Electronic Supplementary Information (ESI)

NMR Spectroscopy and DFT Calculations of a Self-Assembled Arene Ruthenium Rectangle Obtained from a Combination of Coordination and Hydrogen Bonds

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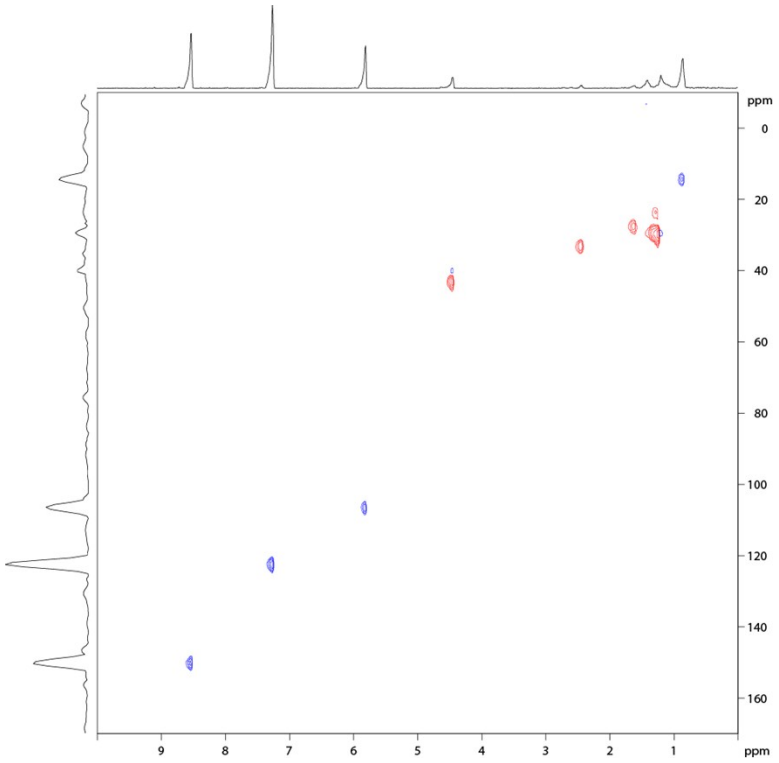

Figure ESI1 ^{1}H-^{13}C multiplicity-edited HSQC spectrum of UPy in $CDCl_3$ at B_0 = 9.4 T and T = 298 K.

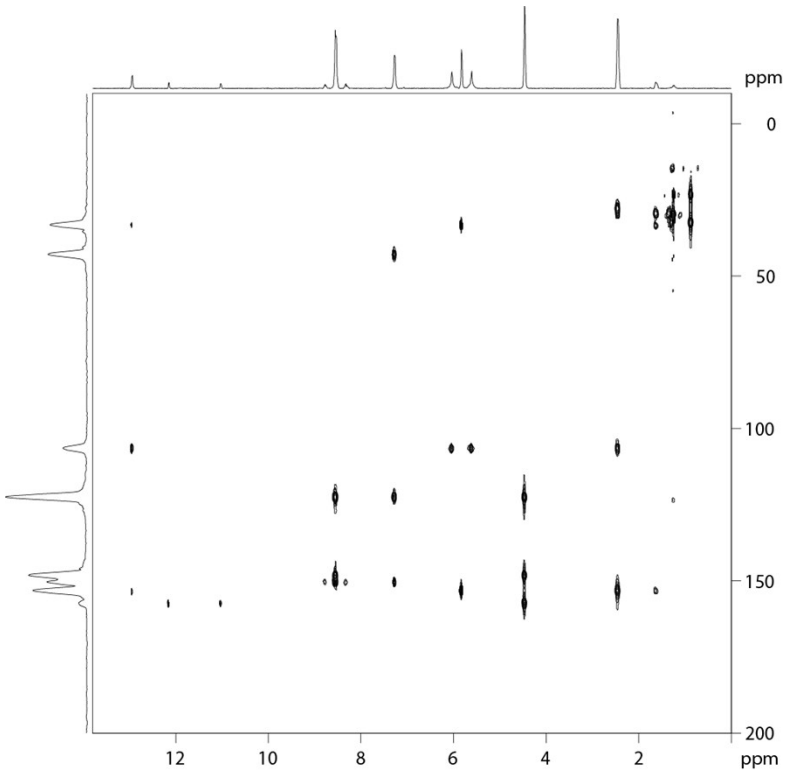

Figure ESI2 ^{1}H-^{13}C HMBC spectrum of UPy in $CDCl_3$ at B_0 = 9.4 T and T = 298 K.

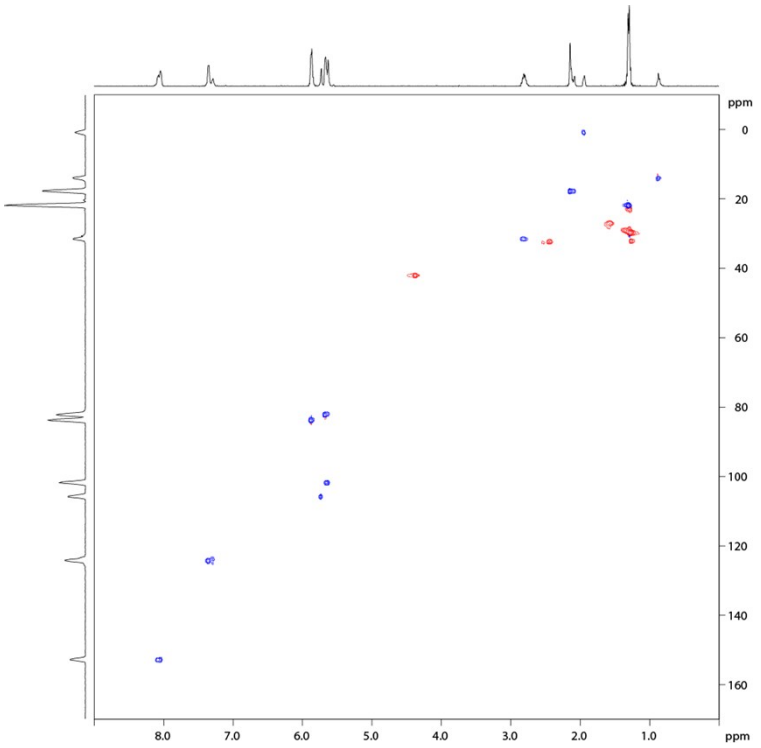

Figure ESI3 ^{1}H-^{13}C multiplicity-edited HSQC spectrum of the rectangular self-assembly in $CDCl_3$ at B_0 = 9.4 T and T = 298 K.

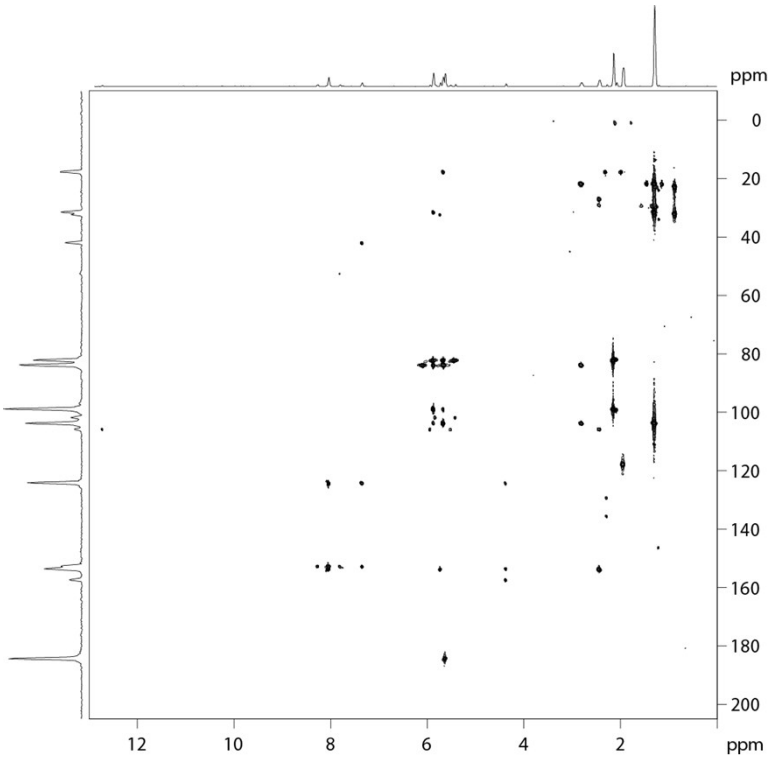

Figure ESI4 ^{1}H-^{13}C HMBC spectrum of the rectangular self-assembly in $CDCl_3$ at B_0 = 9.4 T and T = 298 K.

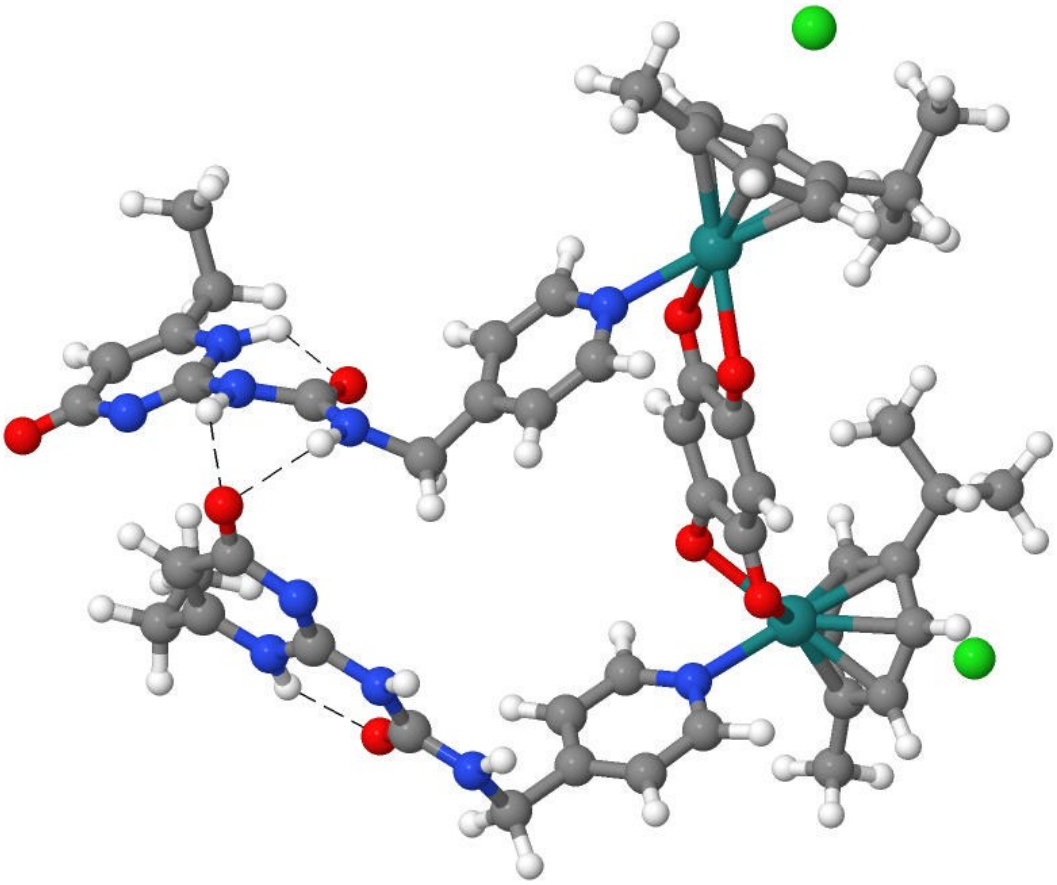

Figure ESI5 Half-rectangle structure obtained from a PM7 semiempirical optimization performed on an initial geometry generated by disassembling the H-bonding networks between the two Upy dimers in a full rectangle. The H-bonds are shown as black dashed lines. Both carbonyl groups of the urea moieties appear to retain the *intra*Upy H-bonding with the NH of the pyrimidinones, whereas the only *inter*UPy H-bonding is found between the two NH of *one* urea moiety and one carbonyl of the pyrimidinone. The second urea moiety features both NHs not being involved in any H-bond interaction. The heat of formation of this half-rectangle structure, as calculated with MOPAC2012/PM7, is +54.3 kcal/mol higher than half of that of the full rectangle. This is consistent with the energy required to disassemble an isolated Upy dimer into its constituent monomers, i.e., 52.1 kcal/mol, thus indicating that the interactions between the two Upy do not contribute significantly to the stability of this half-rectangle system.

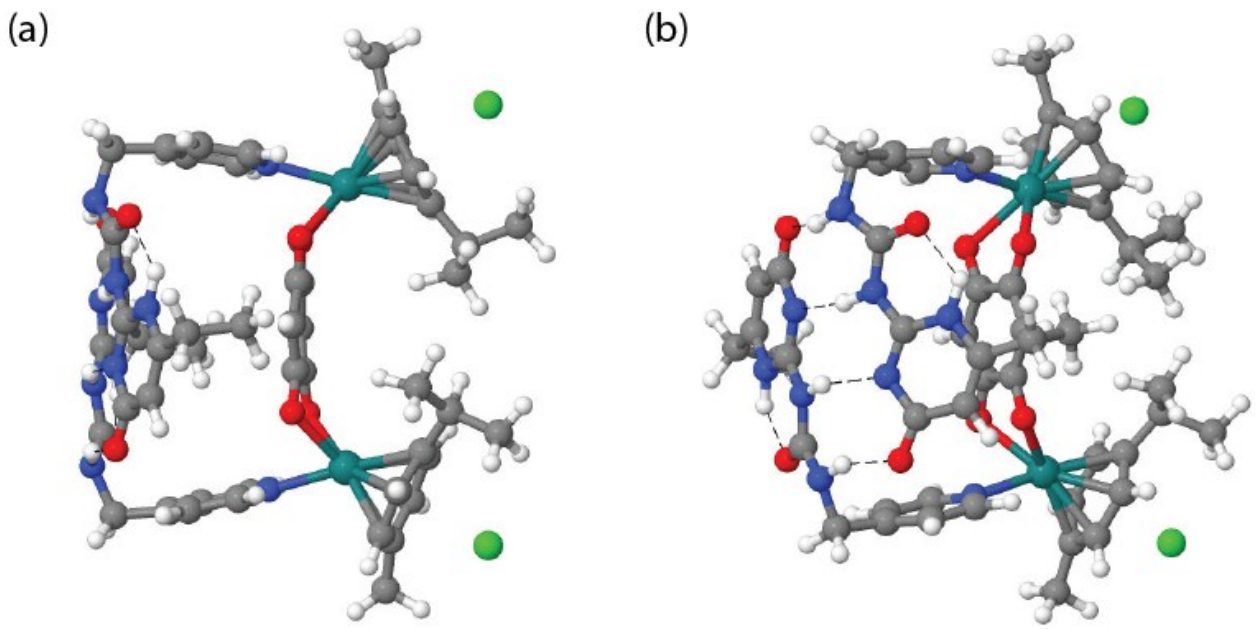

Figure ESI6 (a) Half-rectangle structure obtained from a PM7 semiempirical optimization performed on an initial geometry generated by manipulation of the C(8)-N(9)-C(10)-C(11) dihedral angles of a previously optimized UPy H-bonded dimer so as to favor coordination of the Ru centres of a single arene-Ru clip with minimal distortion of the H-bonding network. (b) Skewed view of the same structure of (a) where one can appreciate the integrity of the H-bonding network. The heat of formation of this half-rectangle structure, as calculated with MOPAC2012/PM7, is +11.02 kcal/mol higher than half of that of the full rectangle.

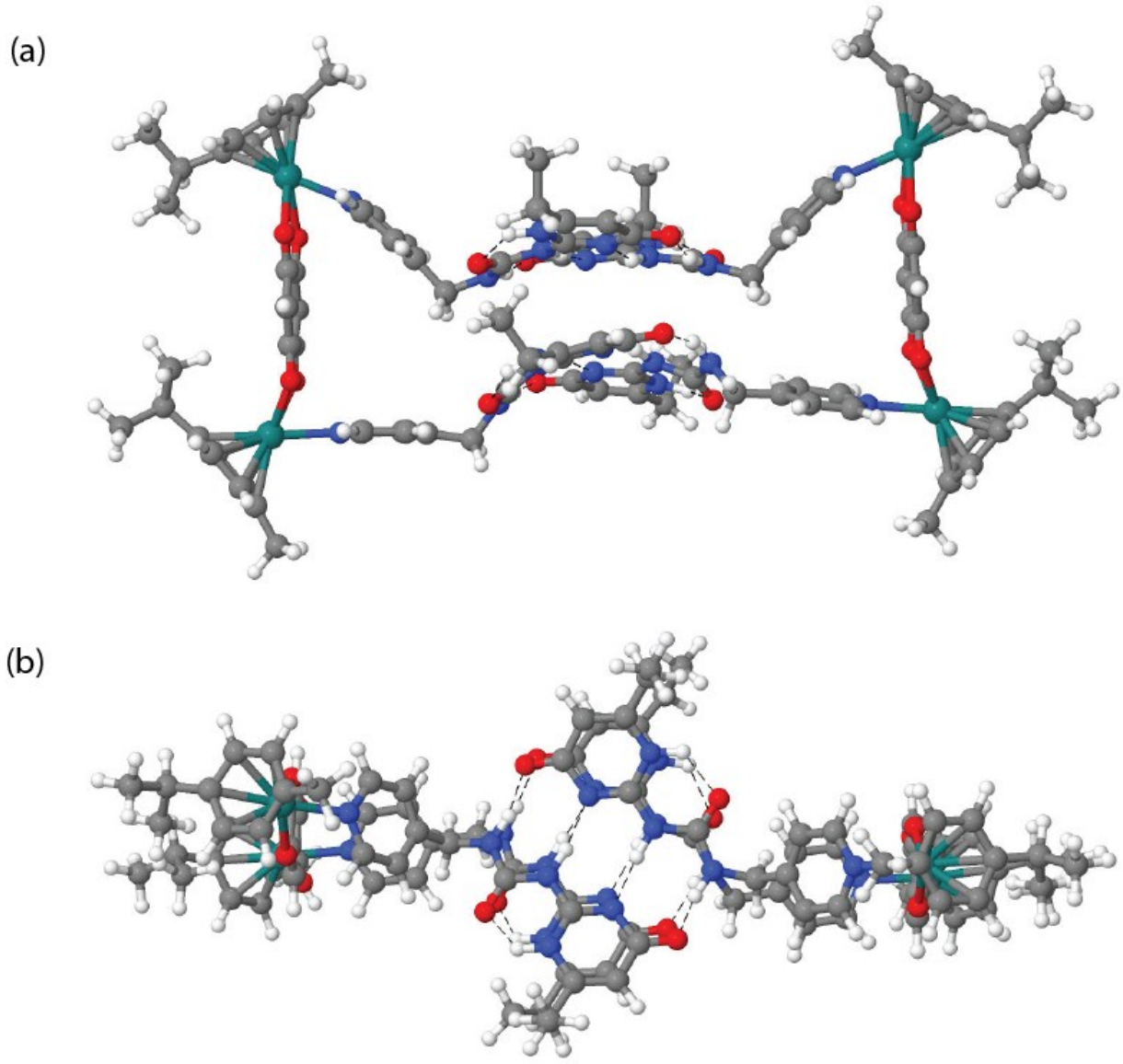

Figure ESI7 (a) Structure of the full rectangle as optimized with DFT methods employing the M06 functional, so as to include for dispersion effects, and the 6-31+G(d,p) basis set. (b) Top view of the structure of (a), where one can appreciate the integrity of the H-bonding network. This structure is very similar to those obtained with the B3LYP method as shown in Fig. 8(b) and (c) of the manuscript, hence the inclusion of dispersion corrections by means of the M06 functional does not result in substantially different interatomic distances from those of the histograms of Fig. 4 and 7.

Table ESI1: Distances as measured by ROE experiments and as calculated with DFT methods and used for the histogram of Fig. 4. It is worth noting that the two experimental sets of data are related to the fact that calculations of distances based on ROE enhancements have been performed assuming either a monomeric or a dimeric *reference* distance.

Irradiated site	NOE response site	Exp $r_{monomer}$ (Å)	Exp r_{dimer} (Å)	DFT $r_{monomer}$ (Å)	DFT r_{dimer} (Å)
H(2)	H(16)	2.78	2.48	3.49	3.14
	H(6)	4.44	3.97	4.22	3.77
	H(7)	4.90	4.38	5.63	4.17
	H(9)	4.24	3.79	7.63	3.86
	H(10)	4.96	4.44	7.74	5.05
	H(12)	5.27	4.71	8.15	4.69
	H(13)	5.44	4.87	10.09	5.21
H(10)	H(13)	4.22	3.83	4.01	3.57
	H(12)	2.73	2.48	2.25	2.03
	H(7)	4.93	4.48	3.92	3.46
	H(6)	4.31	3.92	4.07	3.48
	H(2)	4.83	4.39	7.74	4.91
H(13)	H(2)	5.39	4.80	10.09	5.21
	H(10)	4.22	3.76	4.01	3.57
	H(9)	5.29	4.71	4.80	4.15

Table ESI2: Differences between distances as measured by ROE experiments and those calculated with DFT methods as shown in the histogram of Fig. 4.

Irradiated site	NOE response site	Δr monomer (Å)	Δr dimer (Å)
H(2)	H(16)	0.72	0.66
	H(6)	0.22	0.20
	H(7)	0.73	0.21
	H(9)	3.39	0.07
	H(10)	2.77	0.62
	H(12)	2.88	0.02
	H(13)	4.65	0.34
H(10)	H(13)	0.21	0.26
	H(12)	0.48	0.46
	H(7)	1.01	1.03
	H(6)	0.24	0.44
	H(2)	2.90	0.52
H(13)	H(2)	4.71	0.41
	H(10)	0.21	0.19
	H(9)	0.49	0.56

Table ESI3: Experimental and DFT calculated chemical shifts used for the correlations of Fig. 5.

Experimental			DFT Calculated			
			Monomer		Dimer	
Site	^{13}C δ (ppm)	^{1}H δ (ppm)	^{13}C δ (ppm)	^{1}H δ (ppm)	^{13}C δ (ppm)	^{1}H δ (ppm)
1	152.8	-	152.27	-	155.55	-
2	106.1	5.8	111.08	5.35	107.15	5.23
3	173.2	-	168.87	-	173.93	-
5	154.5	-	151.66	-	156.91	-
6	-	13	-	10.30	-	12.79
7	-	12.2	-	5.54	-	11.60
8	157	-	155.95	-	159.81	-
9	-	11	-	3.47	-	10.77
10	42.5	4.5	42.75	4.15	43.13	4.25
11	147.7	-	150.14	-	151.54	-
12	122.1	7.3	122.37	6.82	122.83	6.95
13	150	8.5	153.90	8.56	153.87	8.32
15	32.7	2.45	27.48	1.85	27.76	1.87

Table ESI4: Distances as measured by ROE experiments and as calculated with DFT methods and used for the histogram of Fig. 7. The irradiated site is H(13) in all cases. It is worth noting that, although equivalent when reported to their second decimal place, the three experimental sets of data are related to the fact that calculations of distances based on ROE enhancements have been performed assuming three different *reference* distances, according to the considered structure.

NOE response site	Rectangle (Å)		Shrunk (Å)		Counterions (Å)	
	r_{exp} (Å)	r_{DFT} (Å)	r_{exp} (Å)	r_{DFT} (Å)	r_{exp} (Å)	r_{DFT} (Å)
H(2’)	2.28	3.02	2.28	2.88	2.28	2.85
H(5’)	2.20	2.28	2.20	2.26	2.20	2.26
H(6’)	2.61	2.87	2.61	2.94	2.60	2.91

Table ESI5: Differences between distances as measured by ROE experiments and those calculated with DFT methods as shown in the histogram of Fig. 7. The irradiated site is H(13) in all cases.

NOE response site	Δr Rectangle (Å)	Δr Shrunk (Å)	Δr Counterions (Å)
H(2’)	0.74	0.60	0.57
H(5’)	0.08	0.05	0.05
H(6’)	0.27	0.33	0.31

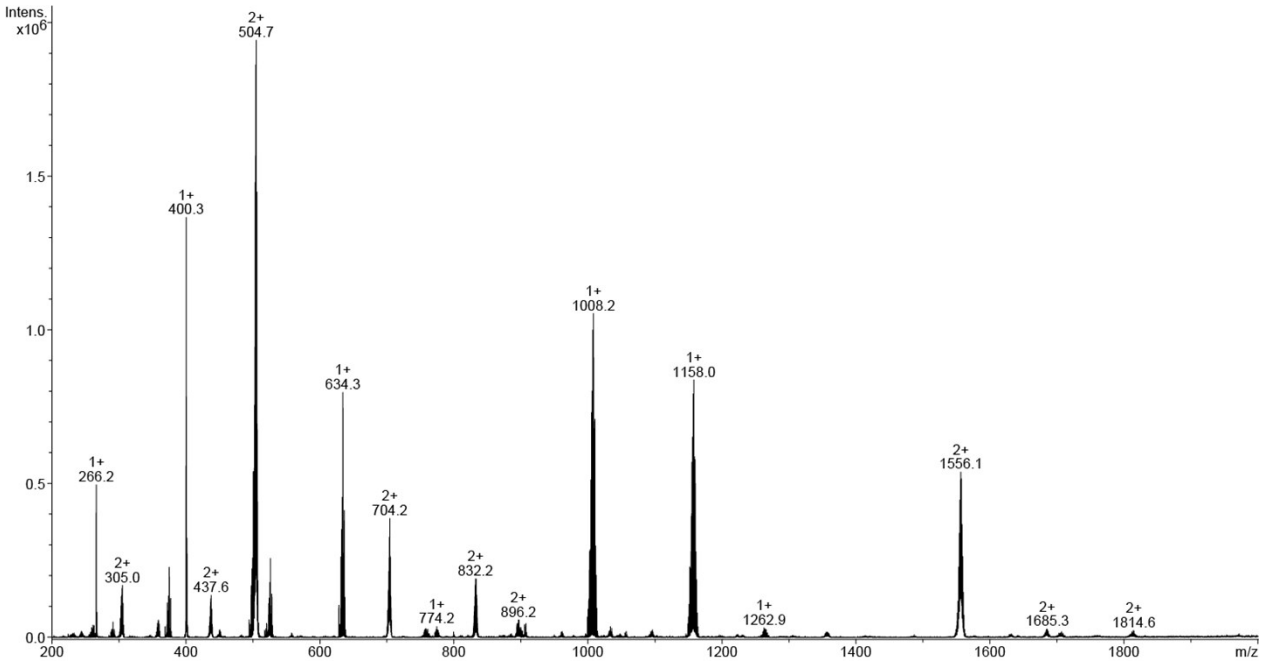

Figure ESI8 ESI-MS spectrum of the rectangular self-assembly in acetonitrile recorded with a Bruker ion trap MS.

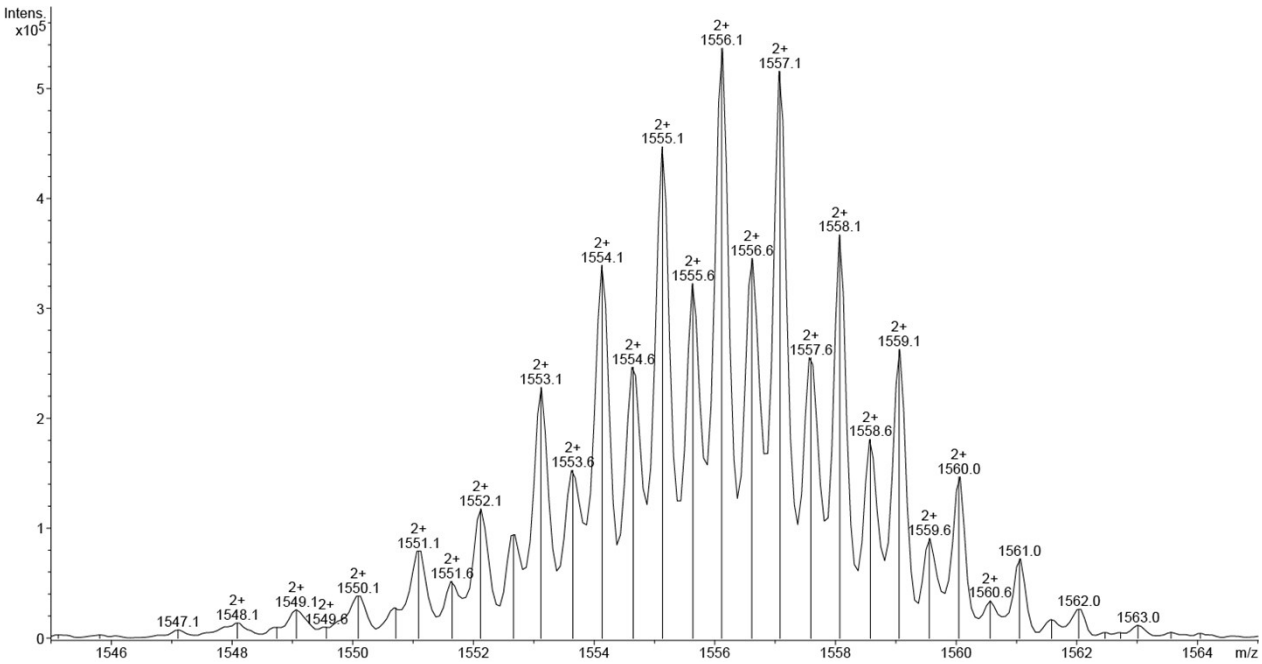

Figure ESI9 Expansion of the MS spectrum of fig. ESI8.

The .xyz file for the structure shown in Figure ES5 is given below.

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134
 Half-rectangle
 H    12.63951633   -3.09283184   -2.75210002
 H     9.23857318    0.27807550   -2.26762746
 C    13.35548926   -0.93451155   -1.18336711
 H     9.71136185    6.67813498   -0.96812221
 C    12.38156091   -3.70105355   -1.87833360
 H    11.52658543   -5.28556717   -3.09837613
 H    11.78548969    5.32574558   -1.16382644
 C     9.33778735    0.12263559   -1.19688077
 O     9.27170962   -2.22644428   -1.33014008
 C    13.83897323   -2.18097121   -0.43117474
 C    10.07730834    6.13943554   -0.08927368
 O     9.41898811    2.41303503   -0.65577182
 C    15.21663063   -2.63186361   -0.92761431
 C    11.74397605   -4.95774945   -2.07712443
 C    12.88846832   -3.34393151   -0.60086841
 C    11.26520726    5.36402508   -0.20124459
 C     9.39467258   -1.16732017   -0.68004628
 H    13.91099146   -1.92534904    0.65760090
 C     9.43419945    1.21178019   -0.33367070
Ru    10.64745856   -3.86003196   -0.45945411
 C     9.53342529    6.43965532    1.19020802
 C    13.47796801    3.29765238   -0.24689042
 C    11.64419548   -5.88926138   -1.00763803
Ru     9.71020079    4.14343923    0.86468789
 C    14.26390308    5.48900961    0.75095873
 C    11.89879004    4.84317988    0.95913640
 C    12.64521428   -4.21178024    0.49983195
 C     9.53444959   -1.38824760    0.83681597
 C    13.30821493    4.30107493    0.90112592
 C     9.47918835    0.99207721    1.18392892
 C    10.08173866    5.79717788    2.33479722
 C    12.01008693   -5.46763274    0.30308740
 O     9.58219515   -2.59308338    1.16462438
 H    13.10783695   -3.99759426    1.46922216
 O     9.42785246    2.05090499    1.83426169
 C     9.50990427   -0.30153758    1.70387581
 C    11.26732098    5.01826409    2.22200973
 H     9.72091913    6.07318099    3.33014524
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H	11.78807442	4.71285954	3.13528424
H	5.18500481	1.83395167	2.43943709
H	7.37631567	3.07264425	2.78402344
H	3.23080668	4.44167680	-8.11616764
H	2.67068919	4.88589314	-6.49823342
C	5.70557499	2.27697719	1.59158898
C	6.90245767	2.96704717	1.79406091
H	3.71500317	0.69920290	0.93365218
H	1.49863733	4.48597063	-7.75933239
C	2.48130662	4.21756489	-7.34739354
N	7.58607249	3.51569300	0.76273337
C	5.20866499	2.15046535	0.29354156
C	4.02144334	1.26579402	0.01764139
H	4.32370016	0.49427119	-0.74164790
O	3.57247244	1.96047365	-2.62648698
H	2.90827945	2.71835309	-4.32689258
C	2.53133506	2.74560425	-6.93604861
H	3.54990378	2.47735968	-6.58607391
C	7.05901255	3.46947003	-0.48855300
C	5.87516605	2.78774997	-0.75627782
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H	2.35161969	2.09608664	-7.82104351
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H	7.66720159	3.97164943	-1.26473567
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H	-0.17546924	2.08509222	-7.17632066
N	-0.27203483	2.06002464	-3.76317623
C	-0.76305592	1.91100853	-5.09111352
O	-1.90556822	1.55940818	-5.25576924
H	6.63541607	-5.59624987	2.30093390
H	9.01253747	-4.87054737	1.71457245
H	0.28920051	-1.96151419	-5.36232643

H	1.59421592	-2.00486539	-4.16853692
C	6.87274272	-5.24678264	1.29781687
C	8.17584392	-4.86055564	0.98714206
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H	0.73998668	-0.49003997	-4.50254978
C	0.61126988	-1.57531026	-4.38619390
N	8.51405484	-4.42408497	-0.25194627
C	5.89444932	-5.18001322	0.30332367
C	4.47156103	-5.56874750	0.61003801
H	3.96979314	-6.01216790	-0.29074371
O	2.68332899	-4.15812745	-0.94668994
H	1.31762178	-3.06351203	-1.71251423
C	-0.42044859	-1.89682452	-3.30449103
H	-0.62707931	-2.98601165	-3.26932704
C	7.56933835	-4.36333933	-1.21918250
C	6.24443215	-4.72871189	-0.96937505
N	3.72060156	-4.39789680	1.08075152
C	2.92901576	-3.72581798	0.16694563
H	-1.39768087	-1.42262566	-3.57108535
N	0.97706199	-2.18445216	-1.30626045
H	4.05158881	-3.96309146	1.92872325
C	0.05437630	-1.37591356	-1.98515186
H	7.91787299	-3.99631913	-2.20114816
H	5.49730915	-4.65532291	-1.76290323
N	2.38715124	-2.51478144	0.63604862
C	1.47779294	-1.72347091	-0.09405107
C	-0.32388128	-0.18760544	-1.45015935
H	2.57705469	-2.17881205	1.58577761
H	-1.05555450	0.46630218	-1.94417449
N	1.17732433	-0.55970479	0.44498182
C	0.28708533	0.31222035	-0.22949984
O	0.15341592	1.44175303	0.20367119
C	11.33408130	-7.31669936	-1.27878509
H	10.69451556	-7.46206790	-2.15711367
H	10.87709638	-7.83255447	-0.42697975
H	12.30456742	-7.83573930	-1.49297479
H	15.98027439	-1.86994449	-0.76267377
H	15.20598698	-2.89415899	-1.99413173
H	15.54010663	-3.56413172	-0.42790566
H	13.91138464	-0.04584493	-0.86559274
H	12.28985392	-0.74812062	-1.00024116
H	13.49308711	-1.03075851	-2.26601875

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H 14.43847921 2.77731900 -0.17106349
H 13.45256809 3.78883352 -1.22570825
H 14.07563277 6.25423833 1.52909362
H 14.11201503 6.02526734 -0.19400348
H 15.30922993 5.18256066 0.81553076
C 8.53247914 7.52685283 1.34664381
H 7.88276121 7.39429125 2.21972661
H 7.89892458 7.66437627 0.46242895
H 9.09441955 8.48381024 1.49770198
Cl 14.39070423 -5.94832094 -1.32147670
Cl 11.89364973 7.90349572 1.41165737

The .xyz file for the structure shown in Figure ESI6 is given below.

134
Half rectangle 2
H -10.88350705 5.73934975 2.65493438
H -9.04520809 0.04181010 3.03272698
H -13.46389356 -2.29806533 1.71361850
H -12.21891554 3.65442002 2.51034505
H -12.90965798 -4.34337521 2.98995223
C -11.06192610 5.29325658 1.67201467
H -9.72590492 7.65098474 1.50567854
H -13.73302296 -1.13124099 -0.33072774
C -9.10339615 -0.02288916 1.95127414
C -11.82890657 4.09522829 1.58750997
C -13.00592874 -3.13730083 1.18107054
O -8.83226784 2.29117060 1.59457049
O -9.60289925 -2.32484595 1.90213986
C -12.68050134 -4.31496871 1.92046746
H -13.27319805 1.90794187 1.19010877
C -9.00567195 1.13037316 1.17522165
C -9.35844756 -1.24307684 1.33181959
H -11.20475300 8.10099824 0.62113759
H -15.57877369 -2.88105518 -0.60996992
C -10.29711303 7.44469975 0.59299266
C -13.60694821 -2.01472794 -1.00972985
C -10.76749033 6.03850700 0.49951313
H -12.08599788 -6.72373531 3.02185771
H -14.79305524 3.93724864 1.27881815
H -15.56254728 -1.69197353 -1.93939270

C	-12.95910233	-3.13795525	-0.23404167
Ru	-9.99258748	3.85086587	0.32961247
C	-12.29087690	3.62071434	0.33077754
H	-13.10766349	-0.65414927	-2.64006759
C	-14.99040908	-2.48963367	-1.46278611
C	-13.38098105	2.57481147	0.29623923
Ru	-10.91961058	-3.75578424	0.64072118
C	-12.31240145	-5.50347323	1.24527713
H	-9.69805748	7.75938577	-0.26939416
H	-13.33679845	-7.24588626	1.86567745
H	-11.69700553	-1.43547875	-1.89392105
C	-12.74150079	-1.58787396	-2.20205007
C	-12.30898818	-6.81150122	1.95190412
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H	-15.56989557	2.62000297	0.36287656
C	-9.06736283	1.03384763	-0.36047503
C	-9.29339394	-1.35819532	-0.20180636
C	-11.08388581	5.47029190	-0.76966871
H	-14.01276112	0.86179338	-0.88955142
H	-12.30578224	1.30012858	-1.11579695
H	-14.92961710	-3.34054773	-2.15350844
C	-11.86063877	4.28459982	-0.84990655
C	-13.31381245	1.70427164	-0.96316042
C	-12.46837029	-4.29760776	-0.90430843
O	-9.02023827	2.13873568	-0.93523770
C	-12.13265741	-5.46135591	-0.17333850
O	-9.38625253	-2.52938051	-0.61847242
H	-11.61330321	-7.53689267	1.51396027
H	-12.74275573	-2.33995035	-2.99758886
H	-14.84465505	4.03029683	-0.44973236
C	-9.10931931	-0.21526540	-0.97718820
H	-10.92541536	6.06542903	-1.67373848
H	-12.52505115	-4.34520139	-1.99654418
H	-12.27999654	3.99036097	-1.81758910
H	-13.59396129	2.26631647	-1.86127349
H	-11.94464052	-6.39683792	-0.70914399
H	-9.05713955	-0.29326738	-2.05645095
H	-6.39962196	0.27241456	5.87899768
H	-6.24819651	-1.47496466	5.65688390
H	-6.11894776	-0.77595879	7.27512064
C	-5.85640523	-0.61904721	6.22120084
H	-6.52793851	-5.07512255	3.30639504

H	-5.77148275	4.21916066	-2.56483299
H	-4.52306451	-6.12809493	2.31115513
H	-8.24457042	4.19922343	-1.90196074
H	-3.88836552	1.95465081	4.68936538
H	-8.65027540	-1.50919422	-4.03412519
C	-4.34559870	-0.46014968	6.04750178
C	-3.85530343	1.05355310	4.08572880
C	-4.03463443	-0.18905540	4.60751494
C	-3.62876183	1.22517646	2.65960908
O	-3.46890321	2.30060486	2.10739105
H	-3.42668040	4.24139057	-1.89184625
N	-3.94973420	-1.31261092	3.78781331
N	-3.62279266	0.06709555	1.85857057
C	-3.77734981	-1.12910467	2.41408764
H	-4.16236434	-2.26041057	4.14790377
N	-3.75605506	-2.23758136	1.57458910
C	-6.06977555	4.22204211	-1.51434173
H	-3.97093918	0.37013189	6.68619371
H	-8.18375969	0.19959525	-3.99876227
H	-3.23750633	2.19378638	0.30348894
C	-7.41782380	4.20394561	-1.16569853
H	-3.72311812	-2.04401564	0.54545669
H	-8.94117603	-4.30911714	3.00882641
H	-3.95457901	0.11289546	-0.07224629
C	-4.09806570	-3.54678671	2.00104596
N	-4.05474479	-4.50566985	1.00998220
C	-6.99413697	-5.06851538	2.31867268
O	-4.33115514	-3.78627559	3.17929205
H	-4.11106646	-4.20514369	0.01215953
N	-3.40716250	2.49532502	-0.67707541
N	-4.28347751	0.34494924	-1.04049168
C	-4.79798887	-5.74629871	1.29782731
H	-3.81591159	-1.36462377	6.41768274
C	-8.14893211	-0.71489929	-4.60599379
N	-4.58521399	-1.94104012	-1.33842243
O	-4.90798695	-4.15387676	-1.60441589
C	-8.31165604	-4.63786455	2.16473388
C	-4.74879758	-0.71094338	-1.81252971
C	-3.66499179	3.93672978	-0.84429736
C	-4.11075589	1.66346099	-1.52510615
C	-5.11313970	4.17653663	-0.49740545
C	-5.09489826	-3.03662203	-2.05920637

N	-7.81549524	4.14088592	0.12992898
H	-8.75138155	-0.53032270	-5.50387689
C	-6.27187269	-5.44940651	1.18657572
N	-5.39872332	-0.43177279	-3.01641425
C	-5.81670154	-2.76187425	-3.29056755
O	-4.55954482	1.99955910	-2.61221436
H	-4.46950988	-6.51795416	0.56034124
H	-5.52226864	0.55048327	-3.30752730
H	-6.23013048	-3.61426591	-3.81847698
C	-5.96397763	-1.48359545	-3.73182872
C	-6.89244912	4.16184764	1.11857902
C	-5.52555087	4.18380945	0.83534231
N	-8.89274755	-4.56699781	0.94374143
H	-2.97037101	4.49545285	-0.17289322
C	-6.71657024	-1.10368274	-4.97031947
C	-6.89461267	-5.43293211	-0.06229747
H	-7.29204008	4.12266994	2.14484088
H	-4.79420229	4.15578293	1.65007484
H	-6.72230533	-1.95271822	-5.68959280
C	-8.20841880	-4.97490561	-0.15196149
H	-6.35464887	-5.73348266	-0.96582556
H	-6.21690262	-0.27211076	-5.51361877
H	-8.76094867	-4.88787801	-1.10466478
Cl	-14.98493696	-5.37293962	0.37643463
Cl	-13.50149447	6.47412304	0.54599116

The .xyz file for the structure shown in Figure ESI7 is given below.

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H	12.78775433	-3.96674809	-2.50320433
H	9.82459865	0.24830993	-2.30271761
C	13.75498937	-1.66430828	-1.13129144
H	9.96310781	6.70274749	-1.52473329
C	12.46795284	-4.39427287	-1.54223724
H	11.22003078	-5.90530737	-2.49443622
H	12.12716748	5.48278847	-1.39868945
C	9.89594425	0.18321799	-1.21808849
O	9.87047381	-2.17126950	-1.14941902
C	14.17906314	-2.91089005	-0.34551170
C	10.29056389	6.30308381	-0.55719006
O	9.92794630	2.51289400	-0.84360685

C	15.46316527	-3.51346251	-0.92457485
C	11.59225315	-5.51553895	-1.53752991
C	13.08287094	-3.95325019	-0.34181142
C	11.52524783	5.59759783	-0.48622019
C	9.95158683	-1.05899961	-0.59198056
H	14.37821009	-2.59713273	0.71517967
C	9.95540567	1.33394226	-0.43889032
Ru	10.78496816	-3.98261430	-0.09094706
C	9.57747260	6.63317689	0.62109657
C	13.78749656	3.62782991	-0.13154573
C	11.32314003	-6.21946948	-0.33539444
Ru	9.95927079	4.35232021	0.54780310
C	14.44487674	5.92953162	0.69161378
C	12.07573174	5.23092719	0.76890249
C	12.73039917	-4.59438994	0.87634237
C	10.06404325	-1.15605142	0.93712981
C	13.50036926	4.73754059	0.88383080
C	9.97348536	1.23300268	1.09229745
C	10.07626434	6.17520197	1.87069547
C	11.86421351	-5.71960100	0.87868884
O	10.13512193	-2.33053944	1.35011674
H	13.24961647	-4.32003114	1.80570590
O	9.89601686	2.34385038	1.65132195
C	10.01321704	-0.00784971	1.71997698
C	11.31249268	5.47866031	1.94481802
H	9.56838500	6.46986457	2.79797704
H	13.65941187	4.31292862	1.91126040
H	11.71996400	-6.28043489	1.81178474
H	10.02810265	-0.07512734	2.80703369
H	11.74892660	5.26828289	2.93109454
H	-12.48076702	-4.34502819	2.61649306
H	-9.82956144	0.40073208	2.32579611
H	-14.00636858	-2.71142115	1.74848315
C	-12.21369038	-4.63751783	1.59139932
H	-10.80408240	-6.15414388	2.26567764
H	-11.88849860	5.64846662	1.75357770
C	-9.93623358	0.33231786	1.24430551
O	-9.98682192	-2.02206827	1.18336225
C	-14.16266970	-3.23760552	0.76851277
C	-10.28670912	6.47600296	0.53121414
O	-9.87462967	2.65854395	0.86309835
C	-15.40374395	-4.13127740	0.87959465

C	-11.26426767	-5.67339293	1.39255663
C	-12.96459823	-4.12034516	0.49553303
C	-11.48309534	5.73481721	0.73573209
C	-10.04338904	-0.90926923	0.62510071
C	-14.35391646	-2.17033690	-0.31348390
C	-9.98648093	1.48307135	0.46425831
Ru	-10.69726341	-3.91266539	0.10053802
C	-9.82900977	6.76481248	-0.78173699
H	-13.75379981	4.45571425	0.94251026
C	-11.03348462	-6.20708788	0.09431374
Ru	-10.08896310	4.48683878	-0.51419339
C	-14.68829258	5.75530695	-0.52205605
C	-12.25258065	5.27950960	-0.37080005
C	-12.65111207	-4.57583096	-0.80819089
C	-10.16992200	-1.00833208	-0.90174214
C	-13.63530827	4.70626861	-0.14599618
C	-10.10557393	1.37971842	-1.06163322
C	-10.54548687	6.22891149	-1.88176039
C	-11.69918676	-5.61713590	-1.00650668
O	-10.21175424	-2.18422164	-1.31464646
H	-13.24973588	-4.23592141	-1.66500862
O	-10.07444398	2.48879778	-1.62862977
C	-10.16179158	0.13855032	-1.68720266
C	-11.74243054	5.48707724	-1.67874116
H	-10.24873603	6.48950847	-2.90501487
C	-13.82790260	3.41663561	-0.95063605
H	-11.59021420	-6.04732286	-2.01062925
H	-10.21701039	0.06938224	-2.77240351
H	-12.34931387	5.20463666	-2.55069199
H	5.88544708	1.54271498	2.37184285
H	7.75655617	3.25941123	2.51872856
H	1.77331065	4.88382777	-6.80068203
H	1.74354781	5.07482266	-5.04235281
C	6.32455349	1.96481911	1.46205152
C	7.33861146	2.92006820	1.55521846
H	5.00755196	-0.30446045	0.88902006
H	0.22848478	4.92456133	-5.93916058
C	1.26320454	4.56037521	-5.88214452
N	7.91123477	3.45794134	0.44922360
C	5.89445559	1.55645865	0.19870749
C	4.91441851	0.41896862	0.03712422
H	5.15019575	-0.15654620	-0.89559507

O	3.59535272	1.34826944	-2.24714402
H	2.45886522	2.27525085	-3.47365091
C	1.32713317	3.04038615	-5.73732447
H	2.38822958	2.71102594	-5.75578267
C	7.42032006	3.13910085	-0.77679874
C	6.41236946	2.18990715	-0.93393279
N	3.53823169	0.89634424	0.00290214
C	2.99777092	1.31513423	-1.17545487
H	0.85579160	2.56048122	-6.62613992
N	1.43446603	2.33615365	-3.38600610
H	3.02869763	0.95507953	0.91442647
C	0.62106135	2.61455458	-4.48664230
H	7.90593262	3.65186554	-1.62549662
H	6.03456138	1.93789103	-1.93202298
N	1.63621684	1.70403512	-1.07661135
C	0.83367652	1.93912619	-2.18871992
C	-0.73045354	2.52358575	-4.37373824
H	1.13426478	1.50498344	-0.16901968
O	2.54060521	1.28946517	2.52901416
H	-1.40843319	2.74595281	-5.19418869
N	-0.47646393	1.80221390	-2.05101604
C	-1.34320259	2.11673729	-3.11986822
C	1.34352057	1.42746330	2.72320930
N	0.47439741	1.26017597	1.62822771
O	-2.54280731	2.01846054	-2.93321004
H	-1.13048903	1.24267355	-0.26672481
H	1.43084107	1.98933098	4.81870055
C	0.74747657	1.79488769	3.99591781
C	-0.83858988	1.38223104	1.79013554
N	-1.63250773	1.29836985	0.65674081
H	-3.04226483	1.25732379	-1.44364117
H	-0.33798910	4.37272282	5.30475097
C	-0.60149634	1.91238740	4.11974472
N	-1.42973713	1.63775817	3.03010055
N	-3.57840471	1.01691094	-0.57835941
C	-3.04200224	1.13930384	0.66987267
H	-5.04705413	0.06645468	-1.71578044
C	-1.34020914	3.92244651	5.33928174
H	-1.89355782	4.29610842	4.47043716
H	-2.45539721	1.66617391	3.10518090
C	-1.27422556	2.39298254	5.36828271
H	-5.80990490	2.04394093	1.44205953

H	-0.70440282	2.05908194	6.26605426
C	-4.96875708	0.61596994	-0.74059740
O	-3.67092507	1.10682221	1.72159875
H	-1.83777261	4.31485777	6.23725755
H	-5.25358895	-0.12147145	0.05906570
C	-6.30861481	2.34709032	0.51182716
H	-2.28898663	1.96370608	5.49468781
C	-5.93966242	1.77113352	-0.70650724
H	-7.70336959	3.75080635	1.46631192
C	-7.34116853	3.28393128	0.53559690
C	-6.55331891	2.21905999	-1.87815600
H	-6.24924251	1.83507778	-2.85564794
N	-8.00567718	3.64203487	-0.59384290
C	-7.58436770	3.15551678	-1.78898705
H	-8.14525331	3.51928456	-2.66839351
H	6.35186666	-4.19728289	2.75027862
H	8.84060324	-4.10513345	2.24810715
H	3.37461837	-0.45223222	-6.13924808
H	3.14518727	0.01015757	-4.44964490
C	6.70496782	-4.12987261	1.71814972
C	8.07383988	-4.07243409	1.45290983
H	4.23216198	-4.87367103	1.92510713
H	1.96663017	0.51110037	-5.67614532
C	2.61505709	-0.31259799	-5.35715534
N	8.55309310	-3.98000632	0.18752258
C	5.80081587	-4.11916983	0.65311479
C	4.33918225	-4.41314186	0.90847382
H	4.00590890	-5.18882921	0.16696596
O	3.52198314	-3.12605922	-1.42836837
H	2.74921136	-2.04813452	-2.75244054
C	1.80478512	-1.58819533	-5.13475806
H	2.47341554	-2.47843853	-5.13005564
C	7.67649264	-3.90760616	-0.84501869
C	6.29657482	-3.97266903	-0.64404895
N	3.44501475	-3.25756019	0.85459418
C	3.00959860	-2.81280075	-0.35923425
H	1.11813841	-1.76101874	-5.99489773
N	1.77061330	-1.71819469	-2.69734255
H	3.00415215	-2.94549341	1.74580032
C	1.02942256	-1.49329351	-3.85655258
H	8.13333542	-3.80231425	-1.84353942
H	5.60783533	-3.92529204	-1.49809804

N	1.87538114	-1.95164650	-0.31570631
C	1.11659362	-1.71488865	-1.46434532
C	-0.29670006	-1.20817553	-3.76719005
H	1.35947288	-1.83256491	0.59010555
O	2.39906310	-2.74433473	3.35051773
H	-0.90979310	-0.99372999	-4.63854134
N	-0.17867811	-1.46535177	-1.33425207
C	-0.96700259	-1.20475526	-2.47590902
C	1.18492891	-2.75461040	3.46610446
N	0.41235497	-2.41831608	2.33294728
O	-2.16434125	-1.04408859	-2.31523728
H	-1.09161489	-1.65867009	0.48353072
H	1.06970203	-3.35382036	5.55275361
C	0.47168675	-3.14760455	4.66726203
C	-0.90667481	-2.51690899	2.37128052
N	-1.63642226	-2.12963026	1.24591567
H	-3.00090529	-1.42196808	-0.72150889
H	-1.42199591	-1.91000963	6.95002853
C	-0.88029698	-3.28662242	4.64965300
N	-1.60198385	-2.96349513	3.49832176
N	-3.52394328	-2.14449198	-0.18239957
C	-2.91952042	-2.65992492	0.95288689
H	-4.18929816	-2.70497552	-2.08484790
C	-2.23307901	-2.55547033	6.58600626
H	-2.89878043	-1.93920430	5.97178777
H	-2.59850059	-3.20825569	3.41685670
C	-1.68918009	-3.75788425	5.81757689
H	-5.58497340	-2.90195185	1.48077579
H	-1.06143294	-4.38682345	6.49307787
C	-4.30592085	-3.06163884	-1.02286370
O	-3.46649461	-3.44025004	1.71471206
H	-2.80585688	-2.88013925	7.46636347
H	-3.87424051	-4.09805483	-0.99455670
C	-6.25503653	-3.11782803	0.63940106
H	-2.51781382	-4.42760283	5.50137805
C	-5.76786234	-3.17732810	-0.66673093
H	-8.04717218	-3.34068897	1.89513490
C	-7.60899481	-3.36524076	0.88262171
C	-6.67671836	-3.45406626	-1.69810630
H	-6.35094826	-3.49453290	-2.73881852
N	-8.47698165	-3.64944770	-0.11862029
C	-8.01604749	-3.69121591	-1.39471727

H	-8.78450474	-3.91718739	-2.15888836
C	10.66153431	-7.55130317	-0.36356748
H	10.00820796	-7.68857412	-1.23774572
H	10.04649460	-7.73881859	0.52972046
H	11.42098580	-8.35984836	-0.40363155
H	16.29216808	-2.79336151	-0.87066990
H	15.35355168	-3.79595214	-1.97785635
H	15.78391103	-4.40939268	-0.37684297
H	14.41536801	-0.81773515	-0.90318667
H	12.72563737	-1.36842406	-0.88547526
H	13.80230092	-1.82023999	-2.21564892
H	13.02742801	2.83790158	-0.07840098
H	14.76404015	3.16601221	0.06175133
H	13.80737535	3.99374790	-1.16404040
H	14.21609949	6.74350514	1.39249768
H	14.39097886	6.34475376	-0.32190852
H	15.49127724	5.63861016	0.86251423
C	8.43767954	7.58868241	0.57759696
H	7.63901669	7.32517266	1.28914175
H	7.97293885	7.65709795	-0.41806359
H	8.77843200	8.61127571	0.83735073
C	-8.74002721	7.75393060	-1.00340520
H	-8.15762968	7.54992313	-1.91578580
H	-8.02065096	7.79289360	-0.17063158
H	-9.16162024	8.77391833	-1.11320440
H	-14.67513539	5.99173848	-1.59282289
H	-14.54102222	6.69730760	0.02213741
H	-15.70141640	5.39949642	-0.28081563
H	-13.00150494	2.71410736	-0.77709347
H	-13.88007908	3.60168487	-2.03024648
H	-14.76072337	2.91164746	-0.66883478
C	-10.26695137	-7.47157179	-0.07093021
H	-9.42616175	-7.55470687	0.63510664
H	-9.84883085	-7.59117485	-1.08248836
H	-10.92345257	-8.34896393	0.10579057
H	-15.07977969	-1.41159713	0.01046604
H	-14.73820719	-2.58996753	-1.25060629
H	-13.41245162	-1.65497934	-0.54024053
H	-16.29997210	-3.53783878	1.11219517
H	-15.29846841	-4.88052958	1.67379598
H	-15.60839924	-4.67093247	-0.05328712
H	-9.78687157	6.93077190	1.39525017

The .xyz file for the monomer shown in Figure 9 and used for the calculations of interatomic distances and chemical shifts shown in Fig. 4 and 5, respectively, is given below.

35
Monomer

C	3.744060	0.587230	0.549740
N	2.419860	0.447720	0.162600
C	1.972110	-0.769350	-0.250650
N	0.627990	-0.869640	-0.630690
N	2.675570	-1.848440	-0.323260
C	4.033600	-1.803920	0.051420
O	4.732590	-2.802270	-0.003440
C	4.541560	-0.502260	0.503010
H	0.396860	-1.810220	-0.920550
C	-0.326530	0.136860	-0.653880
O	-0.081020	1.293620	-0.319070
N	-1.559530	-0.271240	-1.075140
C	4.171860	1.964460	0.975090
C	-2.686110	0.644680	-1.196970
H	-1.704460	-1.235780	-1.332210
H	-7.259460	0.000930	-0.418860
C	-6.244170	-0.030850	-0.033600
C	-5.170790	0.302180	-0.859160
H	-5.349900	0.593610	-1.888760
C	-3.875930	0.252250	-0.344030
C	-3.728790	-0.139560	0.988300
H	-2.748340	-0.198520	1.446670
C	-4.864610	-0.454030	1.729200
H	-4.771230	-0.758940	2.767600
N	-6.108640	-0.405350	1.240320
H	-2.991930	0.719480	-2.244990
H	-2.314380	1.626060	-0.895070
H	3.501540	2.317490	1.768060
C	4.191350	2.985740	-0.176310
H	5.166930	1.885190	1.416810
H	3.200850	3.122240	-0.618120
H	4.872240	2.664900	-0.968120
H	4.526970	3.959190	0.188730
H	1.748860	1.214000	0.170730
H	5.580420	-0.442610	0.798280

The .xyz file for the H-bond dimer shown in Figure 9 and used for the calculations of interatomic distances and chemical shifts shown in Fig. 4 and 5, respectively, is given below.

```
70
H-Bond dimer
C    0.756710    4.328450   -0.410410
N   -0.363120    3.526870   -0.355150
C   -0.255170    2.171790   -0.396290
N   -1.409360    1.428410   -0.352210
N    0.894710    1.542350   -0.477720
C    2.066970    2.282901   -0.547800
O    3.159780    1.704941   -0.641140
C    1.968010    3.731461   -0.506260
H   -1.260690    0.407770   -0.407510
C   -2.715210    1.950420   -0.319380
O   -2.926480    3.169759   -0.266070
N   -3.681450    1.015859   -0.344290
C    0.522179    5.812710   -0.371560
C   -5.084420    1.393389   -0.429680
H   -3.437559    0.019019   -0.472050
H   -9.155349   -0.623652    0.662520
C   -8.130709   -0.406822    0.950190
C   -7.303709    0.310408    0.093440
H   -7.682420    0.647658   -0.866820
C   -5.987180    0.576559    0.474780
C   -5.573329    0.093609    1.716360
H   -4.559249    0.254359    2.063310
C   -6.478579   -0.616481    2.502150
H   -6.171879   -1.003841    3.468750
N   -7.739649   -0.871932    2.140300
H   -5.435300    1.304589   -1.462890
H   -5.152900    2.450389   -0.161870
H   -0.067631    6.053100    0.520680
C   -0.191301    6.354080   -1.623230
H    1.490149    6.303351   -0.252950
H   -1.183571    5.914060   -1.748530
H    0.389299    6.143250   -2.524380
H   -0.316441    7.436260   -1.544210
H   -1.326640    3.880820   -0.292590
H    2.880600    4.308971   -0.550510
H    0.059762   -6.046420    0.516210
```

H 6.165510 0.947592 3.487820
H 4.557071 -0.286559 2.060020
C 6.474740 0.575322 2.514830
H 5.153711 -2.447409 -0.205370
C 5.571011 -0.120888 1.716220
H -1.492228 -6.294990 -0.269070
C -0.523408 -5.804380 -0.379890
O 2.928551 -3.160939 -0.282740
N 7.738640 0.833682 2.162890
H 1.326112 -3.872400 -0.303640
C 5.986651 -0.583278 0.467700
C -0.757598 -4.320010 -0.417080
C 5.084411 -1.382239 -0.450570
N 0.362471 -3.518490 -0.362510
C 2.715901 -1.941579 -0.332700
H 0.322232 -7.426550 -1.549260
C -1.969079 -3.722830 -0.509290
C 0.199212 -6.344030 -1.626990
N 3.681801 -1.006749 -0.359880
C 8.131680 0.387642 0.965560
C 7.303641 -0.312548 0.091850
C 0.254861 -2.163360 -0.401180
H -2.881838 -4.300261 -0.552860
N 1.409411 -1.420069 -0.359500
H 5.435981 -1.268469 -1.485480
C -2.067959 -2.274150 -0.547090
H 1.193192 -5.905360 -1.743400
N -0.895309 -1.533790 -0.478370
H 9.159230 0.607032 0.686570
H 3.437351 -0.009699 -0.484170
H 1.260121 -0.399370 -0.412600
H 7.684101 -0.634228 -0.873010
O -3.161099 -1.696051 -0.635960
H -0.373718 -6.130560 -2.532450

The .xyz file for the rectangle shown in Figure 8(a) and used for the calculations of the interatomic distances shown in the histogram of Fig. 7 is given below.

264
Rectangle
H 12.576406 -4.562234 -2.486841
H 10.599311 0.242896 -2.394534

C	14.262005	-2.526610	-2.203616
H	11.295677	5.779588	-2.216673
C	12.493951	-4.828282	-1.442000
H	10.908782	-6.239503	-1.821777
H	13.292873	4.547408	-1.446398
C	10.699991	0.208674	-1.318121
O	10.814603	-2.139922	-1.238102
C	14.471997	-3.255389	-0.872003
C	11.517820	5.750265	-1.158093
O	10.736603	2.549271	-1.079670
C	15.791463	-4.055008	-0.880941
C	11.522029	-5.772638	-1.062444
C	13.338645	-4.186809	-0.486150
C	12.679794	5.048969	-0.711120
C	10.808486	-1.010420	-0.654213
H	14.545218	-2.504454	-0.078171
C	10.777780	1.381791	-0.574779
Ru	11.126673	-3.828599	-0.003950
C	10.648290	6.378070	-0.250383
C	14.794461	3.169686	0.228324
C	11.314912	-6.095896	0.309628
Ru	10.859150	4.168541	0.270456
C	15.277168	5.276999	1.554405
C	12.986543	4.930073	0.651444
C	13.075325	-4.471424	0.867187
C	10.933716	-1.057914	0.853858
C	14.216084	4.220579	1.179726
C	10.933656	1.332603	0.931724
C	10.930226	6.227048	1.142968
C	12.081219	-5.407633	1.269223
O	11.002674	-2.226210	1.357423
H	13.609541	-3.922115	1.632894
O	11.025676	2.461573	1.508330
C	10.972731	0.112626	1.602023
C	12.051967	5.505867	1.575905
H	10.242696	6.632879	1.873663
H	13.910501	3.713423	2.100861
H	11.904871	-5.578182	2.322738
H	11.071760	0.077814	2.678645
H	12.203542	5.353618	2.637217
H	-12.143425	-4.703146	2.610401
H	-10.520964	0.159923	2.424889

H	-13.839356	-3.054976	2.140052
C	-12.140127	-4.981751	1.563696
H	-10.407035	-6.247164	1.785969
H	-13.173307	4.572816	1.805435
C	-10.679049	0.137824	1.355037
O	-10.694061	-2.212415	1.239259
C	-14.254829	-3.587171	1.277570
C	-11.462384	5.777150	1.249450
O	-10.810736	2.479409	1.157771
C	-15.356339	-4.535363	1.797665
C	-11.136280	-5.847274	1.094197
C	-13.130043	-4.421441	0.699081
C	-12.655069	5.044621	0.979691
C	-10.779519	-1.073231	0.677401
C	-14.833492	-2.549787	0.310341
C	-10.832375	1.319472	0.635589
Ru	-11.012086	-3.891568	0.003662
C	-10.720590	6.356099	0.203738
H	-14.568092	3.414221	0.234313
C	-11.049429	-6.169777	-0.291059
Ru	-10.977798	4.114690	-0.169727
C	-15.608656	5.173030	-0.420825
C	-13.143075	4.864248	-0.326479
C	-12.984976	-4.695181	-0.672854
C	-11.006997	-1.104283	-0.819386
C	-14.460615	4.152743	-0.566916
C	-11.044568	1.287445	-0.863543
C	-11.167127	6.126654	-1.131811
C	-11.962554	-5.555332	-1.168347
O	-11.098929	-2.264719	-1.333737
H	-13.631052	-4.203719	-1.387221
O	-11.167545	2.424669	-1.420753
C	-11.104516	0.077049	-1.547384
C	-12.335339	5.386803	-1.384081
H	-10.582277	6.498781	-1.962564
C	-14.545738	3.417908	-1.909350
H	-11.883421	-5.726666	-2.233532
H	-11.260239	0.054262	-2.617610
H	-12.605705	5.179634	-2.410302
H	6.552574	3.154541	2.973062
H	8.893364	3.844747	2.595295
H	3.193021	5.048729	-6.513590

H	3.363394	5.228326	-4.766827
C	6.914450	3.281436	1.960139
C	8.226646	3.677964	1.760365
H	4.591237	2.134139	2.100475
H	2.041588	6.039716	-5.612246
C	2.638482	5.126857	-5.577474
N	8.751921	3.827996	0.533245
C	6.093232	3.017120	0.866460
C	4.714410	2.410711	1.052994
H	4.673797	1.493212	0.458824
O	3.686531	2.866757	-1.534549
H	2.613147	3.477541	-2.913265
C	1.741377	3.890665	-5.391984
H	2.356576	2.983901	-5.395059
C	7.950170	3.626623	-0.530057
C	6.631908	3.231402	-0.403438
N	3.575751	3.249116	0.711387
C	3.063147	3.246810	-0.535569
H	1.050330	3.806044	-6.231215
N	1.631857	3.758587	-2.947375
H	2.995048	3.570705	1.507812
C	0.936398	3.929608	-4.125796
H	8.404604	3.748716	-1.503607
H	6.028701	3.058205	-1.284877
N	1.746900	3.705000	-0.604485
C	0.998169	3.825104	-1.750867
C	-0.396627	4.141139	-4.054526
H	1.208609	3.807599	0.271035
O	2.165379	3.965947	2.985104
H	-0.989526	4.283024	-4.946304
N	-0.292378	4.008439	-1.629009
C	-1.068176	4.139962	-2.771847
C	0.932315	3.860220	3.068766
N	0.161126	3.834373	1.915516
O	-2.300961	4.234055	-2.672041
H	-1.330943	3.805736	-0.001711
H	0.845063	3.800950	5.246436
C	0.255644	3.742972	4.343006
C	-1.130180	3.640648	2.014372
N	-1.873406	3.623027	0.857987
H	-3.111208	3.667150	-1.266905
H	-2.171254	5.488987	6.074985

C	-1.077755	3.527162	4.389257
N	-1.768913	3.466256	3.197219
N	-3.687942	3.260346	-0.507794
C	-3.185534	3.162712	0.740135
H	-4.644659	2.210219	-1.989122
C	-2.773879	4.588099	5.950131
H	-3.497087	4.773219	5.153169
H	-2.750191	3.190217	3.133953
C	-1.885094	3.370714	5.644719
H	-6.118039	3.151361	1.387999
H	-1.195467	3.199831	6.471871
C	-4.804948	2.431957	-0.933597
O	-3.814849	2.702281	1.700649
H	-3.329806	4.421715	6.873730
H	-4.774654	1.484870	-0.386766
C	-6.728451	3.276006	0.502768
H	-2.505383	2.471722	5.559102
C	-6.195407	3.012187	-0.760275
H	-8.504304	3.803362	1.591172
C	-8.054375	3.646879	0.620358
C	-7.031172	3.203318	-1.858559
H	-6.673475	3.036919	-2.867304
N	-8.868465	3.781611	-0.445085
C	-8.350008	3.582340	-1.668038
H	-9.025767	3.698229	-2.504716
H	6.569772	-4.014608	2.473717
H	8.954091	-3.440047	2.135155
H	3.118042	-2.734081	-6.938354
H	3.398093	-2.458115	-5.219114
C	7.009018	-4.111584	1.485235
C	8.346233	-3.791386	1.310329
H	4.764608	-5.490740	1.642074
H	2.085518	-1.610851	-6.046930
C	2.623316	-2.558576	-5.982281
N	8.970654	-3.933921	0.125313
C	6.263420	-4.601051	0.411437
C	4.862418	-5.158104	0.607594
H	4.758015	-6.034484	-0.036167
O	3.795487	-4.513956	-1.904916
H	2.646201	-4.007878	-3.213470
C	1.659374	-3.715034	-5.671357
H	2.210905	-4.660926	-5.647904

C	8.237241	-4.324510	-0.936181
C	6.899731	-4.663769	-0.831732
N	3.748492	-4.252289	0.358599
C	3.203075	-4.176817	-0.874265
H	0.918365	-3.803498	-6.466229
N	1.673614	-3.689713	-3.220251
H	3.185021	-3.976283	1.182779
C	0.929386	-3.547348	-4.371765
H	8.755122	-4.385230	-1.886103
H	6.357999	-4.997468	-1.709431
N	1.892205	-3.686712	-0.885714
C	1.097620	-3.556033	-2.000877
C	-0.385535	-3.258113	-4.250409
H	1.378626	-3.608538	0.005948
O	2.355453	-3.597454	2.681137
H	-1.014760	-3.137545	-5.120171
N	-0.176781	-3.302078	-1.829367
C	-0.992156	-3.155563	-2.941437
C	1.131853	-3.780368	2.790282
N	0.313242	-3.671288	1.675454
O	-2.209209	-2.955270	-2.795931
H	-1.249708	-3.543493	-0.175148
H	1.148667	-4.187250	4.931023
C	0.518867	-4.118325	4.056135
C	-0.966983	-3.921494	1.797434
N	-1.764342	-3.799453	0.682019
H	-3.073834	-3.567929	-1.372326
H	-1.973242	-2.790878	6.112430
C	-0.803167	-4.391821	4.121601
N	-1.547104	-4.287285	2.965782
N	-3.648426	-4.005356	-0.630337
C	-3.087378	-4.236262	0.576978
H	-4.628319	-4.925642	-2.180717
C	-2.508900	-3.711546	5.873691
H	-3.279313	-3.474772	5.136675
H	-2.526245	-4.575076	2.899341
C	-1.542100	-4.792791	5.363632
H	-5.987169	-4.224766	1.316651
H	-0.807084	-5.027054	6.133996
C	-4.757133	-4.824503	-1.102892
O	-3.681237	-4.783136	1.512960
H	-3.009103	-4.057582	6.778915

H	-4.672548	-5.825150	-0.667111
C	-6.652996	-4.141202	0.467345
H	-2.093840	-5.717465	5.163061
C	-6.168276	-4.338629	-0.827339
H	-8.408402	-3.767878	1.657166
C	-8.001374	-3.897418	0.663216
C	-7.076917	-4.191077	-1.874748
H	-6.760522	-4.295968	-2.905342
N	-8.884158	-3.839996	-0.352537
C	-8.412820	-3.941997	-1.606035
H	-9.136459	-3.838461	-2.403865
C	10.296081	-7.117637	0.715111
H	9.448368	-7.140910	0.029819
H	9.932153	-6.945673	1.727881
H	10.762883	-8.107582	0.694218
H	16.626712	-3.390181	-1.106987
H	15.771055	-4.837457	-1.643556
H	15.988472	-4.526689	0.083537
H	15.054472	-1.790180	-2.344064
H	13.302930	-2.006998	-2.240499
H	14.315627	-3.211809	-3.053447
H	14.042499	2.438311	-0.076497
H	15.602250	2.632394	0.726899
H	15.221056	3.622026	-0.670289
H	14.893934	6.006870	2.270504
H	15.619820	5.818385	0.669320
H	16.141958	4.788944	2.006295
C	9.456284	7.162284	-0.711328
H	8.606926	7.038636	-0.039151
H	9.154572	6.881437	-1.720053
H	9.712518	8.225930	-0.725354
C	-9.488203	7.167069	0.469912
H	-8.732783	7.020795	-0.302206
H	-9.053306	6.935784	1.441830
H	-9.756604	8.227932	0.470424
H	-15.541920	5.950976	-1.185248
H	-15.601479	5.657132	0.557442
H	-16.569226	4.669302	-0.540137
H	-13.707115	2.735554	-2.057848
H	-14.578014	4.113923	-2.751322
H	-15.468692	2.837563	-1.946860
C	-9.999052	-7.115093	-0.790781

H -9.072431 -7.027366 -0.223387
H -9.786647 -6.964639 -1.848635
H -10.362573 -8.140087 -0.668459
H -15.557752 -1.926942 0.836812
H -15.364999 -3.018311 -0.522039
H -14.061328 -1.894761 -0.099934
H -16.146789 -3.957599 2.279023
H -14.970053 -5.248673 2.529145
H -15.804802 -5.101227 0.976972
H -11.116532 5.872087 2.270118

The .xyz file for the rectangle shown in Figure 8(b) and used for the calculations of the interatomic distances shown in the histogram of Fig. 7 is given below.

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Rectangle shrunk
H -12.322633 -3.773888 3.100312
H -10.696681 0.904707 2.045572
C -14.298031 -2.192638 2.015487
H -9.062643 6.608566 0.078944
C -12.129729 -4.345297 2.198212
H -10.332838 -5.232996 3.034372
H -11.436885 6.017489 0.402016
C -10.702644 0.643834 0.992749
O -10.698675 -1.684090 1.391953
C -14.333118 -3.465898 1.155686
C -9.643232 6.259551 -0.768954
O -10.626198 2.887678 0.255312
C -15.421548 -4.445244 1.656802
C -10.967849 -5.162668 2.157206
C -13.011409 -4.212076 1.083807
C -11.012554 5.940017 -0.593520
C -10.733819 -0.694380 0.587760
H -14.590314 -3.175821 0.127418
C -10.647383 1.634890 0.010018
Ru -10.847190 -3.598590 0.531041
C -9.008679 6.087061 -2.040037
C -13.757457 4.702122 -0.158363
C -10.620978 -5.872326 0.970017
Ru -9.990111 4.114153 -1.349361
C -14.059165 6.564267 -1.865523
C -11.832819 5.469260 -1.671369

C	-12.589396	-4.847889	-0.116288
C	-10.812997	-1.057714	-0.885750
C	-13.327796	5.242089	-1.531695
C	-10.561917	1.262088	-1.461629
C	-9.781843	5.535598	-3.091817
C	-11.426872	-5.670891	-0.181952
O	-10.955665	-2.303065	-1.131242
H	-13.152195	-4.672976	-1.029225
O	-10.363407	2.239406	-2.256605
C	-10.691567	-0.070624	-1.867529
C	-11.166773	5.235088	-2.899538
H	-9.316816	5.320135	-4.048434
H	-13.607102	4.501491	-2.294264
H	-11.152885	-6.136329	-1.123156
H	-10.683068	-0.332558	-2.920124
H	-11.711330	4.762910	-3.712488
H	12.505534	-4.086862	-2.727409
H	10.147546	0.485089	-2.618902
H	14.275473	-2.690344	-1.948869
C	12.367538	-4.477609	-1.722834
H	10.625395	-5.642104	-2.303382
H	11.189059	5.690411	-2.266349
C	10.363486	0.486566	-1.555946
O	10.654441	-1.855296	-1.441071
C	14.495258	-3.237615	-1.021518
C	9.448141	6.291487	-1.127324
O	10.105364	2.825473	-1.330663
C	15.664645	-4.207356	-1.312403
C	11.269990	-5.350708	-1.480552
C	13.257830	-4.056078	-0.693234
C	10.815889	5.914426	-1.270697
C	10.647341	-0.706139	-0.884275
C	14.879719	-2.212672	0.056174
C	10.356171	1.679900	-0.827711
Ru	11.072488	-3.500297	-0.190295
C	8.892264	6.516925	0.161374
H	13.261202	4.959401	-1.324658
C	11.003737	-5.826188	-0.165830
Ru	9.842235	4.404753	0.053859
C	13.920052	6.827497	-0.477334
C	11.690877	5.764423	-0.158829
C	12.912480	-4.465502	0.626941

C	10.959067	-0.704652	0.602759
C	13.169114	5.479789	-0.360806
C	10.634361	1.675193	0.667647
C	9.726494	6.283211	1.294457
C	11.819880	-5.339477	0.893595
O	11.218880	-1.848348	1.108155
H	13.468251	-4.068965	1.470265
O	10.562809	2.814545	1.237574
C	10.935438	0.484939	1.335536
C	11.087763	5.906034	1.127319
H	9.315572	6.373378	2.294770
C	13.793915	4.589941	0.724882
H	11.603156	-5.624613	1.917941
H	11.141613	0.483923	2.400417
H	11.666735	5.670790	2.014303
H	-5.903866	0.950306	-1.911475
H	-7.713327	2.481227	-2.671862
H	-2.371354	5.854668	6.312814
H	-2.697440	5.386821	4.635759
C	-6.425626	1.573725	-1.190937
C	-7.419884	2.442903	-1.628591
H	-5.245992	-0.463305	0.120089
H	-1.155128	6.159005	5.057200
C	-1.916246	5.449831	5.403237
N	-8.112952	3.229411	-0.778305
C	-6.135011	1.490223	0.176850
C	-5.163931	0.453606	0.712483
H	-5.414914	0.213961	1.748681
O	-3.787537	1.794159	2.769037
H	-2.490105	2.805406	3.694263
C	-1.288024	4.070785	5.697491
H	-2.061102	3.387433	6.079905
C	-7.768200	3.228002	0.526534
C	-6.791601	2.380102	1.035734
N	-3.777050	0.877969	0.661591
C	-3.213351	1.544470	1.696458
H	-0.532815	4.167420	6.484436
N	-1.485294	2.918080	3.537323
H	-3.346662	0.914015	-0.281198
C	-0.635189	3.459692	4.487432
H	-8.337896	3.880682	1.178250
H	-6.572533	2.389139	2.099022

N	-1.879937	1.888550	1.456498
C	-0.994396	2.394497	2.381747
C	0.701005	3.439380	4.235136
H	-1.458741	1.609215	0.554449
O	-2.959909	0.963855	-1.994062
H	1.412468	3.847611	4.943385
N	0.285561	2.355224	2.088270
C	1.210751	2.849704	3.005030
C	-1.742385	0.921440	-2.271988
N	-0.802625	1.138698	-1.270505
O	2.428339	2.766029	2.756137
H	0.972139	1.572597	0.348521
H	-1.986323	0.503276	-4.405488
C	-1.259356	0.652706	-3.616435
C	0.478257	1.031710	-1.554685
N	1.384037	1.261140	-0.545529
H	2.898093	1.723233	1.357180
H	0.700890	2.353547	-5.917258
C	0.073849	0.549850	-3.856948
N	0.944150	0.729980	-2.795664
N	3.363996	1.183702	0.607093
C	2.743325	0.922463	-0.559697
H	4.663501	0.302285	1.943255
C	1.404383	1.524193	-5.790430
H	2.225590	1.871041	-5.152505
H	1.953999	0.578706	-2.869358
C	0.698696	0.288984	-5.199898
H	5.575078	1.847147	-1.417962
H	-0.088503	-0.049937	-5.880595
C	4.681861	0.664746	0.910774
O	3.295638	0.409016	-1.553506
H	1.823800	1.282751	-6.772134
H	4.873669	-0.191437	0.256122
C	6.131875	2.164429	-0.540886
H	1.415906	-0.538828	-5.108864
C	5.791321	1.683350	0.731309
H	7.536728	3.367031	-1.658096
C	7.216135	3.020666	-0.682040
C	6.533808	2.151341	1.820008
H	6.296263	1.838636	2.832491
N	7.963308	3.419279	0.371333
C	7.607741	3.010124	1.605073

H	8.228325	3.351869	2.426044
H	-6.550438	-4.162308	-2.294804
H	-8.974980	-3.840495	-1.850805
H	-2.740390	-0.323209	6.700762
H	-2.968668	-0.175450	4.947418
C	-6.882829	-3.907859	-1.292044
C	-8.245593	-3.739941	-1.054456
H	-4.373725	-4.558745	-1.460514
H	-1.596518	0.630109	5.734359
C	-2.215062	-0.275304	5.739621
N	-8.732618	-3.463027	0.171410
C	-5.966489	-3.784434	-0.240812
C	-4.500750	-4.153343	-0.448009
H	-4.261050	-4.961408	0.261290
O	-3.478443	-3.082844	1.975592
H	-2.359772	-2.217684	3.214987
C	-1.338781	-1.531134	5.559782
H	-1.964779	-2.429238	5.660382
C	-7.855330	-3.276476	1.181405
C	-6.481295	-3.427165	1.016128
N	-3.506188	-3.082824	-0.316480
C	-2.926904	-2.841497	0.889519
H	-0.594497	-1.581068	6.360812
N	-1.388858	-1.900513	3.129455
H	-2.977638	-2.864850	-1.179803
C	-0.617111	-1.587465	4.236834
H	-8.282555	-3.021074	2.145621
H	-5.814008	-3.302070	1.863430
N	-1.639480	-2.298663	0.813285
C	-0.829020	-2.005563	1.891735
C	0.712313	-1.362322	4.043000
H	-1.129480	-2.363005	-0.082804
O	-2.164155	-2.813415	-2.640416
H	1.366442	-1.119954	4.873328
N	0.453692	-1.833107	1.659247
C	1.301227	-1.537460	2.721126
C	-0.941421	-3.040856	-2.762992
N	-0.097589	-2.779585	-1.687166
O	2.531224	-1.528792	2.518776
H	1.466614	-2.427326	0.115612
H	-1.007486	-3.822896	-4.811256
C	-0.362060	-3.640937	-3.959212

C	1.159221	-3.161291	-1.751731
N	1.958386	-2.905535	-0.656128
H	3.311330	-2.400586	1.356367
H	1.918531	-2.973302	-6.413222
C	0.941764	-4.034529	-3.967492
N	1.701803	-3.779558	-2.837941
N	3.801059	-3.070122	0.743460
C	3.216893	-3.466359	-0.416839
H	4.710751	-3.773829	2.456969
C	2.529553	-3.758974	-5.946586
H	3.305295	-3.274769	-5.336786
H	2.645960	-4.160554	-2.716237
C	1.649055	-4.717089	-5.110887
H	5.960116	-3.509551	-1.154917
H	0.895414	-5.184996	-5.755014
C	4.822767	-3.902680	1.373699
O	3.748616	-4.263996	-1.204544
H	3.033062	-4.315500	-6.744917
H	4.614100	-4.960442	1.150032
C	6.683090	-3.493995	-0.347058
H	2.273233	-5.533977	-4.714083
C	6.268199	-3.635764	0.985024
H	8.390904	-3.283933	-1.658308
C	8.039294	-3.384724	-0.637233
C	7.263541	-3.613352	1.970336
H	7.010574	-3.697760	3.023599
N	8.991487	-3.411058	0.319712
C	8.602116	-3.497486	1.606979
H	9.389237	-3.472372	2.353042
C	-9.414850	-6.768554	0.929715
H	-8.634348	-6.434872	1.620245
H	-8.991944	-6.841532	-0.076716
H	-9.716884	-7.780445	1.236313
H	-16.398935	-3.950869	1.652849
H	-15.214387	-4.771906	2.684600
H	-15.493784	-5.337595	1.024646
H	-15.256881	-1.671610	1.931426
H	-13.508171	-1.503733	1.698390
H	-14.151366	-2.415700	3.079130
H	-13.198773	3.803483	0.123655
H	-14.821869	4.448338	-0.184261
H	-13.630061	5.448619	0.635200

H -13.805865 6.931779 -2.866525
H -13.807049 7.349033 -1.139855
H -15.142775 6.409461 -1.828002
C -7.560120 6.442255 -2.236111
H -7.099620 5.850725 -3.033346
H -6.978778 6.308621 -1.318456
H -7.490346 7.502098 -2.522976
C 7.459828 6.945472 0.328564
H 7.025781 6.569584 1.260230
H 6.834680 6.618431 -0.508350
H 7.422523 8.044893 0.364201
H 13.853785 7.397169 0.459031
H 13.519717 7.452078 -1.284281
H 14.980002 6.647309 -0.686056
H 13.237953 3.655979 0.862400
H 13.851144 5.101135 1.693847
H 14.820282 4.335899 0.441074
C 9.868481 -6.775574 0.099888
H 9.051017 -6.645877 -0.616289
H 9.472215 -6.667011 1.113996
H 10.239124 -7.806229 -0.002338
H 15.711949 -1.599536 -0.304122
H 15.218817 -2.693524 0.981449
H 14.048470 -1.543555 0.302930
H 16.551014 -3.642343 -1.621110
H 15.420997 -4.913828 -2.113850
H 15.929327 -4.786097 -0.417901
H 8.823804 6.389437 -2.009646

The .xyz file for the rectangle shown in Figure 8(c) and used for the calculations of the interatomic distances shown in the histogram of Fig. 7 is given below.

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Shrunk rectangle with counterions
H -12.695085 -2.092225 2.191603
H -9.651601 1.819436 1.524797
C -13.929269 -0.190395 0.620056
H -6.297168 6.832630 -0.149268
C -12.476528 -2.773343 1.380828
H -11.348659 -4.096797 2.656987
H -8.749952 6.897929 -0.319301
C -9.536201 1.510441 0.494335

O	-10.127746	-0.723031	0.942069
C	-14.084861	-1.495973	-0.165803
C	-6.772289	6.577888	-1.087049
O	-8.853917	3.643991	-0.239911
C	-15.445912	-2.163036	0.125290
C	-11.671554	-3.899274	1.644334
C	-13.004994	-2.521862	0.095862
C	-8.169837	6.643284	-1.195512
C	-9.800292	0.192925	0.122996
H	-14.046323	-1.256555	-1.233793
C	-9.102425	2.417793	-0.469454
Ru	-10.693160	-2.586579	0.081891
C	-5.970588	6.317417	-2.226032
C	-11.200147	6.331040	-1.476556
C	-11.429167	-4.854766	0.633828
Ru	-7.603040	4.582540	-1.712350
C	-10.390653	8.229354	-2.960780
C	-8.829373	6.398731	-2.429143
C	-12.504655	-3.332072	-0.946268
C	-9.702937	-0.225533	-1.328890
C	-10.288763	6.721997	-2.644496
C	-8.855208	1.953689	-1.891063
C	-6.625679	5.790645	-3.352262
C	-11.696005	-4.459402	-0.693341
O	-10.065826	-1.417833	-1.587117
H	-12.754356	-3.084413	-1.970476
O	-8.318578	2.810446	-2.661420
C	-9.204317	0.661150	-2.279826
C	-8.033944	5.879480	-3.464463
H	-6.044326	5.436195	-4.191986
H	-10.611546	6.165820	-3.530589
H	-11.391532	-5.093904	-1.514082
H	-9.068374	0.343678	-3.305327
H	-8.510359	5.536899	-4.374199
H	11.568403	-2.425922	-3.720754
H	8.316690	1.239519	-2.642232
H	13.267187	-0.981354	-2.966517
C	11.657270	-3.016054	-2.817431
H	10.168201	-4.445746	-3.461865
H	8.545505	6.672133	-1.628056
C	8.736514	1.191749	-1.646090
O	9.360874	-1.066458	-1.860423

C	13.645653	-1.587492	-2.136534
C	6.809105	6.602182	-0.346631
O	8.202047	3.430129	-1.140183
C	14.918221	-2.315580	-2.618440
C	10.827652	-4.150233	-2.657867
C	12.595862	-2.635309	-1.841842
C	8.201165	6.628728	-0.602450
C	9.314086	0.010618	-1.185226
C	13.955576	-0.649742	-0.965242
C	8.695290	2.305921	-0.810646
Ru	10.449752	-2.670967	-0.986134
C	6.331182	6.640830	0.975167
H	10.779994	6.697335	-0.893442
C	10.992818	-4.993263	-1.544757
Ru	7.791625	4.752625	0.501186
C	10.861687	8.382672	0.441365
C	9.148345	6.608643	0.437956
C	12.518451	-3.323325	-0.603933
C	9.923862	-0.053402	0.199373
C	10.609300	6.884534	0.171843
C	9.232700	2.215492	0.604185
C	7.262022	6.331503	1.997900
C	11.709497	-4.461888	-0.445163
O	10.473138	-1.157673	0.513309
H	13.100664	-2.976715	0.238700
O	9.079388	3.256313	1.317511
C	9.839579	1.043848	1.052961
C	8.642237	6.353293	1.738023
H	6.912424	6.187020	3.010920
C	11.571893	6.001056	0.971650
H	11.727796	-5.001554	0.491876
H	10.237138	0.985397	2.057578
H	9.328085	6.165480	2.552224
H	-5.129970	0.109375	-1.122269
H	-5.847514	2.107974	-2.401047
H	-1.238247	5.184175	6.201424
H	-1.723320	4.462440	4.666815
C	-5.432116	1.007137	-0.600331
C	-5.804171	2.125202	-1.321186
H	-5.565280	-1.062775	1.156873
H	-0.073349	5.058259	4.878514
C	-0.900588	4.552141	5.378783

N	-6.208967	3.260633	-0.728536
C	-5.466812	1.050302	0.791601
C	-5.123790	-0.173822	1.606031
H	-5.497220	-0.080214	2.623873
O	-3.411140	0.994425	3.458505
H	-1.941787	1.786007	4.182280
C	-0.458689	3.180232	5.914879
H	-1.291705	2.705915	6.444317
C	-6.139126	3.338853	0.610730
C	-5.775047	2.263371	1.398618
N	-3.679847	-0.370937	1.648061
C	-2.942814	0.367686	2.502254
H	0.345901	3.308735	6.640212
N	-0.934143	1.690709	4.026247
H	-3.270662	-0.670442	0.750011
C	0.027760	2.259136	4.834211
H	-6.452284	4.273964	1.052024
H	-5.767212	2.363270	2.476032
N	-1.576908	0.327754	2.230104
C	-0.581359	0.883014	2.996126
C	1.323246	1.975450	4.579651
H	-1.268647	-0.147794	1.371549
O	-3.053523	-1.023520	-1.053919
H	2.116743	2.389885	5.184875
N	0.654521	0.594496	2.689400
C	1.681537	1.094001	3.483489
C	-1.878364	-1.022902	-1.445826
N	-0.857096	-0.813830	-0.531544
O	2.850410	0.783374	3.238204
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H	1.242900	-2.342402	5.675168
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C	0.908460	-5.700331	-3.132031
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H	5.431958	-4.037200	-0.813122
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C	6.264567	-4.221721	1.168715
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C	8.566929	-3.525877	1.269756
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H	-10.118402	8.825472	-2.086537
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C	4.876403	6.806809	1.276729
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