.27450900	0.23606500
H	1.38706400	-0.11941700	-0.00180400
O	3.42037400	2.27995300	0.39453600
N	-0.05054300	1.66720300	0.03578700
N	-3.04511700	-1.96181500	-0.23631600
H	-2.07213000	-2.15014900	-0.47563700
N	-2.38152100	0.23246900	-0.11029300
H	-1.43974200	-0.14390200	-0.23785100
N	3.01176800	-1.90882200	0.21896300
H	2.10103200	-2.10989400	-0.19351600
C	2.40864800	1.63476200	0.25144000
C	-3.45484200	-0.68705800	-0.02938000
C	1.08538100	2.36088000	0.05938100
C	-2.51508400	1.59026000	-0.08359800
C	3.37132600	-0.62358300	0.45714600
C	-1.19126200	2.34034700	-0.09542100
C	-4.00585200	-3.04251500	-0.17331600
C	3.99109800	-2.96353100	0.37036600
C	1.13359500	3.74754100	-0.05991400
H	2.09912400	4.23369900	-0.02484100
C	-1.24785400	3.72624100	-0.22134300
H	-2.21782700	4.19490500	-0.31867500
C	-0.05878600	4.43943100	-0.20882100
H	-0.06167400	5.51884300	-0.30823400
H	-3.56357900	-3.89720500	-0.68858300
H	-4.90507200	-2.74444900	-0.71921800
H	3.44463900	-3.90453500	0.45973800
H	4.53318600	-2.79590900	1.30425300
C	-4.37960200	-3.41097400	1.26124700
H	-3.48995200	-3.70620900	1.82110300
H	-4.83126200	-2.54593600	1.74863800
H	-5.09579600	-4.23696400	1.27763100
C	4.98109900	-3.02166000	-0.79194300
H	4.45284900	-3.18616500	-1.73320800
H	5.52070600	-2.07534600	-0.85176500
H	5.70423900	-3.82929200	-0.64894500
Cl	0.05569600	-1.87797100	-0.99568100

L1+Br⁻: cis-cis

O	-3.56619900	2.38727300	0.00046700
O	-4.59211700	-0.18510500	0.48325000
O	4.43765800	-0.02767700	1.07247600
N	2.28727400	0.48077500	0.37430800
H	1.38661000	0.07218100	0.12020100
O	3.39503100	2.49837500	0.44099000
N	-0.06834100	1.85016600	0.08641600
N	-3.06707400	-1.79209100	-0.00519900
H	-2.12143700	-1.98713100	-0.33048400
N	-2.39667500	0.40404700	0.02560200
H	-1.46025200	0.02609300	-0.12635400
N	3.00328200	-1.69745800	0.51393400
H	2.13668600	-1.92194800	0.02624500
C	2.38911600	1.84133500	0.31527900
C	-3.46446200	-0.51096200	0.18739600
C	1.06555400	2.54737600	0.06368900
C	-2.53243400	1.76202100	-0.01357900
C	3.35446300	-0.39672700	0.67899700
C	-1.21069900	2.51118600	-0.08681500
C	-4.02794300	-2.86784500	0.12232700
C	3.99961800	-2.73105600	0.70296100
C	1.11036200	3.92282200	-0.14895700
H	2.07446300	4.41300600	-0.14599900
C	-1.27097000	3.88528300	-0.30481100
H	-2.24236800	4.34479600	-0.42835300
C	-0.08366700	4.60043200	-0.34342200
H	-0.08918800	5.67058000	-0.51539100
H	-3.60954600	-3.73486900	-0.39221100
H	-4.94968700	-2.57971100	-0.39069900
H	3.46852700	-3.67362500	0.85013400
H	4.55062500	-2.50505100	1.61839500
C	-4.33904600	-3.20189900	1.57972800
H	-3.42727500	-3.49119300	2.10593400
H	-4.76324300	-2.32312400	2.06717700
H	-5.05910300	-4.02190700	1.64642100
C	4.97210100	-2.83559800	-0.47096100
H	4.43038300	-3.05219200	-1.39395200
H	5.49984700	-1.88769000	-0.58692800
H	5.70684500	-3.62729800	-0.30094200
Br	0.08548300	-1.79943200	-1.15591700

L1: trans-trans

N	-0.00004900	1.15193200	-0.05370400
C	1.13938600	1.83644700	0.01662200
C	1.19426500	3.21956300	0.15828900
H	2.16213000	3.70007200	0.20987600
C	-0.00013700	3.92185600	0.22936800
H	-0.00017200	4.99921700	0.34014500
C	-1.19449500	3.21952800	0.15788100
H	-2.16238900	3.70001600	0.20911500
C	-1.13952800	1.83641200	0.01626900
C	2.44548800	1.07905300	-0.05760700
O	3.50217100	1.67737700	0.00873100
N	2.30883900	-0.26472900	-0.19700300
H	1.36797800	-0.63437700	-0.23062600
C	3.31617400	-1.26732800	-0.28870300
O	2.97496900	-2.42343300	-0.38890600
N	4.58538200	-0.82177400	-0.26322100
H	4.74731900	0.16757500	-0.13479300
C	-2.44557400	1.07895800	-0.05826100
O	-3.50230300	1.67726400	0.00752100
N	-2.30881100	-0.26486800	-0.19716300
H	-1.36791200	-0.63448000	-0.23011600
C	-3.31605500	-1.26757700	-0.28848100
O	-2.97474400	-2.42373700	-0.38780100
N	-4.58531300	-0.82210700	-0.26375300
H	-4.74737400	0.16729500	-0.13587100
C	-5.68278600	-1.77818800	-0.30591300
H	-5.45382900	-2.52042000	-1.07276500
H	-6.57339100	-1.23248500	-0.62064700
C	-5.90785700	-2.46808100	1.03569700
H	-5.01236500	-3.02371800	1.31708400
H	-6.12810700	-1.73509300	1.81426600
C	5.68297400	-1.77769800	-0.30602800
H	6.57355000	-1.23161100	-0.62017600
H	5.45421300	-2.51931900	-1.07353000
C	5.90792700	-2.46867200	1.03504400
H	6.12793500	-1.73629900	1.81426000
H	5.01246300	-3.02466500	1.31581600
H	-6.74336400	-3.16793100	0.97076400
H	6.74353300	-3.16836400	0.96968300

L1: TS1

N	0.02385900	1.17629100	-0.03292400
C	1.16947200	1.85515700	-0.06852700
C	1.23755000	3.24350600	-0.05324800
H	2.20860900	3.71958900	-0.08079300
C	0.04839200	3.95881800	-0.00488000
H	0.05797000	5.04174400	0.00756700
C	-1.15103800	3.26314900	0.02784700
H	-2.11539100	3.75222200	0.06797000
C	-1.10980900	1.87190300	0.01541400
C	2.46122400	1.07470200	-0.13318300
O	3.53261200	1.64895300	-0.12706900
N	2.29027600	-0.27235000	-0.20239200
H	1.33811500	-0.61214900	-0.19460700
C	3.26386500	-1.30399700	-0.28419900
O	2.88726400	-2.45403200	-0.33345500
N	4.54546100	-0.89598100	-0.30980900
H	4.73813700	0.09271700	-0.22375500
C	-2.42006000	1.11784700	0.06843800
O	-3.47609100	1.70308200	0.09429100
N	-2.29415200	-0.24062000	0.04734400
H	-1.36112200	-0.61491200	0.15468300
C	-3.41539700	-1.06497900	0.45218200
O	-3.85738400	-1.05022400	1.56868600
N	-3.85183500	-1.85354800	-0.55331700
H	-3.51584500	-1.65144300	-1.48090100
C	-5.02600200	-2.69600700	-0.36686400
H	-4.93148900	-3.16186200	0.61508800
H	-4.98925700	-3.48607700	-1.11856000
C	-6.32697900	-1.90466400	-0.45074000
H	-6.33033400	-1.12152700	0.30867300
H	-6.43660400	-1.43932000	-1.43240000
C	5.61337500	-1.88499500	-0.35025100
H	6.50917300	-1.37855500	-0.71222300
H	5.33802500	-2.64680900	-1.08190500
C	5.86041400	-2.53372200	1.00788100
H	6.13098200	-1.78176900	1.75162700
H	4.95666900	-3.04777100	1.33785000
H	-7.18377300	-2.55942600	-0.28070500
H	6.66961900	-3.26372900	0.94123300

L1: cis-trans

N	0.08855000	1.36078800	-0.02144400
C	1.18664600	2.11163700	0.02222600
C	1.15656000	3.50354600	0.01132900
H	2.09439300	4.04205000	0.04553200
C	-0.07600700	4.13665400	-0.04053600
H	-0.13987600	5.21785300	-0.04685200
C	-1.22809200	3.36206300	-0.08613700
H	-2.22151400	3.78819900	-0.13066100
C	-1.09051300	1.97964800	-0.07720300
C	2.54131600	1.42806600	0.08623800
O	3.55248100	2.07622800	0.08075300
N	2.44666900	0.05690200	0.13423800
H	1.50398000	-0.30604600	0.13700300
C	3.52249300	-0.83633800	0.34108300
O	4.62599600	-0.49102100	0.66552200
N	3.13743600	-2.14163500	0.17665400
H	2.32755600	-2.33060500	-0.39407600
C	-2.33907800	1.13186100	-0.14055300
O	-3.43932000	1.64662500	-0.17493800
N	-2.09520100	-0.20579400	-0.16010400
H	-1.12690100	-0.49180000	-0.11999700
C	-3.00582000	-1.29305300	-0.23223500
O	-2.56118400	-2.42016600	-0.23305600
N	-4.30683200	-0.96154100	-0.30576300
H	-4.55845800	0.01667100	-0.25902400
C	-5.31487400	-2.01214200	-0.34390300
H	-4.96999700	-2.78156100	-1.03676100
H	-6.22471000	-1.57254700	-0.75465100
C	-5.57182900	-2.62463900	1.02890600
H	-4.65072800	-3.06707800	1.41061200
H	-5.91737600	-1.86501700	1.73266600
C	4.14979700	-3.18697400	0.27137600
H	3.63247000	-4.12812600	0.46511100
H	4.76059500	-2.95509400	1.14407400
C	5.02814000	-3.28302800	-0.97173600
H	4.42982300	-3.51476100	-1.85606000
H	5.54362600	-2.33514900	-1.13186600
H	-6.33060600	-3.40687400	0.96191100
H	5.77713800	-4.06830200	-0.85140300

L1: TS2

N	0.10732800	1.34852600	-0.03303500
C	1.21588400	2.08483000	-0.10792800
C	1.20462600	3.47199700	-0.21556000
H	2.15006200	3.99480700	-0.27427700
C	-0.02052500	4.12213900	-0.23807900
H	-0.07015000	5.20140100	-0.31638900
C	-1.18123100	3.36595300	-0.15687900
H	-2.17127700	3.80225800	-0.16498000
C	-1.06427200	1.98410300	-0.05814100
C	2.56328400	1.38890300	-0.07036900
O	3.58340500	2.01521400	-0.16664700
N	2.45912500	0.02204900	0.06293100
H	1.51419600	-0.32879500	0.13145600
C	3.53223200	-0.85948600	0.31833000
O	4.62810200	-0.50502900	0.65629500
N	3.14936100	-2.17312500	0.18770500
H	2.38852700	-2.36829100	-0.44548100
C	-2.33417700	1.16856100	0.02954900
O	-3.41894800	1.69650000	0.06338100
N	-2.13995400	-0.18421200	0.01545600
H	-1.18482400	-0.50388500	0.09524700
C	-3.20409300	-1.06885100	0.43734700
O	-3.67025600	-1.04170900	1.54312400
N	-3.55837500	-1.93438400	-0.54099300
H	-3.25823600	-1.71285900	-1.47687600
C	-4.68706700	-2.83518500	-0.34061200
H	-4.58198900	-3.25990300	0.65860700
H	-4.59371400	-3.64774100	-1.06294000
C	-6.02976700	-2.12404300	-0.47190000
H	-6.09519400	-1.32080100	0.26331900
H	-6.14626100	-1.69469100	-1.46916400
C	4.16581900	-3.20899000	0.33687900
H	3.64959000	-4.14933200	0.53839200
H	4.74812900	-2.95195300	1.22179800
C	5.08246900	-3.32906500	-0.87615400
H	4.51197100	-3.58052100	-1.77366800
H	5.60094800	-2.38364400	-1.04063000
H	-6.85036900	-2.82289800	-0.29932300
H	5.82868700	-4.11013800	-0.71765500

L1: cis-cis

N	-0.03006900	1.48779500	-0.03132000
C	1.10673800	2.18197400	0.02185200
C	1.15780000	3.56863200	-0.06756600
H	2.12069500	4.05783200	-0.00154200
C	-0.03203000	4.26226900	-0.23818800
H	-0.03315800	5.34250700	-0.31746800
C	-1.22051800	3.54910700	-0.30402100
H	-2.18456900	4.02182900	-0.43781100
C	-1.16782200	2.16420600	-0.18488500
C	2.41209800	1.42971500	0.18721700
O	3.44604500	2.01340200	0.36743000
N	2.26351200	0.06573800	0.06465400
H	1.32353900	-0.25078700	-0.12620500
C	3.25888400	-0.89522000	0.34748900
O	4.23165700	-0.67760200	1.01518500
N	2.93821500	-2.12292300	-0.18624500
H	2.39584600	-2.10876900	-1.03787000
C	-2.47600700	1.39728000	-0.22457300
O	-3.50481400	1.94961500	-0.50315800
N	-2.32497800	0.06257000	0.08476800
H	-1.38315400	-0.21448800	0.32432400
C	-3.37972800	-0.84945600	0.30855700
O	-4.53488600	-0.53423000	0.39258800
N	-2.91551400	-2.13236700	0.47076600
H	-2.03204000	-2.36530100	0.04373600
C	-3.88772400	-3.21036500	0.61260400
H	-4.64385800	-2.85982200	1.31501300
H	-3.37469800	-4.05800400	1.07043800
C	-4.54165800	-3.60519600	-0.70733700
H	-5.06305200	-2.74648600	-1.13244000
H	-3.79510900	-3.95580600	-1.42428000
C	3.91144800	-3.20346800	-0.05509300
H	3.38420500	-4.14300500	-0.23060800
H	4.24802700	-3.19929100	0.98166700
C	5.10363400	-3.05517600	-0.99429500
H	4.78063100	-3.05110000	-2.03838100
H	5.62655600	-2.12161100	-0.78304600
H	-5.26633600	-4.40681100	-0.55190500
H	5.80359700	-3.88188400	-0.85890400

L1+F⁻: trans-trans

N	-0.03001600	1.17986500	-0.05205200
C	1.13157800	1.81929500	0.01005100
C	1.20294800	3.20912300	0.14192700
H	2.18293400	3.66427200	0.18816400
C	0.02562200	3.93876500	0.21018500
H	0.05194000	5.01800000	0.31330800
C	-1.18951400	3.26814000	0.14693800
H	-2.14614400	3.77054200	0.19672100
C	-1.15176400	1.88387500	0.01489000
C	2.43327700	1.02556000	-0.05899600
O	3.47059700	1.71125100	0.01592000
N	2.27238700	-0.28664800	-0.18671600
H	0.91811700	-1.07408000	-0.25674700
C	3.36014500	-1.16458800	-0.25771300
O	3.18701600	-2.37258300	-0.32558800
N	4.62630300	-0.63850300	-0.26202100
H	4.71097300	0.36199600	-0.13315000
C	-2.45235600	1.12391300	-0.05423100
O	-3.51164900	1.73749400	0.00789800
N	-2.32467700	-0.22312800	-0.18250700
H	-1.37485000	-0.64094800	-0.21603400
C	-3.37381300	-1.16863800	-0.26051600
O	-3.13097400	-2.35185200	-0.34515300
N	-4.63477500	-0.66360700	-0.24271500
H	-4.74606300	0.33405300	-0.12102200
C	-5.76257000	-1.57223600	-0.26580700
H	-5.57637800	-2.33136100	-1.02884600
H	-6.64073000	-0.99767800	-0.56888900
C	-5.99965900	-2.25295000	1.08105500
H	-5.11603100	-2.83330200	1.34940800
H	-6.18144800	-1.50860100	1.85950900
C	5.76949300	-1.51988300	-0.27069700
H	6.64127900	-0.93536400	-0.57821800
H	5.60195200	-2.29706700	-1.02070200
C	6.02125900	-2.18177700	1.08513200
H	6.18684800	-1.42377800	1.85464300
H	5.14405600	-2.77096100	1.35527500
H	-6.85981800	-2.92580000	1.03206300
H	6.89368800	-2.84123900	1.04844800
F	0.08192400	-1.59895700	-0.30553100

L1+F⁻: TS1

N	-0.06067700	1.16278400	0.06727600
C	1.08429100	1.81955000	-0.05996400
C	1.13092100	3.21483300	-0.12373200
H	2.09822700	3.68850400	-0.22301600
C	-0.05813200	3.92772400	-0.06209500
H	-0.05153500	5.01114400	-0.11041200
C	-1.25828400	3.23646800	0.05940300
H	-2.22367200	3.72328600	0.10645900
C	-1.19452100	1.84989800	0.12351500
C	2.38613900	1.03061100	-0.15085700
O	3.41806100	1.72049600	-0.24049200
N	2.23532600	-0.29221100	-0.12714700
H	0.93356100	-1.08877700	0.02181000
C	3.32331600	-1.16642700	-0.22588200
O	3.16554100	-2.37524600	-0.13113400
N	4.56811000	-0.63908500	-0.45600000
H	4.65287800	0.36928600	-0.42071300
C	-2.46405900	1.04342300	0.24637200
O	-3.56326500	1.57047300	0.20484000
N	-2.25544900	-0.28606300	0.38538200
H	-1.30072000	-0.68640100	0.36699100
C	-3.39274900	-1.14127800	0.53881800
O	-3.88552100	-1.41891500	1.60309800
N	-3.85121400	-1.60883600	-0.65045200
H	-3.43174000	-1.23311500	-1.48472800
C	-5.11059900	-2.32419600	-0.71970400
H	-5.12679000	-3.03056900	0.11182600
H	-5.12493400	-2.89761000	-1.64892700
C	-6.30948300	-1.38250700	-0.62811900
H	-6.25690100	-0.82253200	0.30665800
H	-6.30121800	-0.66837300	-1.45416000
C	5.71789100	-1.51144000	-0.49229500
H	6.52989100	-0.97818000	-0.99483100
H	5.46381400	-2.38648200	-1.09506400
C	6.15942300	-1.97386100	0.89717700
H	6.41785500	-1.11500100	1.52138200
H	5.33481900	-2.51282300	1.36550100
H	-7.24830200	-1.94136600	-0.65517100
H	7.02727700	-2.63759500	0.83748200
F	0.11015200	-1.65119700	0.11213100

L1+F⁻: cis-trans

N	0.22570600	1.45491900	0.00162000
C	-0.97545100	2.00503300	0.10226700
C	-1.14746200	3.39020600	0.14914100
H	-2.15264300	3.78050300	0.23145600
C	-0.02401200	4.20374300	0.08983500
H	-0.12784100	5.28272300	0.12460300
C	1.23454900	3.62209700	-0.01309200
H	2.15204400	4.19406200	-0.06092400
C	1.29897700	2.23496200	-0.05420200
C	-2.20044900	1.10168500	0.17166300
O	-3.28955200	1.69077700	0.26351600
N	-1.94609700	-0.20943700	0.12344000
H	-0.68882900	-0.85908200	0.01236300
C	-2.96354300	-1.17379300	0.17884800
O	-2.70090900	-2.36110100	0.06171700
N	-4.24936700	-0.75387200	0.38557800
H	-4.41502900	0.24455300	0.38471900
C	2.64503700	1.53732300	-0.16509800
O	3.67261800	2.17241500	-0.20814800
N	2.49002100	0.18050700	-0.20206700
H	1.52123100	-0.15643600	-0.14905500
C	3.49016500	-0.80011200	-0.28006600
O	4.68017300	-0.58156000	-0.34542700
N	2.94292000	-2.04834000	-0.27928000
H	1.93622100	-2.14423700	-0.17972800
C	3.80447300	-3.20977800	-0.30644600
H	4.58342600	-3.04252500	-1.05467000
H	3.20130700	-4.05972700	-0.63156100
C	4.45412000	-3.49456100	1.04713400
H	5.06335500	-2.63787100	1.33904200
H	3.68951300	-3.65863500	1.80933300
C	-5.32560400	-1.71733900	0.37877400
H	-6.19110000	-1.25503600	0.86112600
H	-5.02171600	-2.57649000	0.98141200
C	-5.68710100	-2.19568800	-1.02793200
H	-5.99141200	-1.35202600	-1.65196800
H	-4.81016500	-2.66526800	-1.47516700
H	5.09410000	-4.37974200	0.99594200
H	-6.50308500	-2.92378400	-0.99990100
F	0.21083400	-1.39381400	-0.06003300

L1+F⁻: TS2

N	0.26873700	1.55962000	0.01703000
C	-0.87236200	2.22202700	0.14260300
C	-0.91573000	3.61660600	0.15386000
H	-1.88067100	4.09552300	0.25598500
C	0.27595800	4.31966300	0.03442400
H	0.27522600	5.40409400	0.04289800
C	1.47168400	3.62064400	-0.09689900
H	2.43488400	4.10433800	-0.19555800
C	1.40650700	2.23284100	-0.10055400
C	-2.16369700	1.42636800	0.26452200
O	-3.22125500	2.05691300	0.30463100
N	-1.99707300	0.10351500	0.30764500
H	-0.86723200	-0.63612100	0.17563500
C	-3.17890000	-0.65709700	0.45127200
O	-3.65043700	-1.02616700	1.50608700
N	-3.73240500	-1.01544700	-0.74680100
H	-3.27774800	-0.69352500	-1.58303100
C	2.67109500	1.40281900	-0.24032800
O	3.75523900	1.92690600	-0.34281300
N	2.38196600	0.06511700	-0.22991800
H	1.38807200	-0.17278200	-0.13589300
C	3.27911700	-1.01025800	-0.29560400
O	4.48209200	-0.91277200	-0.40356500
N	2.61390100	-2.19894000	-0.22883000
H	1.60824200	-2.18891700	-0.08026300
C	3.36233800	-3.43634900	-0.22127900
H	4.14609100	-3.36382600	-0.97928400
H	2.68174400	-4.23809400	-0.51535700
C	3.99676400	-3.73585300	1.13632300
H	4.67867000	-2.92554000	1.39820200
H	3.22861200	-3.81259900	1.90870200
C	-4.92869700	-1.82602700	-0.80570200
H	-5.38725100	-1.68362900	-1.78753600
H	-5.62506700	-1.45036400	-0.05187900
C	-4.64732700	-3.30514800	-0.54680100
H	-3.95090500	-3.70022100	-1.28977000
H	-4.19835300	-3.41103700	0.44151600
H	4.55979800	-4.67276200	1.10751100
H	-5.56936900	-3.89227800	-0.58067900
F	-0.05069300	-1.32664000	0.02946300

L1+F⁻: cis-cis

N	0.00008300	1.69694700	-0.00968700
C	-1.14453300	2.36313900	0.05806000
C	-1.19963700	3.74680000	0.19816100
H	-2.16799100	4.22713600	0.24874300
C	0.00022700	4.44445700	0.26839900
H	0.00028400	5.52309700	0.37867100
C	1.20001700	3.74668800	0.19801500
H	2.16842100	4.22693500	0.24845700
C	1.14476900	2.36302600	0.05794100
C	-2.43513300	1.56016800	-0.02065900
O	-3.50039500	2.13325100	0.02928700
N	-2.20231500	0.22512400	-0.14279000
H	-1.22188600	-0.10582300	-0.15875400
C	-3.17530000	-0.79376200	-0.23393500
O	-4.37467000	-0.61041200	-0.22499100
N	-2.57810000	-2.00732000	-0.33985900
H	-1.54696500	-2.03724100	-0.30274200
C	2.43528700	1.55993900	-0.02091500
O	3.50060000	2.13295900	0.02856700
N	2.20234000	0.22487000	-0.14261700
H	1.22189500	-0.10600800	-0.15836800
C	3.17524300	-0.79408900	-0.23387000
O	4.37462900	-0.61087900	-0.22464100
N	2.57792900	-2.00756000	-0.34020300
H	1.54679300	-2.03737400	-0.30308000
C	3.39422800	-3.19661800	-0.41050900
H	4.21899600	-3.01372200	-1.10516000
H	2.77745100	-3.99767800	-0.82405200
C	3.96327100	-3.60312300	0.94893000
H	4.59203900	-2.79587200	1.32735100
H	3.15501100	-3.78131300	1.66134200
C	-3.39451400	-3.19626000	-0.41066500
H	-2.77780200	-3.99726200	-0.82442100
H	-4.21919100	-3.01301600	-1.10533200
C	-3.96376300	-3.60313300	0.94857500
H	-3.15561300	-3.78161200	1.66104200
H	-4.59249800	-2.79593600	1.32717100
H	4.56768500	-4.51115300	0.86806800
H	-4.56825400	-4.51108000	0.86735900
F	-0.00002600	-1.37325100	-0.21457100

L4: trans-trans

O	3.50528300	1.59005700	0.55680900
O	3.49979000	-2.14130500	-1.23349500
N	2.58384500	-0.19391300	-0.52699900
H	1.78039800	-0.52590600	-1.04022000
N	4.82364800	-0.71732500	-0.05290800
H	4.85193200	0.18352400	0.40479600
C	2.54239200	1.04748000	0.05222800
C	-0.00007600	1.03129400	0.00010500
H	0.00003200	-0.05365200	0.00024200
C	1.20562300	1.72899700	0.01930300
C	3.67663600	-1.10310200	-0.63594000
C	5.98107600	-1.60132300	-0.09060700
H	6.85899000	-0.98997200	0.12166200
H	6.07775400	-1.99142000	-1.10564500
C	5.86400300	-2.75426100	0.90087900
H	4.99194500	-3.36141600	0.65485800
H	5.75656600	-2.37631100	1.91926400
C	1.20127600	3.12222900	0.04710800
H	2.15128000	3.63987600	0.09934600
C	-0.00019600	3.81627700	-0.00031000
H	-0.00026100	4.89897100	-0.00049400
O	-3.50550200	1.58969900	-0.55665800
O	-3.49943100	-2.14192900	1.23315500
N	-2.58397500	-0.19397000	0.52758300
H	-1.78037300	-0.52598900	1.04053700
N	-4.82390300	-0.71734200	0.05401600
H	-4.85215200	0.18328500	-0.40411900
C	-2.54256700	1.04726400	-0.05201000
C	-1.20583400	1.72886600	-0.01929800
C	-3.67658100	-1.10337900	0.63629100
C	-5.98086300	-1.60195600	0.09076000
H	-6.85914700	-0.99079400	-0.12055200
H	-6.07715200	-1.99332300	1.10533600
C	-5.86335600	-2.75365200	-0.90210700
H	-4.99089100	-3.36059200	-0.65696200
H	-5.75637600	-2.37450500	-1.92009600
C	-1.20159500	3.12210200	-0.04750900
H	-2.15165200	3.63964300	-0.09989500
H	6.75173300	-3.38838600	0.85715700
H	-6.75068500	-3.38837700	-0.85890200

L4: TS1

O	3.47245500	1.40923000	0.72207400
O	3.77636800	-1.74424800	1.18309000
N	2.53288700	-0.40435400	-0.24492100
H	1.76912100	-0.78215900	-0.78227300
N	4.47744700	-1.47130200	-0.95925500
H	4.40041900	-0.83091800	-1.73374400
C	2.50128700	0.88107200	0.23366900
C	-0.03255400	0.95137300	0.05614400
H	-0.06479600	-0.12965400	0.14259200
C	1.19532100	1.60699900	0.08041200
C	3.64956700	-1.26311200	0.09117200
C	5.73217800	-2.18645500	-0.75254200
H	6.07972300	-2.53612900	-1.72586200
H	5.50094700	-3.06139400	-0.14402300
C	6.78058200	-1.32247500	-0.05989200
H	6.39597400	-0.97636900	0.90051800
H	7.03032900	-0.45051900	-0.66812400
C	1.24014400	2.99741500	0.00400600
H	2.20605700	3.48403100	0.06650500
C	0.06807300	3.72561200	-0.15038700
H	0.10681300	4.80506900	-0.22774800
O	-3.49680500	1.59472200	-0.68058300
O	-3.66100400	-2.07878600	1.21745800
N	-2.67085300	-0.16946800	0.50667900
H	-1.89652600	-0.50587500	1.06013100
N	-4.90903800	-0.64069600	-0.02593600
H	-4.89783100	0.25027700	-0.50334100
C	-2.56826500	1.04563800	-0.12040500
C	-1.21131300	1.68360100	-0.07319000
C	-3.79000700	-1.04620300	0.59773900
C	-6.08964900	-1.49345100	-0.00691500
H	-6.94702000	-0.86216200	-0.24339500
H	-6.21796900	-1.87188300	1.00895700
C	-5.98067700	-2.65844100	-0.98528500
H	-5.12721700	-3.28239800	-0.71677800
H	-5.84554100	-2.29315400	-2.00506200
C	-1.15499900	3.07011300	-0.20254100
H	-2.08287300	3.61287200	-0.33463200
H	7.69405600	-1.89403400	0.11463100
H	-6.88300500	-3.27232700	-0.95253100

L4: cis-trans

O	3.46025900	1.94092900	0.72829800
O	4.41196900	-0.72375100	1.24691200
N	2.66582600	-0.04012800	-0.09640800
H	1.94187300	-0.42837200	-0.68051900
N	3.84914300	-1.96392700	-0.57994800
H	3.54852400	-1.82601600	-1.53330700
C	2.55460100	1.29348800	0.27985700
C	0.02200500	1.14345600	0.04517500
H	0.07046200	0.07274200	0.21335300
C	1.19481700	1.89478500	0.04185000
C	3.73608300	-0.89226900	0.27005600
C	4.93999900	-2.90947300	-0.36316800
H	4.68744200	-3.82738600	-0.89680500
H	4.95307600	-3.13649000	0.70300500
C	6.29699500	-2.36924300	-0.80133300
H	6.53848800	-1.47075200	-0.23216600
H	6.29361400	-2.12315200	-1.86600800
C	1.13149400	3.27477900	-0.14240400
H	2.05459100	3.84056300	-0.10527100
C	-0.09020100	3.89339400	-0.37028100
H	-0.13387800	4.96346500	-0.53015900
O	-3.46808900	1.46155800	-0.78959500
O	-3.38399500	-2.08557500	1.33853200
N	-2.53191800	-0.15280500	0.52146500
H	-1.74402200	-0.39409700	1.10438700
N	-4.72633200	-0.81496400	0.01218200
H	-4.77316600	0.04296500	-0.52083300
C	-2.51050900	1.02359100	-0.18269100
C	-1.20756900	1.76736800	-0.15998300
C	-3.58471400	-1.10277200	0.65950500
C	-5.84468500	-1.74539000	0.07914700
H	-6.74592100	-1.18411100	-0.17072500
H	-5.93597300	-2.08941400	1.11096400
C	-5.66614900	-2.93849500	-0.85358800
H	-4.77210200	-3.49587800	-0.57055500
H	-5.56290200	-2.60636900	-1.88832600
C	-1.25705500	3.14045200	-0.39182100
H	-2.22113800	3.59735200	-0.57857100
H	7.07831600	-3.11154000	-0.62658500
H	-6.52611300	-3.60806300	-0.78802300

L4: TS2

O	3.34200000	1.71513400	1.19836300
O	4.14491600	-1.05570200	1.35521100
N	2.62157300	-0.05682400	-0.05826500
H	1.98892900	-0.29282000	-0.80691300
N	3.86374600	-1.87791400	-0.75222100
H	3.72132600	-1.52804300	-1.68832700
C	2.48985300	1.19875200	0.52923400
C	0.00844300	1.19321400	-0.02542600
H	0.00539600	0.10839000	0.00086500
C	1.19129000	1.88868900	0.21671200
C	3.62321700	-0.99809200	0.27592100
C	4.92439500	-2.86635200	-0.57943400
H	4.76557100	-3.65051400	-1.32191200
H	4.78603100	-3.30799100	0.40762700
C	6.32291600	-2.26934000	-0.69505000
H	6.46253200	-1.50651800	0.07189200
H	6.47287700	-1.81469200	-1.67740700
C	1.18825400	3.28192700	0.21388000
H	2.11220200	3.79961000	0.44168400
C	0.02199200	3.97465700	-0.08349000
H	0.02615900	5.05730800	-0.10477100
O	-3.33556500	1.71364000	-1.24188300
O	-4.87595800	-0.10041400	0.54081200
N	-2.60789400	-0.06252500	-0.01877800
H	-1.98491700	-0.29573100	0.74240100
N	-3.91814800	-1.94159500	-0.36893900
H	-3.09820500	-2.27147900	-0.84860400
C	-2.47951800	1.20418500	-0.56651900
C	-1.16859500	1.88842700	-0.29502600
C	-3.92336200	-0.66589400	0.07920500
C	-5.13010300	-2.74994500	-0.31568100
H	-5.01933800	-3.55375100	-1.04451100
H	-5.96574600	-2.12139400	-0.63006100
C	-5.38957600	-3.30499200	1.08027600
H	-5.50947900	-2.48301200	1.78723200
H	-4.55919800	-3.93378300	1.40705300
C	-1.15086600	3.28037100	-0.35178800
H	-2.07118700	3.79634500	-0.59707500
H	7.08184900	-3.04216200	-0.55842900
H	-6.30292000	-3.90267400	1.08975900

L4: cis-cis

O	3.33597400	1.70593800	1.22054200
O	4.15487600	-1.05678600	1.33910800
N	2.61678900	-0.05310000	-0.05523400
H	1.97900100	-0.28506900	-0.80099000
N	3.86050300	-1.86483000	-0.77079000
H	3.69241300	-1.52122000	-1.70466200
C	2.48379800	1.19344800	0.54804800
C	-0.00010700	1.18787200	0.00001000
H	-0.00009500	0.10265100	-0.00000900
C	1.18033800	1.88340100	0.25308700
C	3.62462800	-0.99438800	0.26391100
C	4.92089700	-2.85565700	-0.61442600
H	4.75414500	-3.63470200	-1.36042900
H	4.79119600	-3.30357100	0.37100400
C	6.31883400	-2.25900400	-0.73911600
H	6.46485600	-1.49947300	0.02993000
H	6.46105200	-1.80033800	-1.72067500
C	1.17027800	3.27634800	0.27932300
H	2.09267900	3.79347900	0.51456200
C	-0.00001300	3.97031000	0.00012000
H	0.00000900	5.05316700	0.00015400
O	-3.33624400	1.70636700	-1.22028700
O	-4.15537300	-1.05663000	-1.33917200
N	-2.61691900	-0.05306700	0.05488200
H	-1.97883900	-0.28541900	0.80026900
N	-3.85995900	-1.86520200	0.77049700
H	-3.69271100	-1.52098000	1.70432500
C	-2.48399700	1.19364700	-0.54806700
C	-1.18049800	1.88348600	-0.25301500
C	-3.62475600	-0.99436100	-0.26417700
C	-4.92045400	-2.85599100	0.61420900
H	-4.75334700	-3.63528600	1.35987100
H	-4.79109600	-3.30357100	-0.37141800
C	-6.31839100	-2.25951200	0.73964400
H	-6.46483100	-1.49976000	-0.02910200
H	-6.46031300	-1.80117900	1.72140100
C	-1.17033600	3.27644400	-0.27913400
H	-2.09271100	3.79363800	-0.51434700
H	7.07828800	-3.03288300	-0.61160400
H	-7.07779000	-3.03345400	0.61218800

L4+F⁻: trans-trans

O	-3.57429100	1.75530600	-0.17608800
O	-3.33573000	-2.27207700	0.65140300
N	-2.46828100	-0.19400900	0.30954900
H	-1.57095800	-0.61828300	0.56910300
N	-4.76710300	-0.61702300	0.06545400
H	-4.84138000	0.36933100	-0.14544900
C	-2.52983300	1.14940500	0.01807700
C	-0.03795700	1.15344200	-0.26478500
H	-0.06456000	0.10904300	-0.53044200
C	-1.21251200	1.84944900	-0.01137500
C	-3.54128800	-1.11331300	0.35996400
C	-5.91175000	-1.50633500	0.06010700
H	-6.80776500	-0.88512800	0.12083800
H	-5.87124800	-2.12984000	0.95654400
C	-5.95473300	-2.39851800	-1.17868900
H	-5.06072400	-3.02273200	-1.20240400
H	-5.98415300	-1.79151200	-2.08602900
C	-1.16895900	3.21805200	0.25635200
H	-2.09864700	3.74588000	0.43235400
C	0.05913100	3.86497600	0.30164400
H	0.10061600	4.92808400	0.51025500
O	3.51100100	1.64561700	-0.54758200
O	3.25247000	-2.38979900	0.17565900
N	2.33908000	-0.31375600	-0.04464400
H	1.11701000	-0.97520200	0.57043600
N	4.59552200	-0.76701400	-0.63903700
H	4.69532500	0.23628800	-0.73668900
C	2.48606700	0.99883800	-0.28092500
C	1.19579900	1.78178900	-0.15570000
C	3.39835700	-1.21854800	-0.14465600
C	5.73500500	-1.65408300	-0.66278900
H	6.47096100	-1.23920100	-1.35733400
H	5.40508900	-2.61804300	-1.05599800
C	6.35822400	-1.86362400	0.71827800
H	5.60457900	-2.28944000	1.38202700
H	6.69602000	-0.91124600	1.13443200
C	1.23787100	3.14771400	0.10794000
H	2.20959100	3.62450600	0.16308900
H	-6.83480400	-3.04651500	-1.16102300
H	7.21198300	-2.54606100	0.66881900
F	0.24671200	-1.34057200	0.92893500

L4+F⁻: TS1

O	-3.58844800	2.03732100	-0.28822200
O	-4.42399100	-0.60000200	1.32111400
N	-2.50861600	0.08957700	0.17534400
H	-1.64954100	-0.35400800	0.51467200
N	-4.02329400	-1.38714900	-0.76054300
H	-3.34501500	-1.40400600	-1.50345300
C	-2.55204100	1.43813400	-0.08776800
C	-0.06354500	1.34095800	-0.32460500
H	-0.14428900	0.30461900	-0.60712100
C	-1.20659200	2.09552200	-0.09760700
C	-3.73534100	-0.63798300	0.33278800
C	-5.17336300	-2.27065600	-0.77631200
H	-5.42327500	-2.47670100	-1.81907400
H	-6.00781700	-1.72581400	-0.33043800
C	-4.92720700	-3.56467600	-0.00426500
H	-4.69162300	-3.32720500	1.03409400
H	-4.08908200	-4.11727800	-0.43347500
C	-1.09445600	3.45466700	0.18602800
H	-1.99866800	4.03104600	0.34393800
C	0.16880700	4.02944400	0.27823300
H	0.26418500	5.08656100	0.49997600
O	3.52127800	1.59951200	-0.41590900
O	2.93560300	-2.44101000	0.04574600
N	2.19264400	-0.28986300	-0.06825100
H	0.93741200	-0.89963800	0.43579700
N	4.46001900	-0.86511600	-0.49038600
H	4.63014700	0.13215700	-0.53568300
C	2.43817500	1.02245400	-0.23783600
C	1.20022800	1.88943400	-0.16002400
C	3.19242400	-1.26114600	-0.15514400
C	5.53108000	-1.83327900	-0.51427300
H	6.36059900	-1.40062900	-1.08065100
H	5.18214100	-2.71934600	-1.05020600
C	5.99478000	-2.24541600	0.88373000
H	5.15324200	-2.69233700	1.41440000
H	6.34089900	-1.37336800	1.44371700
C	1.31204700	3.24850400	0.12298000
H	2.30573200	3.66887800	0.22549000
H	-5.81435500	-4.20244700	-0.02399600
H	6.80860700	-2.97483700	0.83123600
F	0.02999100	-1.26556900	0.74113800

L4+F⁻: cis-trans

O	3.72068300	2.21128800	0.28500000
O	4.74101000	-0.58310700	0.44058700
N	2.60691400	0.21305300	-0.06342000
H	1.67786500	-0.19245800	-0.29759900
N	2.99279500	-2.00968600	0.10624500
H	1.97574600	-2.05272100	-0.02014800
C	2.70880500	1.56963400	0.12003400
C	0.20188900	1.48948600	0.31171400
H	0.28509700	0.46752300	0.65227200
C	1.34935400	2.22945800	0.04813800
C	3.57154100	-0.77761600	0.18499000
C	3.78753800	-3.18892900	0.36163700
H	3.10148100	-4.00338500	0.60248300
H	4.41898000	-3.00799700	1.23694600
C	4.67365400	-3.56553500	-0.82511800
H	5.35396600	-2.73968600	-1.03840200
H	4.06282800	-3.75577500	-1.71003000
C	1.23159000	3.55826200	-0.34495400
H	2.13690600	4.12741600	-0.52428300
C	-0.03211700	4.11896200	-0.52037900
H	-0.12450800	5.15368800	-0.83013700
O	-3.38152500	1.68956000	0.25850200
O	-2.76127600	-2.36503000	0.07868700
N	-2.06691400	-0.19235900	0.08591200
H	-1.10750400	-0.60402800	-0.11292000
N	-4.32523300	-0.77381700	0.44949900
H	-4.50168700	0.22210700	0.43358500
C	-2.28000300	1.15881400	0.15528300
C	-1.05416600	2.01635500	0.05720700
C	-3.05705500	-1.19405100	0.19521400
C	-5.39505300	-1.74720100	0.50930900
H	-6.23575400	-1.28089400	1.02825200
H	-5.05427100	-2.59251700	1.11087600
C	-5.82116800	-2.24590300	-0.87073100
H	-4.96868800	-2.72150100	-1.35715600
H	-6.16079600	-1.41359000	-1.49132100
C	-1.17535400	3.34696300	-0.34231900
H	-2.16544900	3.75121100	-0.51691300
H	5.26414200	-4.45953000	-0.60480900
H	-6.63132900	-2.97555600	-0.78943600
F	0.37913100	-1.20183600	-0.28458500

L4+F⁻: TS2

O	3.81892400	2.02083500	0.12021800
O	4.60535500	-0.84554100	0.30494900
N	2.51599900	0.11945300	-0.07059200
H	1.54904600	-0.20282900	-0.23011200
N	2.71599000	-2.11880500	0.20641700
H	1.69367100	-2.08008800	0.14490000
C	2.74455700	1.47288100	0.04155700
C	0.25949100	1.62045300	0.37192800
H	0.28099800	0.62321500	0.78490200
C	1.44588800	2.24465500	0.00641200
C	3.40587600	-0.94338300	0.16061300
C	3.42543600	-3.35721700	0.42880400
H	2.70789600	-4.08679200	0.81007900
H	4.18282900	-3.19367300	1.20054200
C	4.10261800	-3.87913600	-0.83792400
H	4.82408800	-3.13941000	-1.18870800
H	3.36205700	-4.04512500	-1.62319700
C	1.41225100	3.55323400	-0.46635700
H	2.34737800	4.03712900	-0.72492600
C	0.18775200	4.19957400	-0.61987200
H	0.15959800	5.21823700	-0.99005600
O	-3.32773400	1.99584300	0.32398900
O	-3.64140700	-1.11700200	1.57712700
N	-2.07712700	0.09028800	0.33843900
H	-1.15123800	-0.43355100	0.15667300
N	-3.84917000	-1.02058000	-0.66757000
H	-3.45865100	-0.63340700	-1.50918100
C	-2.24050500	1.44032400	0.29316600
C	-0.96588700	2.22408700	0.13484000
C	-3.24317000	-0.71665500	0.50939200
C	-5.05550200	-1.82275500	-0.69884700
H	-5.55817700	-1.63562200	-1.65020100
H	-5.71019400	-1.47357900	0.10344000
C	-4.76757000	-3.31104000	-0.51680900
H	-4.27551400	-3.46483500	0.44424000
H	-4.10868000	-3.67484000	-1.30776800
C	-1.00288600	3.53002000	-0.34704800
H	-1.96917500	3.99274200	-0.51243400
H	4.62883600	-4.81824300	-0.64485900
H	-5.69361900	-3.89144400	-0.53458600
F	0.12864700	-1.17263500	-0.08277800

L4+F⁻: cis-cis

O	3.35804000	2.34818600	0.55552700
O	4.39883600	-0.40418600	0.56492800
N	2.27959600	0.38398800	0.00058000
H	1.38498400	-0.00548400	-0.32078300
N	2.72162700	-1.83935800	-0.00396000
H	1.71857000	-1.89978900	-0.20438100
C	2.35760800	1.73053000	0.27720700
C	-0.16310200	1.67404900	0.23894800
H	-0.11715800	0.61622400	0.46247700
C	1.01256200	2.41081700	0.16156400
C	3.25493400	-0.60549300	0.22066900
C	3.53972800	-3.01566000	0.18843100
H	2.86775100	-3.86907700	0.30067900
H	4.10417700	-2.90654000	1.11942800
C	4.51448200	-3.24664200	-0.96521500
H	5.18075300	-2.38676600	-1.04598500
H	3.97165700	-3.36050200	-1.90578000
C	0.94451100	3.78372800	-0.05900200
H	1.86900500	4.34864600	-0.09346000
C	-0.29371600	4.39479300	-0.23879000
H	-0.34576600	5.46392800	-0.41029500
O	-3.74741500	1.91303000	0.04442400
O	-4.42501700	-0.94280800	-0.01677600
N	-2.37074900	0.10228400	-0.34948400
H	-1.40026200	-0.17092300	-0.54593400
N	-2.53796300	-2.15903200	-0.42242000
H	-1.51470000	-2.09551700	-0.44257400
C	-2.64978800	1.42577000	-0.08795000
C	-1.39502100	2.26486200	-0.01357800
C	-3.23599700	-1.00089400	-0.23927600
C	-3.20989100	-3.42519700	-0.23681400
H	-2.62397800	-4.19298300	-0.74733100
H	-4.18447100	-3.36471600	-0.72682300
C	-3.40436600	-3.78505200	1.23622700
H	-4.01108100	-3.01525700	1.71573800
H	-2.44014200	-3.83922600	1.74635300
C	-1.46254000	3.63786000	-0.23281500
H	-2.43371600	4.08833900	-0.40349300
H	5.11678400	-4.14333500	-0.79457600
H	-3.91112500	-4.74826300	1.34269300
F	0.06546200	-1.18983800	-0.47793600