

Supporting Information

Host-guest complexes vs supramolecular polymers in chalcogen bonding receptors: experimental and theoretical study

Encarnación Navarro-García^a, Bartomeu Galmés^b, José Luis Esquivel^a, María D. Velasco^a, Adolfo Bastida^c, Fabiola Zapata^a, Antonio Caballero^{a*} and Antonio Frontera^{*b}

^a Departamento de Química Orgánica, Universidad de Murcia, Campus de Espinardo, 30100 Murcia, Spain. E-mail: antocaba@um.es

^b Department of Chemistry, Universitat de les Illes Balears, Crta. de Valldemossa km 7.5, 07122 Palma de Mallorca, Spain E-mail toni.frontera@uib.es

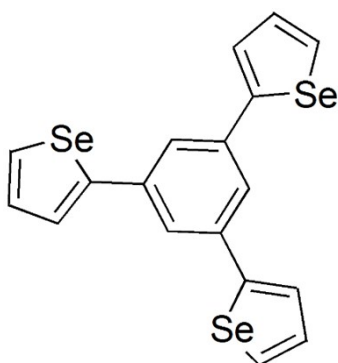
^c Departamento de Química Física, Universidad de Murcia, Campus de Espinardo, 30100 Murcia, Spain

Contents

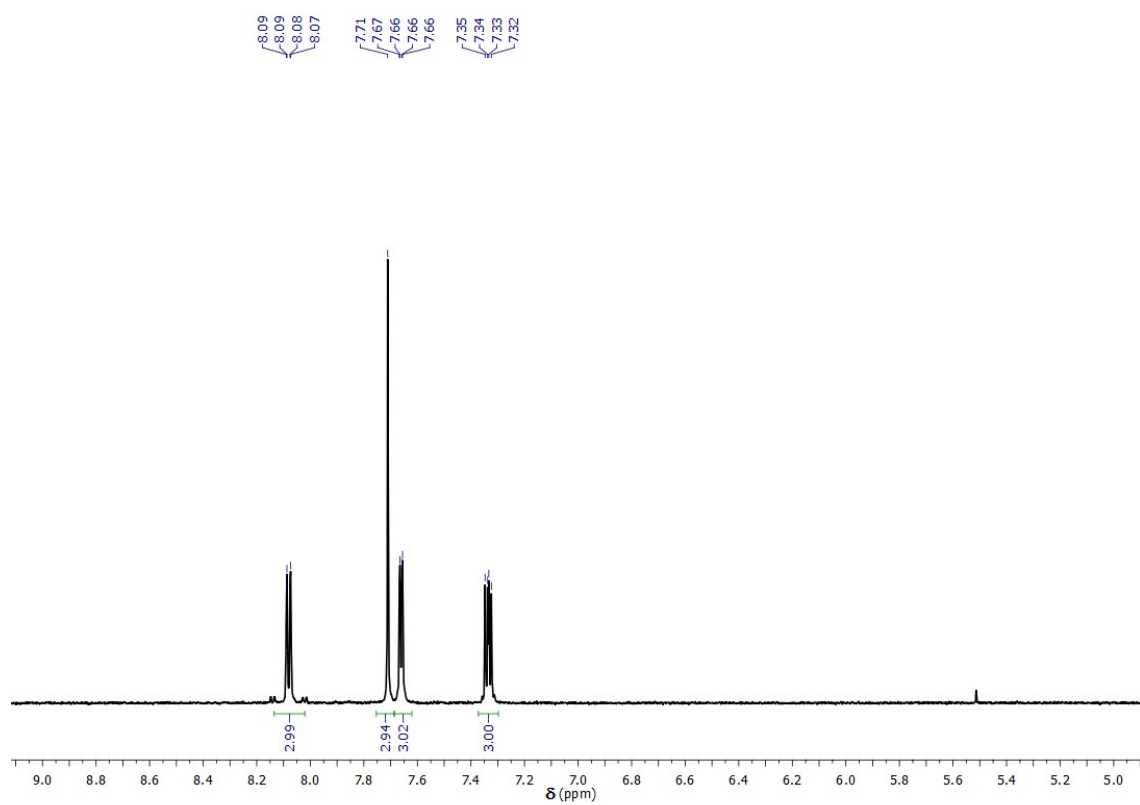
PART I: ¹H NMR, ¹³C NMR and ⁷⁷Se RMN spectra.	S2
PART II: ¹H NMR and ⁷⁷Se RMN Anion Binding Studies.	S6
PART III: Thermodynamic model.	S8
PART IV: Computational Results.	S10

PART I: ^1H NMR, ^{13}C NMR and ^{77}Se RMN spectra.

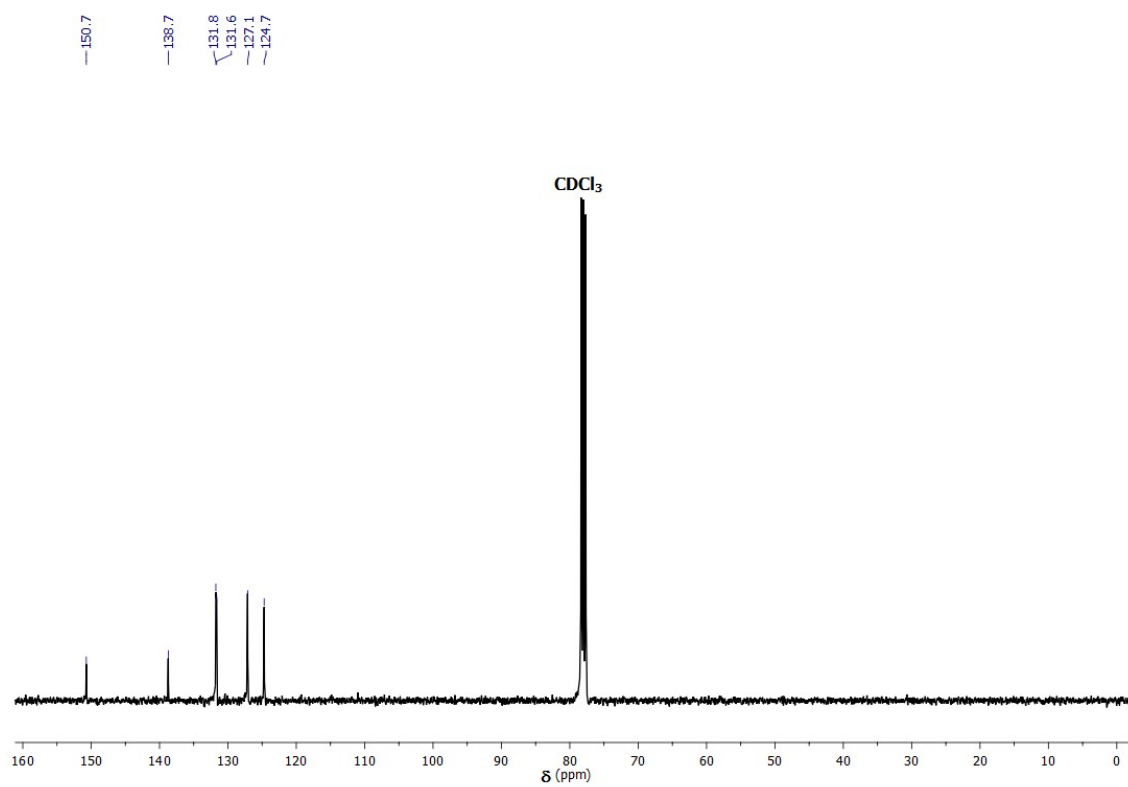
1,3,5-tri(selenophen-2-yl)benzene (2).



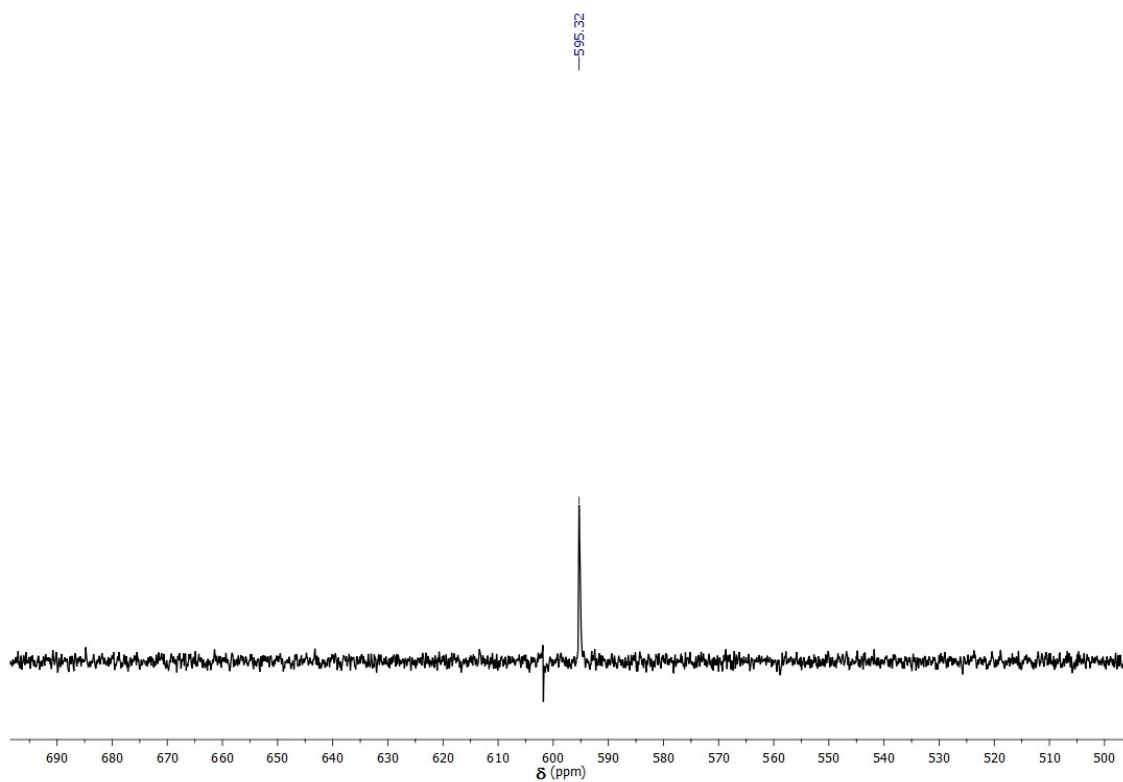
^1H NMR



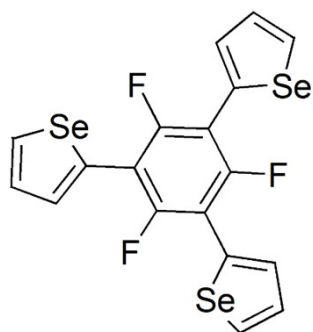
¹³C NMR



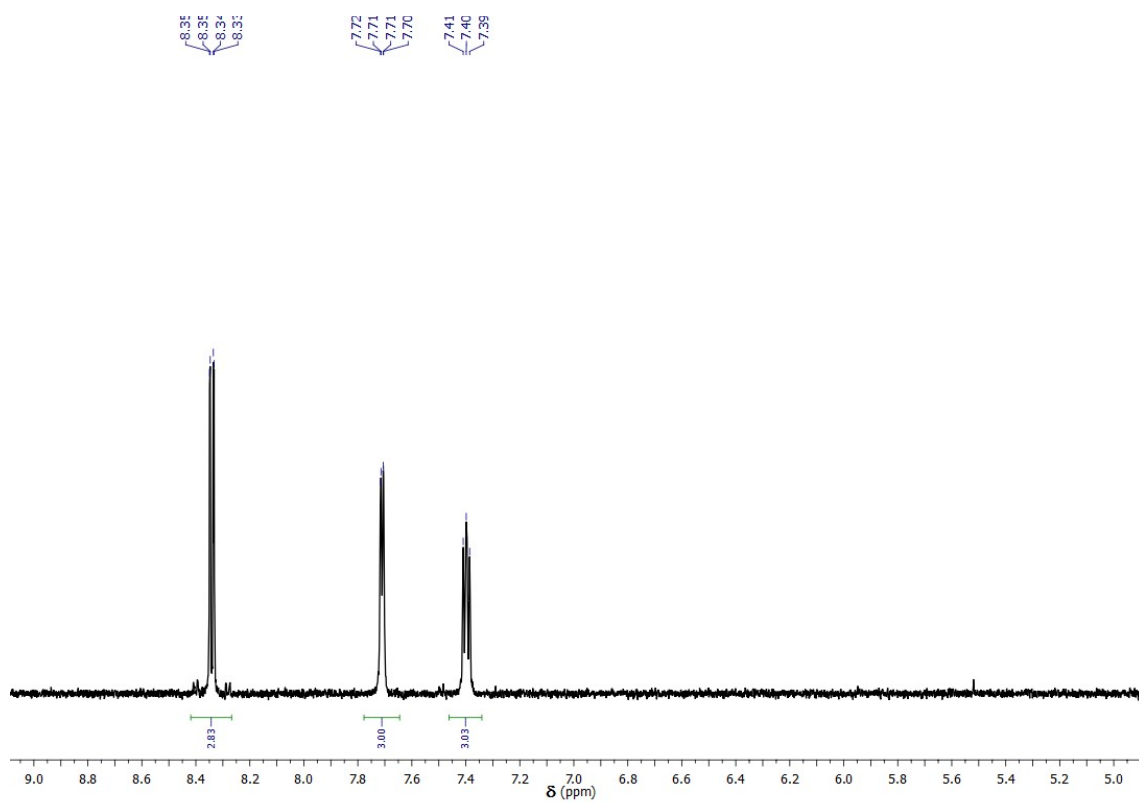
⁷⁷Se NMR



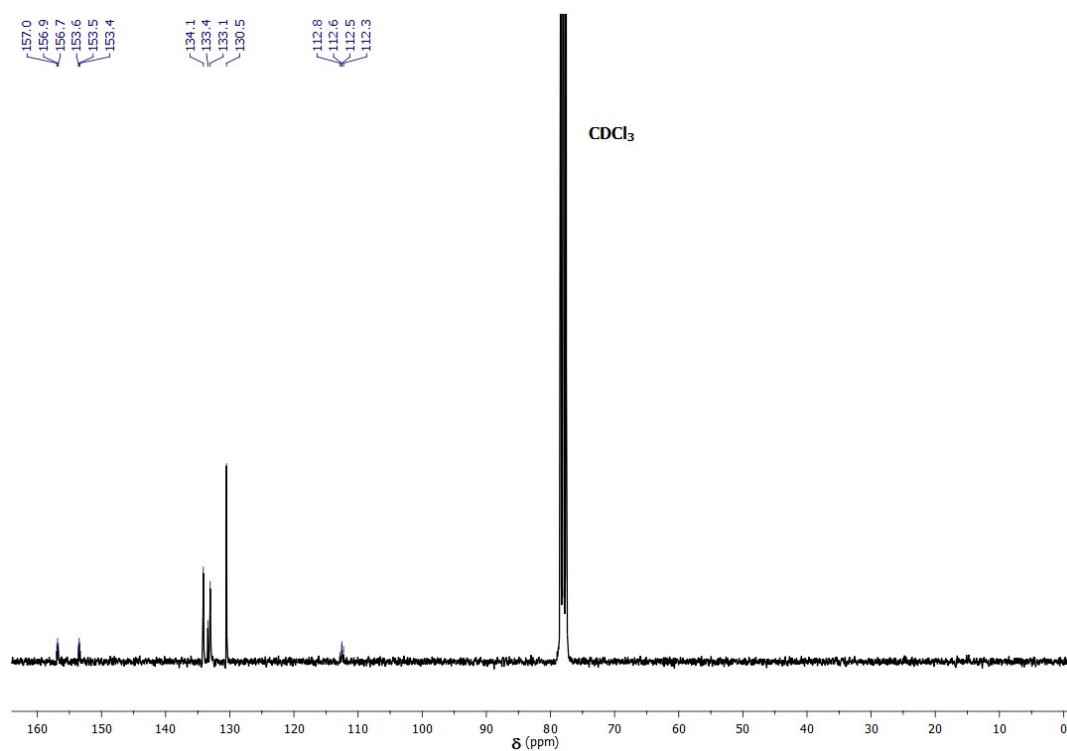
1,3,5-tri(selenophen-2-yl)perfluorobenzene (3).



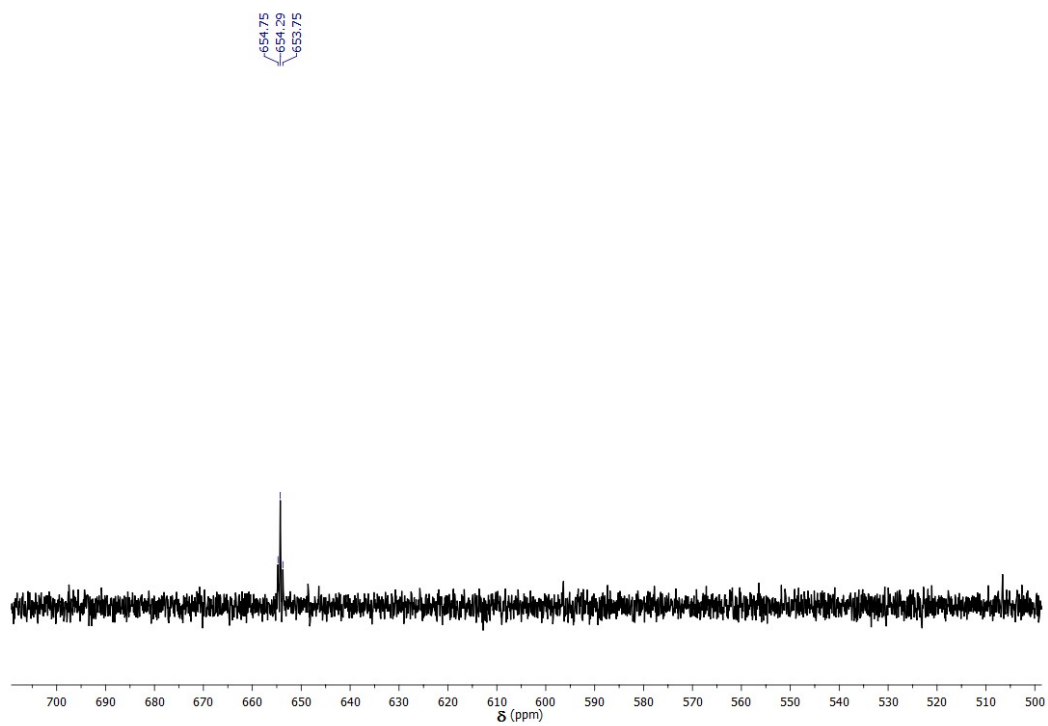
^1H NMR



¹³C NMR



⁷⁷Se NMR



PART II: ^1H NMR Anion Binding Studies.

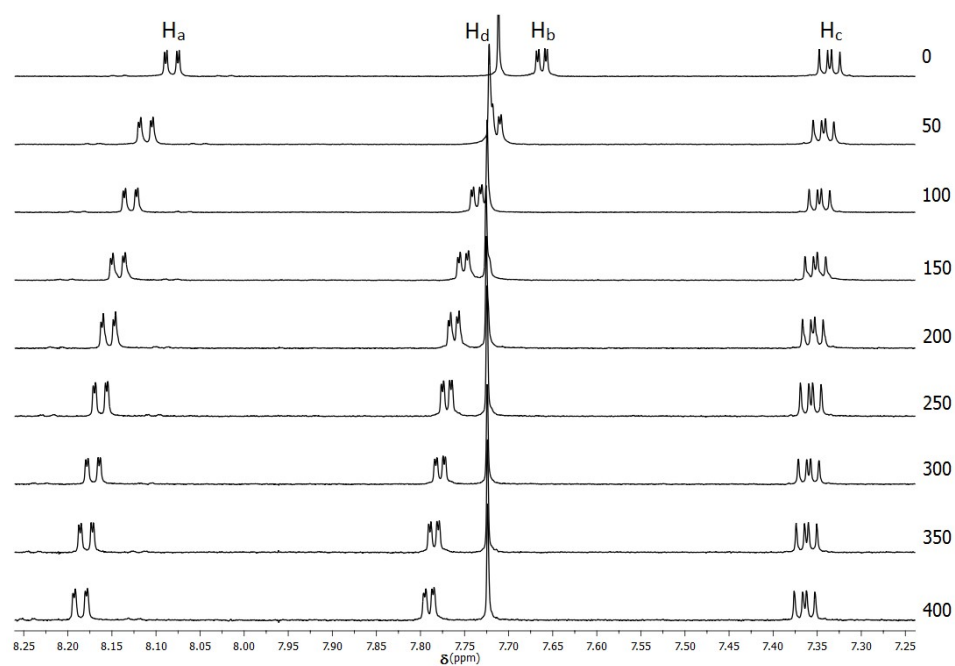


Figure S11 Changes in the ^1H NMR of the receptor **2** ($c = 2.5 \times 10^{-3} \text{ M}$ in tetrahydrofuran- d_8) with the addition of increasing amounts of Cl^- anion.

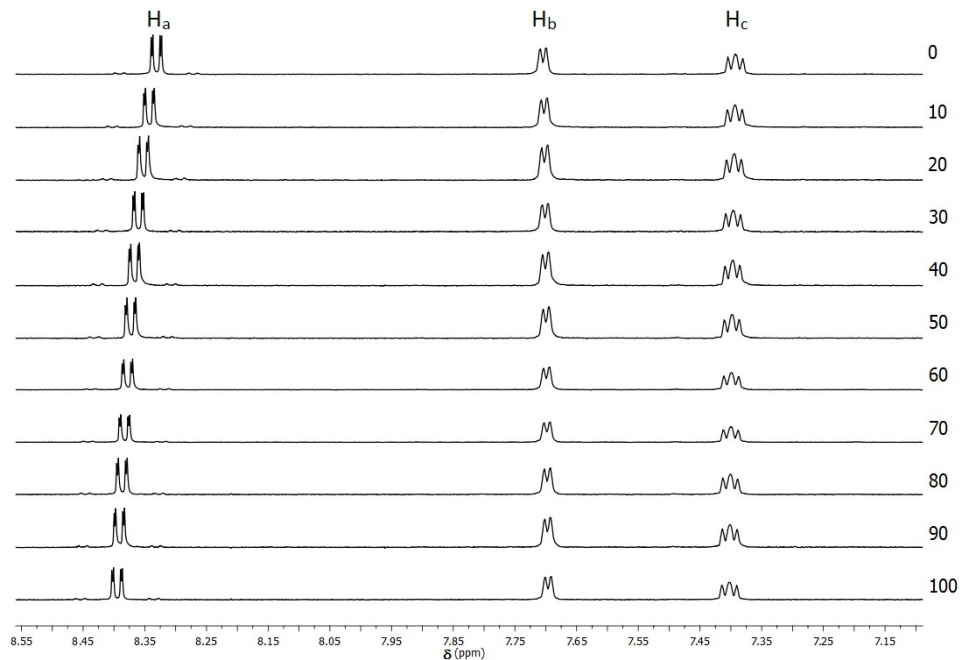


Figure S12 Changes in the ^1H NMR of the receptor **3** ($c = 2.5 \times 10^{-3} \text{ M}$ in tetrahydrofuran- d_8) with the addition of increasing amounts of Cl^- anion.

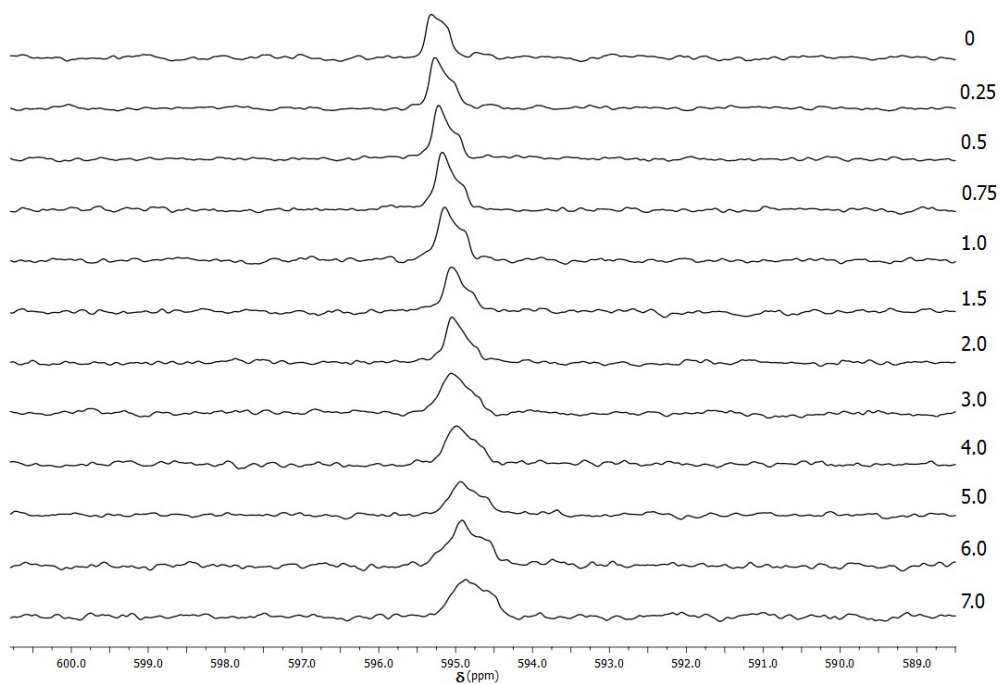


Figure S13 Changes in the ^{77}Se NMR of the receptor **2** ($c = 0.05$ M in tetrahydrofuran- d_8) with the addition of increasing amounts of Cl^- anion.

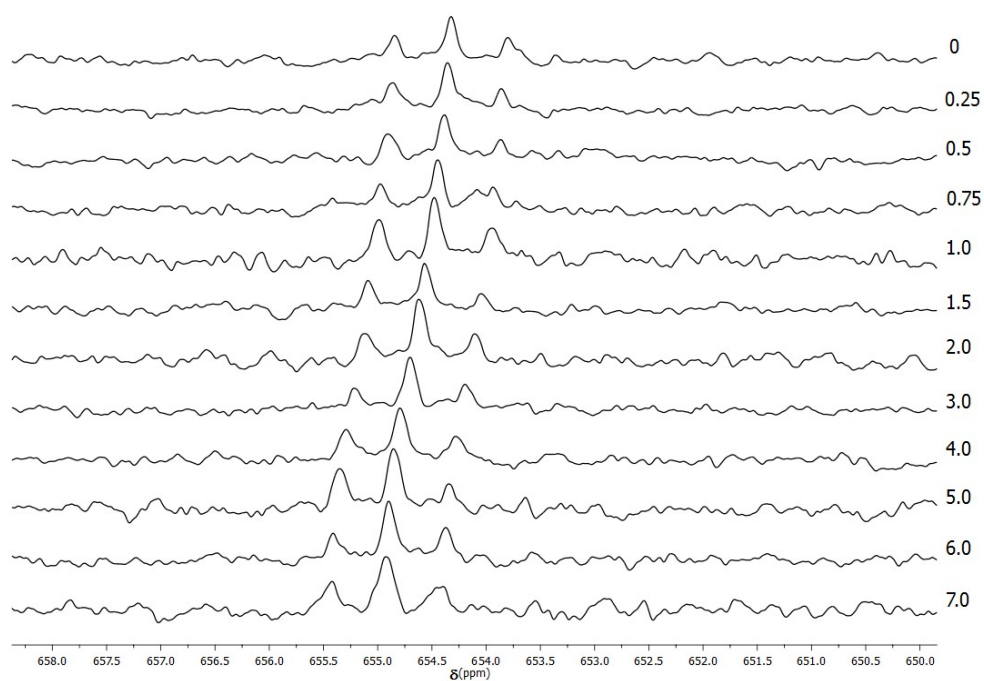


Figure S14 Changes in the ^{77}Se NMR of the receptor **3** ($c = 0.05$ M in tetrahydrofuran- d_8) with the addition of increasing amounts of Cl^- anion.

PART III: Thermodynamic model.

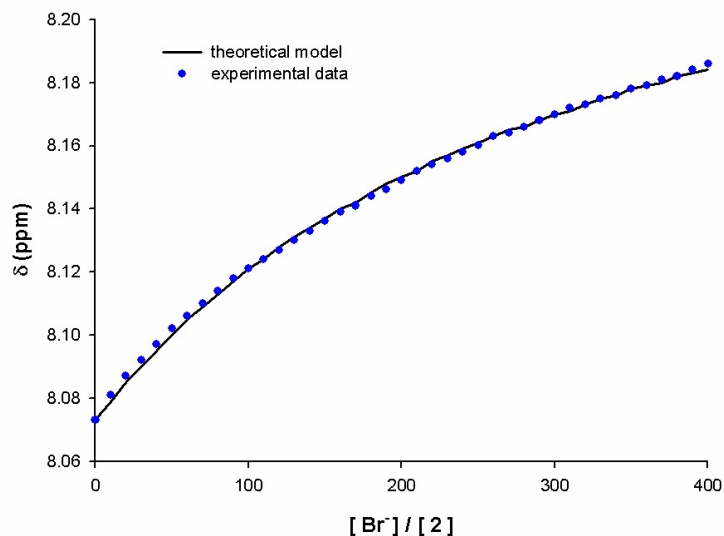


Figure SI5 Changes in the chemical shift of the H_a proton of the receptor **2** upon addition of increasing amounts of Br^- anions. Points represent experimental data, and continuous lines represent fitted curves

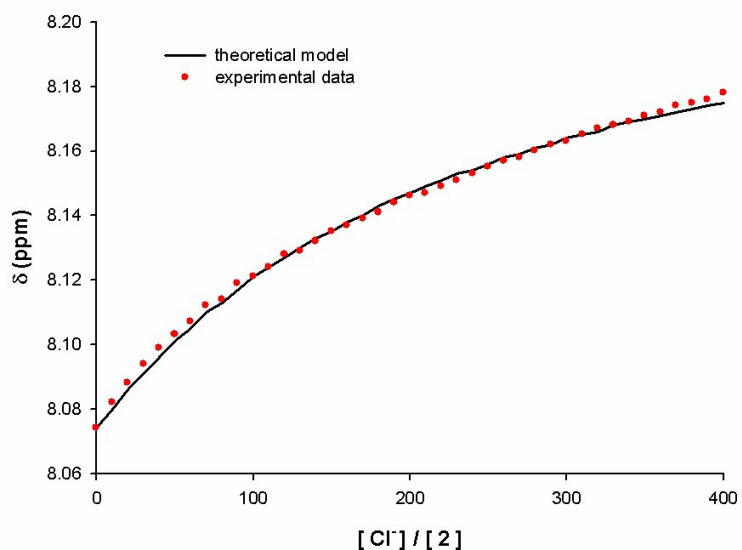


Figure SI6 Changes in the chemical shift of the H_a proton of the receptor **2** upon addition of increasing amounts of Cl^- anions. Points represent experimental data, and continuous lines represent fitted curves

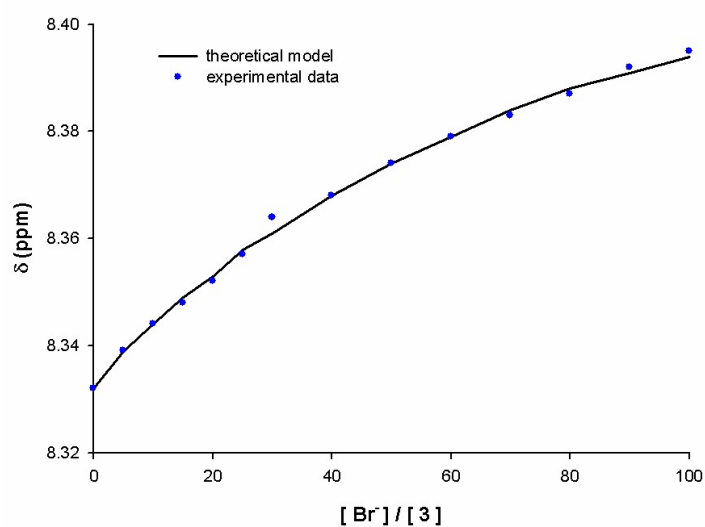


Figure SI7 Changes in the chemical shift of the H_a proton of the receptor **3** upon addition of increasing amounts of Br⁻ anions. Points represent experimental data, and continuous lines represent fitted curves

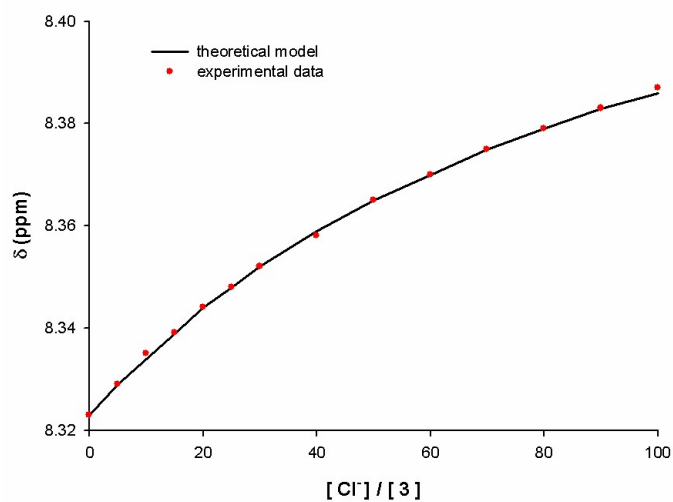


Figure SI8 Changes in the chemical shift of the H_a proton of the receptor **3** upon addition of increasing amounts of Cl⁻ anions. Points represent experimental data, and continuous lines represent fitted curves

PART IV: Computational Results.

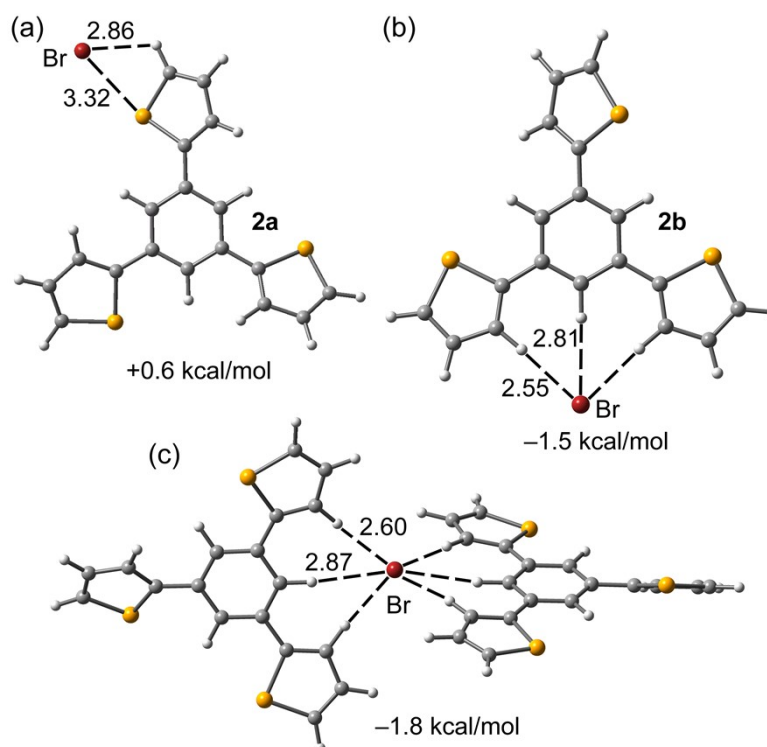


Figure S19 PBE0-D3/def2-TZVP optimized geometries of bromide complexes with receptor **2**. Binding energies are given using THF as solvent.

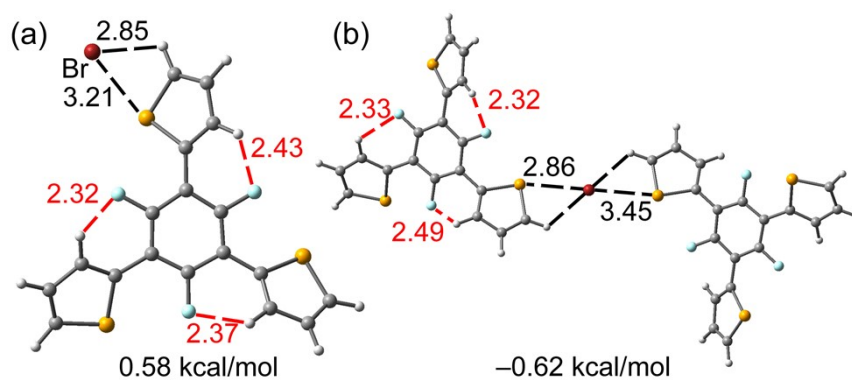


Figure S110 PBE0-D3/def2-TZVP optimized geometries of bromide complexes with receptor **3**. Binding energies are given using THF as solvent.

Cartesian Coordinates

Cl@2a

C	0.0788721	0.4803882	1.3167803
C	0.0900593	1.2317034	0.1363288
C	0.0953162	0.5333161	-1.0738556
C	0.0714251	-0.8590110	-1.1204493
C	0.0495038	-1.5759720	0.0738917
C	0.0512875	-0.9105921	1.2994103
C	0.0676475	-1.5405118	-2.4130708
C	-0.3387315	-1.0533672	-3.6213990
C	-0.2191666	-1.9437028	-4.7203083
H	-0.7412413	-0.0533687	-3.7260557
C	0.2860656	-3.1665727	-4.4169950
H	-0.5118391	-1.6673303	-5.7261952
H	0.4635606	-3.9928892	-5.0885724
C	0.0963074	2.6866858	0.1662870
C	-0.3019834	3.4760758	1.2130138
C	-0.2111805	4.8696193	0.9733345
H	-0.6955395	3.0741801	2.1419165
C	0.2537601	5.2063858	-0.2610678
H	-0.4986965	5.6120009	1.7097014
H	0.4204545	6.1751800	-0.7089845
C	0.0169007	-1.6844545	2.5386014
C	-0.5443002	-2.9106317	2.7515618
C	-0.4196610	-3.4290729	4.0673104
H	-1.0769057	-3.4331330	1.9660543
C	0.2475321	-2.6280196	4.9376365
H	-0.8345802	-4.3868536	4.3589668
H	0.4534674	-2.8155491	5.9807001
Cl	1.2546723	5.8892258	-3.2741359
Se	0.8106144	-1.0661386	4.1164454
Se	0.6511380	3.7453714	-1.3099509
Se	0.6848381	-3.2983378	-2.6127958
H	0.0849930	0.9991749	2.2689437
H	0.1271120	1.0963087	-1.9990066
H	0.0382979	-2.6601077	0.0559579

Cl@2b

C	-0.1774261	0.1935782	1.0862886
C	-0.2460965	1.1902779	0.1098076
C	0.0092855	0.8547198	-1.2196665
C	0.3096311	-0.4544151	-1.5864156
C	0.3756812	-1.4315134	-0.5977311
C	0.1391970	-1.1229114	0.7422201
C	0.5490076	-0.7772688	-2.9901635
C	0.0095195	-0.1864229	-4.0962934
C	0.4329024	-0.7091435	-5.3467182
H	-0.7187702	0.6110436	-4.0105939
C	1.3241738	-1.7309097	-5.2701285
H	0.0634582	-0.3294836	-6.2922977
H	1.7700568	-2.2790290	-6.0863325
C	-0.5772832	2.5599458	0.4942304
C	-0.6186136	3.0930170	1.7493025
C	-0.9927210	4.4617173	1.8116153
H	-0.3897059	2.5123044	2.6497323
C	-1.2620980	5.0530665	0.6195853
H	-1.0581962	4.9903720	2.7554172
H	-1.5639284	6.0741596	0.4386107
C	0.1990060	-2.1493267	1.7800602
C	0.1701774	-1.9737775	3.1328632
C	0.2348732	-3.1677898	3.8985293
H	0.1032418	-0.9866336	3.6034852
C	0.3143897	-4.3201407	3.1851707
H	0.2201808	-3.1494512	4.9818383
H	0.3713670	-5.3305806	3.5622692
Se	1.7318013	-2.1331891	-3.5078767
Se	-1.0566576	3.8582318	-0.7823077

Se	0.3132220	-3.9819967	1.3630785
H	0.5993011	-2.4549904	-0.8843779
H	0.0129788	1.6271600	-1.9810647
H	-0.3743145	0.4467643	2.1273708
Cl	-0.2176412	1.1426153	4.5604926

Cl@2b)₂

C	-0.0281812	-0.7292339	-3.6289921
C	-0.0844435	0.2543021	-4.6190090
C	0.1879572	-0.1016021	-5.9393822
C	0.4969060	-1.4149328	-6.2829520
C	0.5564779	-2.3756976	-5.2783893
C	0.3016572	-2.0483634	-3.9463271
C	0.7584613	-1.7543745	-7.6789069
C	0.2393333	-1.1699498	-8.7979232
C	0.6857034	-1.6998760	-10.0370056
H	-0.4886009	-0.3703769	-8.7313087
C	1.5746054	-2.7215676	-9.9366765
H	0.3359889	-1.3246117	-10.9916770
H	2.0370343	-3.2741866	-10.7404961
C	-0.4141170	1.6317548	-4.2622264
C	-0.4498990	2.1927334	-3.0190728
C	-0.8145595	3.5641645	-2.9809919
H	-0.2179445	1.6340641	-2.1122414
C	-1.0805046	4.1312805	-4.1852947
H	-0.8746631	4.1129677	-2.0487508
H	-1.3738438	5.1506343	-4.3873603
C	0.3634852	-3.0597258	-2.8940059
C	0.3728481	-2.8667801	-1.5429199
C	0.4381244	-4.0492641	-0.7601578
H	0.3357289	-1.8773300	-1.0864637
C	0.4806570	-5.2109405	-1.4610765
H	0.4524991	-4.0180934	0.3226975
H	0.5317790	-6.2174844	-1.0734425
Se	1.9476740	-3.1151027	-8.1653750
Se	-0.8854311	2.9065617	-5.5615549
Se	0.4354888	-4.8971371	-3.2858053
H	0.7957702	-3.4011109	-5.5438470
H	0.2009705	0.6594008	-6.7118958
H	-0.2453965	-0.4643208	-2.5984485
C	-0.1988670	0.7255844	3.6105107
C	0.9181625	1.2187616	4.2890244
C	0.8185848	1.4660196	5.6578999
C	-0.3606255	1.2136313	6.3533695
C	-1.4620844	0.7302713	5.6542295
C	-1.4002357	0.4871446	4.2816440
C	-0.4199243	1.4589503	7.7919359
C	0.5932046	1.3751578	8.7031077
C	0.2461218	1.6817347	10.0452275
H	1.5897343	1.0643888	8.4131586
C	-1.0549395	2.0190816	10.2382730
H	0.9627855	1.6405660	10.8571053
H	-1.5371335	2.2808065	11.1679320
C	2.1598066	1.4803910	3.5641978
C	2.3780207	1.4230248	2.2180763
C	3.7000052	1.7296034	1.8014276
H	1.5997808	1.1583770	1.5020848
C	4.5694154	2.0363599	2.7974793
H	3.9876519	1.7162081	0.7569064
H	5.6135016	2.2971616	2.7089528
C	-2.5610988	-0.0136372	3.5488689
C	-2.6899484	-0.1983248	2.2025963
C	-3.9486844	-0.6942885	1.7732069
H	-1.8902041	0.0189449	1.4946302
C	-4.8542108	-0.9189980	2.7590255
H	-4.1628797	-0.8781872	0.7271871
H	-5.8624438	-1.2930581	2.6609842
Se	-2.0007285	1.9834835	8.6459534
Se	3.7460103	1.9585677	4.4548169
Se	-4.1543254	-0.4999393	4.4219354
H	-2.3782367	0.5218186	6.1986575
H	1.6593768	1.8932673	6.1933743
H	-0.1304486	0.5205499	2.5462147
Cl	-0.0467088	0.3207755	-0.0727151

Br@2a

C	0.0676953	0.6707584	0.9927465
C	0.0800566	1.4000865	-0.1948199
C	0.0787463	0.7156496	-1.4082426
C	0.0670011	-0.6782993	-1.4367115
C	0.0582268	-1.3813286	-0.2361779
C	0.0471389	-0.7256649	0.9992022
C	0.0613092	-1.3726679	-2.7225746
C	-0.4751838	-0.9516142	-3.9052227
C	-0.3217692	-1.8369079	-5.0044649
H	-1.0090767	-0.0119522	-3.9816467
C	0.3440896	-2.9869072	-4.7248472
H	-0.7148560	-1.6168859	-5.9900780
H	0.5697484	-3.7985152	-5.3999181
C	0.0939869	2.8604791	-0.1500590
C	-0.3192477	3.6778631	0.8617076
C	-0.1787412	5.0709547	0.6290937
H	-0.7424847	3.2829958	1.7770710
C	0.3511671	5.4014669	-0.5760862
H	-0.4746963	5.8147219	1.3591729
H	0.5477096	6.3902194	-0.9621562
C	0.0166672	-1.4755557	2.2467508
C	-0.4083846	-2.7677973	2.4084036
C	-0.3437596	-3.2550295	3.7371789
H	-0.8014800	-3.3646829	1.5913127
C	0.1296143	-2.3628379	4.6495344
H	-0.6551365	-4.2567329	4.0111658
H	0.2802912	-2.4631875	5.7149228
Br	1.2329913	-0.0827993	6.9926701
H	0.0550617	-2.4653963	-0.2557048
H	0.0831205	1.1962271	1.9404077
H	0.0963629	1.2665150	-2.3420336
Se	0.7488912	3.8909092	-1.5711410
Se	0.5677561	-0.7379439	3.8996688
Se	0.8671840	-3.0461403	-2.9491248

Br@2b

C	-0.1811451	0.1916628	1.0802407
C	-0.2479453	1.1891480	0.1045313
C	0.0097276	0.8525655	-1.2242484
C	0.3091732	-0.4567514	-1.5906520
C	0.3729051	-1.4336508	-0.6018409
C	0.1356122	-1.1252458	0.7380987
C	0.5498240	-0.7794658	-2.9943127
C	0.0102253	-0.1880580	-4.1000909
C	0.4337373	-0.7099314	-5.3506635
H	-0.7179330	0.6095352	-4.0142525
C	1.3256473	-1.7310509	-5.2741551
H	0.0640094	-0.3303567	-6.2961505
H	1.7727301	-2.2780323	-6.0903906
C	-0.5799645	2.5598929	0.4846306
C	-0.6166705	3.1000229	1.7364552
C	-0.9930548	4.4675688	1.7967347
H	-0.3820515	2.5299387	2.6386390
C	-1.2683588	5.0525289	0.6032825
H	-1.0547407	4.9987339	2.7392185
H	-1.5722723	6.0723321	0.4191935
C	0.1953499	-2.1539762	1.7733796
C	0.1723306	-1.9841659	3.1269205
C	0.2373477	-3.1792274	3.8902722
H	0.1105631	-1.0031406	3.6049571
C	0.3119647	-4.3288871	3.1722271
H	0.2270699	-3.1622910	4.9736986
H	0.3686847	-5.3409116	3.5448491
Se	1.7331225	-2.1344248	-3.5123680
Se	-1.0673431	3.8520260	-0.7943114
Se	0.3044451	-3.9851017	1.3513931
Br	-0.1963170	1.2164063	4.8184544
H	0.5967253	-2.4571753	-0.8874727
H	0.0164283	1.6250616	-1.9854828
H	-0.3798267	0.4444209	2.1192157

Br@(2b)₂

C	-0.0495485	-0.7416803	-3.8592138
---	------------	------------	------------

C	-0.1024033	0.2306269	-4.8603478
C	0.1831431	-0.1390201	-6.1742647
C	0.4998225	-1.4546954	-6.5010607
C	0.5514924	-2.4046397	-5.4858018
C	0.2847573	-2.0638528	-4.1595374
C	0.7792595	-1.8077056	-7.8902252
C	0.2745263	-1.2350808	-9.0219820
C	0.7393413	-1.7760562	-10.2494465
H	-0.4564549	-0.4368212	-8.9739206
C	1.6278828	-2.7955948	-10.1265903
H	0.4042494	-1.4093501	-11.2126138
H	2.1026832	-3.3548522	-10.9184998
C	-0.4460092	1.6103615	-4.5261202
C	-0.4604224	2.2013290	-3.2969118
C	-0.8487374	3.5665383	-3.2808148
H	-0.1972098	1.6713847	-2.3829281
C	-1.1570381	4.0985861	-4.4908588
H	-0.8935187	4.1365399	-2.3606320
H	-1.4740280	5.1074859	-4.7091913
C	0.3340829	-3.0665599	-3.0984161
C	0.3603188	-2.8616462	-1.7497312
C	0.4011750	-4.0366710	-0.9546612
H	0.3511727	-1.8692357	-1.3013512
C	0.4066038	-5.2057549	-1.6444366
H	0.4258087	-3.9936947	0.1275725
H	0.4333877	-6.2092784	-1.2465187
Se	1.9768990	-3.1713800	-8.3468038
Se	-0.9765220	2.8439730	-5.8419748
Se	0.3541191	-4.9088715	-3.4720517
H	0.7946967	-3.4325977	-5.7374488
H	0.2011509	0.6144593	-6.9539669
H	-0.2766457	-0.4661694	-2.8340171
C	-0.1808137	0.7514802	3.8383770
C	0.9308438	1.2482535	4.5227769
C	0.8211749	1.5000157	5.8899592
C	-0.3622677	1.2477345	6.5781914
C	-1.4580040	0.7610124	5.8727353
C	-1.3864180	0.5128915	4.5014632
C	-0.4291646	1.4938232	8.0163058
C	0.5814704	1.4107196	8.9303041
C	0.2300041	1.7150690	10.2716540
H	1.5791713	1.1013017	8.6427655
C	-1.0723173	2.0494256	10.4612005
H	0.9444847	1.6744755	11.0854774
H	-1.5572571	2.3098157	11.3898634
C	2.1793637	1.5041766	3.8085256
C	2.4028727	1.4715572	2.4630011
C	3.7319970	1.7590422	2.0569605
H	1.6254678	1.2391924	1.7369157
C	4.6028773	2.0264384	3.0628514
H	4.0214482	1.7612680	1.0130217
H	5.6521972	2.2685800	2.9842154
C	-2.5406665	0.0017256	3.7659376
C	-2.6708574	-0.1723598	2.4186322
C	-3.9205497	-0.6879737	1.9868059
H	-1.8803600	0.0659066	1.7088278
C	-4.8183946	-0.9389214	2.9732452
H	-4.1335202	-0.8653494	0.9394394
H	-5.8201476	-1.3295849	2.8742464
Se	-2.0137125	2.0133917	8.8661909
Se	3.7709981	1.9298652	4.7150957
Se	-4.1215658	-0.5233239	4.6381990
H	-2.3783499	0.5538514	6.4103599
H	1.6575163	1.9310476	6.4292682
H	-0.1049322	0.5453525	2.7753174
Br	-0.0306238	0.4300237	-0.0933636

Cl@3

C	0.0660700	0.4541616	1.2163853
C	0.0728713	1.1928837	0.0318653
C	0.0644270	0.4188563	-1.1296125
C	0.0386175	-0.9776118	-1.1653644
C	0.0280118	-1.6072161	0.0752626
C	0.0342769	-0.9378359	1.2963599
C	0.0267582	-1.7136378	-2.4291772

C	-0.5421187	-1.3249513	-3.6099859
C	-0.3566550	-2.2047796	-4.7056995
H	-1.0943047	-0.3998662	-3.6987648
C	0.3763993	-3.3141819	-4.4313463
H	-0.7690033	-2.0037958	-5.6869302
H	0.6335069	-4.1170702	-5.1059073
C	0.0949976	2.6505208	0.0226618
C	-0.4924761	3.4807647	0.9429357
C	-0.2895840	4.8655266	0.7353486
H	-1.0796164	3.0981420	1.7683740
C	0.4784718	5.1958826	-0.3396769
H	-0.7133250	5.6215921	1.3858110
H	0.7915831	6.1842472	-0.7306921
C	0.0202282	-1.6622425	2.5665822
C	-0.6038319	-2.8491410	2.8336491
C	-0.4094424	-3.3706004	4.1369995
H	-1.2076140	-3.3534247	2.0917416
C	0.3858491	-2.6173244	4.9401406
H	-0.8647359	-4.2965450	4.4670239
H	0.6568073	-2.8122611	5.9669900
F	0.0906330	1.0625360	-2.2944848
F	0.1087354	1.1210088	2.3716406
F	0.0264655	-2.9468324	0.0903859
Cl	1.5429175	7.9239559	-1.7807472
Se	0.9674305	-1.0907465	4.0791990
Se	1.0128177	3.6848586	-1.2487473
Se	0.9048317	-3.3548723	-2.6622201

Cl@**(3)**₂

C	-1.4816537	-6.6868422	2.1910648
C	-1.6327243	-5.6754709	1.2444354
C	-1.5167423	-6.0936225	-0.0806647
C	-1.2692295	-7.4080751	-0.4885925
C	-1.1296796	-8.3319100	0.5434667
C	-1.2382435	-8.0290721	1.8988517
C	-1.1622022	-7.7715193	-1.9013255
C	-1.7655482	-7.1594516	-2.9658166
C	-1.4449547	-7.6803639	-4.2440676
H	-2.4411215	-6.3261809	-2.8380388
C	-0.5678635	-8.7164692	-4.2371507
H	-1.8677728	-7.2770490	-5.1561562
H	-0.1923277	-9.2671480	-5.0865454
C	-1.8811010	-4.2869619	1.6224826
C	-2.6977531	-3.8746951	2.6417784
C	-2.7350286	-2.4741362	2.8451089
H	-3.2743165	-4.5671522	3.2436010
C	-1.9378196	-1.7554858	2.0087200
H	-3.3485887	-2.0097285	3.6082519
H	-1.7720607	-0.6899279	1.9464854
C	-1.0926319	-9.0555974	2.9295645
C	-1.4334308	-10.3771637	2.8368304
C	-1.1326329	-11.1749344	3.9685974
H	-1.9039220	-10.7830606	1.9521307
C	-0.5336973	-10.5118196	4.9915347
H	-1.3665459	-12.2317556	4.0132796
H	-0.2306884	-10.9125119	5.9472442
F	-1.5561322	-6.3527293	3.4811702
F	-0.8570242	-9.5992727	0.2049369
F	-1.6492887	-5.1677228	-1.0252620
Se	-0.0615684	-9.1615953	-2.5183247
Se	-1.0329261	-2.8109283	0.8035519
Se	-0.3085112	-8.7216847	4.5991359
C	1.1296796	8.3319100	-0.5434667
C	1.2382435	8.0290721	-1.8988517
C	1.4816537	6.6868422	-2.1910648
C	1.6327243	5.6754709	-1.2444354
C	1.5167423	6.0936225	0.0806647
C	1.2692295	7.4080751	0.4885925
C	1.8811010	4.2869619	-1.6224826
C	2.6977531	3.8746951	-2.6417784
C	2.7350286	2.4741362	-2.8451089
H	3.2743165	4.5671522	-3.2436010
C	1.9378196	1.7554858	-2.0087200
H	3.3485887	2.0097285	-3.6082519
H	1.7720607	0.6899279	-1.9464854

C	1.0926319	9.0555974	-2.9295645
C	1.4334308	10.3771637	-2.8368304
C	1.1326329	11.1749344	-3.9685974
H	1.9039220	10.7830606	-1.9521307
C	0.5336973	10.5118196	-4.9915347
H	1.3665459	12.2317556	-4.0132796
H	0.2306884	10.9125119	-5.9472442
C	1.1622022	7.7715193	1.9013255
C	1.7655482	7.1594516	2.9658166
C	1.4449547	7.6803639	4.2440676
H	2.4411215	6.3261809	2.8380388
C	0.5678635	8.7164692	4.2371507
H	1.8677728	7.2770490	5.1561562
H	0.1923277	9.2671480	5.0865454
F	0.8570242	9.5992727	-0.2049369
F	1.6492887	5.1677228	1.0252620
F	1.5561322	6.3527293	-3.4811702
Se	1.0329261	2.8109283	-0.8035519
Se	0.3085112	8.7216847	-4.5991359
Se	0.0615684	9.1615953	2.5183247
Cl	0.0000000	0.0000000	0.0000000

Br@3

C	0.0006694	0.6953020	0.9742573
C	0.0470368	1.4404093	-0.2079232
C	0.0799976	0.6959049	-1.3827338
C	0.0603586	-0.6957827	-1.4337072
C	0.0197227	-1.3378692	-0.1956885
C	-0.0202796	-0.6985458	1.0435508
C	0.0896311	-1.4178370	-2.7047941
C	-0.4508031	-1.0196034	-3.8964604
C	-0.2318382	-1.8859583	-4.9965383
H	-1.0104052	-0.0989635	-3.9873010
C	0.4998665	-2.9946642	-4.7133685
H	-0.6230860	-1.6796004	-5.9855090
H	0.7741600	-3.7915706	-5.3883285
C	0.0653235	2.9027517	-0.1935832
C	-0.5113683	3.7314882	0.7283028
C	-0.2858112	5.1182117	0.5418159
H	-1.0951256	3.3478147	1.5530416
C	0.4878137	5.4339559	-0.5281556
H	-0.6971627	5.8667372	1.2079192
H	0.7809800	6.4181844	-0.8614275
C	-0.0680229	-1.4343669	2.3028115
C	-0.7436761	-2.6092151	2.5094933
C	-0.6015487	-3.1563099	3.8065335
H	-1.3474515	-3.0812864	1.7434620
C	0.1974661	-2.4394092	4.6434477
H	-1.0898575	-4.0749556	4.1109934
H	0.4768337	-2.6250092	5.6707386
F	0.1501926	1.3686496	-2.5402002
F	-0.0234524	1.3663892	2.1211978
F	0.0363925	-2.6732211	-0.2117836
Br	2.1761045	-0.6292065	6.7871504
Se	0.9791293	-3.0527088	-2.9307397
Se	0.8708280	-0.9131434	3.8686631
Se	1.0073823	3.9234284	-1.4551364

Br@3)2

C	-1.5254241	-6.9300358	2.2221857
C	-1.6768316	-5.9157065	1.2786441
C	-1.5567496	-6.3281310	-0.0475519
C	-1.3048806	-7.6405578	-0.4572104
C	-1.1660436	-8.5684121	0.5707105
C	-1.2797476	-8.2716734	1.9276306
C	-1.1974243	-7.9982858	-1.8712771
C	-1.8367670	-7.4071283	-2.9257038
C	-1.5120501	-7.9126245	-4.2091177
H	-2.5416442	-6.6001335	-2.7855458
C	-0.5945457	-8.9132579	-4.2150652
H	-1.9620668	-7.5256878	-5.1151686
H	-0.2072498	-9.4463153	-5.0703926
C	-1.9301694	-4.5292929	1.6621233
C	-2.7473468	-4.1196541	2.6819515

C	-2.7874316	-2.7199010	2.8895248
H	-3.3226646	-4.8152767	3.2810993
C	-1.9927439	-1.9966008	2.0549514
H	-3.4010006	-2.2589032	3.6545509
H	-1.8323404	-0.9295069	1.9977814
C	-1.1408162	-9.3014316	2.9561759
C	-1.4535517	-10.6291830	2.8478504
C	-1.1720208	-11.4266453	3.9845170
H	-1.8902208	-11.0407042	1.9488168
C	-0.6168391	-10.7576750	5.0280636
H	-1.3871034	-12.4878599	4.0170938
H	-0.3351185	-11.1576261	5.9905614
F	-1.6029628	-6.5981712	3.5128340
F	-0.8917377	-9.8329610	0.2248834
F	-1.6884747	-5.4003929	-0.9903209
Se	-0.0497943	-9.3412164	-2.5033980
Se	-1.0883330	-3.0507216	0.8479203
Se	-0.4144503	-8.9617514	4.6513278
C	1.1660436	8.5684121	-0.5707105
C	1.2797476	8.2716734	-1.9276306
C	1.5254241	6.9300358	-2.2221857
C	1.6768316	5.9157065	-1.2786441
C	1.5567496	6.3281310	0.0475519
C	1.3048806	7.6405578	0.4572104
C	1.9301694	4.5292929	-1.6621233
C	2.7473468	4.1196541	-2.6819515
C	2.7874316	2.7199010	-2.8895248
H	3.3226646	4.8152767	-3.2810993
C	1.9927439	1.9966008	-2.0549514
H	3.4010006	2.2589032	-3.6545509
H	1.8323404	0.9295069	-1.9977814
C	1.1408162	9.3014316	-2.9561759
C	1.4535517	10.6291830	-2.8478504
C	1.1720208	11.4266453	-3.9845170
H	1.8902208	11.0407042	-1.9488168
C	0.6168391	10.7576750	-5.0280636
H	1.3871034	12.4878599	-4.0170938
H	0.3351185	11.1576261	-5.9905614
C	1.1974243	7.9982858	1.8712771
C	1.8367670	7.4071283	2.9257038
C	1.5120501	7.9126245	4.2091177
H	2.5416442	6.6001335	2.7855458
C	0.5945457	8.9132579	4.2150652
H	1.9620668	7.5256878	5.1151686
H	0.2072498	9.4463153	5.0703926
F	0.8917377	9.8329610	-0.2248834
F	1.6884747	5.4003929	0.9903209
F	1.6029628	6.5981712	-3.5128340
Se	1.0883330	3.0507216	-0.8479203
Se	0.4144503	8.9617514	-4.6513278
Se	0.0497943	9.3412164	2.5033980
Br	0.0000000	0.0000000	0.0000000

Polymer (Chloride)

C	-0.38897849	-17.81224057	2.65167130
C	-0.84468268	-17.04766103	1.57949907
C	-1.16480738	-17.77792987	0.43563699
C	-1.05781089	-19.16691445	0.31428257
C	-0.58556122	-19.82546316	1.44626541
C	-0.24804321	-19.20015381	2.64444537
C	-1.41519204	-19.86446552	-0.92065155
C	-2.33510922	-19.47938592	-1.85727348
C	-2.44606506	-20.31383435	-2.99720333
H	-2.93592409	-18.58980022	-1.73592566
C	-1.60994413	-21.38324214	-3.00814703
H	-3.14472644	-20.10844420	-3.79909536
H	-1.52912388	-22.14833810	-3.76567055
C	-0.96255998	-15.59406439	1.65519349
C	-1.40446982	-14.88807452	2.74245726
C	-1.37972920	-13.48095462	2.58851090
H	-1.75044777	-15.36976754	3.64931100
C	-0.90166850	-13.04708571	1.39069509
H	-1.71329982	-12.80146486	3.36410232
H	-0.76998112	-12.04343944	1.01371314
C	0.22995725	-19.95889332	3.79906899

C	-0.11655886	-21.23375021	4.15395980
C	0.54005893	-21.75899380	5.29447997
H	-0.84775884	-21.80138040	3.59543462
C	1.43657850	-20.91935690	5.87422850
H	0.33817885	-22.75307861	5.67477282
H	2.03616428	-21.10247707	6.75326960
F	-0.04063870	-17.17490070	3.77149616
F	-0.43239782	-21.15424566	1.36861473
F	-1.60195447	-17.09703608	-0.61907099
Se	-0.56938163	-21.44289692	-1.48417006
Se	-0.43400741	-14.42688600	0.26701118
Se	1.51366731	-19.29784507	4.99444145
C	1.12209883	-4.13113171	-4.44787430
C	0.78458081	-4.75644107	-5.64605426
C	0.92551609	-6.14435431	-5.65328019
C	1.38122028	-6.90893384	-4.58110796
C	1.70134499	-6.17866500	-3.43724588
C	1.59434850	-4.78968042	-3.31589146
C	1.49909758	-8.36253049	-4.65680238
C	1.94100742	-9.06852035	-5.74406614
C	1.91626681	-10.47564025	-5.59011979
H	2.28698538	-8.58682733	-6.65091989
C	1.43820611	-10.90950917	-4.39230398
H	2.24983743	-11.15513001	-6.36571121
H	1.30651872	-11.91315544	-4.01532202
C	0.30658035	-3.99770155	-6.80067788
C	0.65309646	-2.72284466	-7.15556869
C	-0.00352133	-2.19760107	-8.29608886
H	1.38429645	-2.15521448	-6.59704351
C	-0.90004089	-3.03723797	-8.87583739
H	0.19835875	-1.20351626	-8.67638171
H	-1.49962667	-2.85411780	-9.75487849
C	1.95172965	-4.09212935	-2.08095734
C	2.87164683	-4.47720895	-1.14433541
C	2.98260267	-3.64276053	-0.00440556
H	3.47246170	-5.36679465	-1.26568322
C	2.14648173	-2.57335273	0.00653814
H	3.68126405	-3.84815067	0.79748647
H	2.06566149	-1.80825677	0.76406166
F	0.96893542	-2.80234921	-4.37022362
F	2.13849208	-6.85955879	-2.38253790
F	0.57717630	-6.78169417	-6.77310504
Se	0.97054502	-9.52970888	-3.26862007
Se	-0.97712971	-4.65874980	-7.99605034
Se	1.10591924	-2.51369795	-1.51743883
Cl	0.26826880	-11.97829744	-1.50080444
C	-0.92551609	6.14435431	5.65328019
C	-1.38122028	6.90893384	4.58110796
C	-1.70134499	6.17866500	3.43724588
C	-1.59434850	4.78968042	3.31589146
C	-1.12209883	4.13113171	4.44787430
C	-0.78458081	4.75644107	5.64605426
C	-1.95172965	4.09212935	2.08095734
C	-2.87164683	4.47720895	1.14433541
C	-2.98260267	3.64276053	0.00440556
H	-3.47246170	5.36679465	1.26568322
C	-2.14648173	2.57335273	-0.00653814
H	-3.68126405	3.84815067	-0.79748647
H	-2.06566149	1.80825677	-0.76406166
C	-1.49909758	8.36253049	4.65680238
C	-1.94100742	9.06852035	5.74406614
C	-1.91626681	10.47564025	5.59011979
H	-2.28698538	8.58682733	6.65091989
C	-1.43820611	10.90950917	4.39230398
H	-2.24983743	11.15513001	6.36571121
H	-1.30651872	11.91315544	4.01532202
C	-0.30658035	3.99770155	6.80067788
C	-0.65309646	2.72284466	7.15556869
C	0.00352133	2.19760107	8.29608886
H	-1.38429645	2.15521448	6.59704351
C	0.90004089	3.03723797	8.87583739
H	-0.19835875	1.20351626	8.67638171
H	1.49962667	2.85411780	9.75487849
F	-0.57717630	6.78169417	6.77310504
F	-0.96893542	2.80234921	4.37022362
F	-2.13849208	6.85955879	2.38253790
Se	-1.10591924	2.51369795	1.51743883

Se	-0.97054502	9.52970888	3.26862007
Se	0.97712971	4.65874980	7.99605034
C	0.58556122	19.82546316	-1.44626541
C	0.24804321	19.20015381	-2.64444537
C	0.38897849	17.81224057	-2.65167130
C	0.84468268	17.04766103	-1.57949907
C	1.16480738	17.77792987	-0.43563699
C	1.05781089	19.16691445	-0.31428257
C	0.96255998	15.59406439	-1.65519349
C	1.40446982	14.88807452	-2.74245726
C	1.37972920	13.48095462	-2.58851090
H	1.75044777	15.36976754	-3.64931100
C	0.90166850	13.04708571	-1.39069509
H	1.71329982	12.80146486	-3.36410232
H	0.76998112	12.04343944	-1.01371314
C	-0.22995725	19.95889332	-3.79906899
C	0.11655886	21.23375021	-4.15395980
C	-0.54005893	21.75899380	-5.29447997
H	0.84775884	21.80138040	-3.59543462
C	-1.43657850	20.91935690	-5.87422850
H	-0.33817885	22.75307861	-5.67477282
H	-2.03616428	21.10247707	-6.75326960
C	1.41519204	19.86446552	0.92065155
C	2.33510922	19.47938592	1.85727348
C	2.44606506	20.31383435	2.99720333
H	2.93592409	18.58980022	1.73592566
C	1.60994413	21.38324214	3.00814703
H	3.14472644	20.10844420	3.79909536
H	1.52912388	22.14833810	3.76567055
F	0.43239782	21.15424566	-1.36861473
F	1.60195447	17.09703608	0.61907099
F	0.04063870	17.17490070	-3.77149616
Se	0.43400741	14.42688600	-0.26701118
Se	-1.51366731	19.29784507	-4.99444145
Se	0.56938163	21.44289692	1.48417006
Cl	-0.26826880	11.97829744	1.50080444
Cl	0.00000000	0.00000000	0.00000000

Polymer 2D

C	-6.51347498	-8.27285319	-17.68349215
C	-6.44798038	-7.61057143	-16.45919856
C	-6.76152093	-6.25296390	-16.51199046
C	-7.11996601	-5.55663092	-17.67047690
C	-7.14574301	-6.31875388	-18.83520667
C	-6.86367292	-7.68151473	-18.89753430
C	-7.43777629	-4.12911661	-17.64680036
C	-7.95641590	-3.40945683	-16.60521632
C	-8.11528458	-2.01941920	-16.83018651
H	-8.22318539	-3.87366649	-15.66691469
C	-7.71775558	-1.58790646	-18.05436723
H	-8.52093193	-1.35394665	-16.07789655
H	-7.75472658	-0.58075550	-18.44169874
C	-6.06783631	-8.29267451	-15.22518326
C	-6.44906704	-9.55842405	-14.86686810
C	-5.90772070	-10.01881283	-13.64241545
H	-7.11714296	-10.15963997	-15.47211730
C	-5.07608922	-9.13944747	-13.02060148
H	-6.13554319	-10.99581356	-13.23243468
H	-4.53120516	-9.23080598	-12.09242166
C	-6.92349014	-8.42171567	-20.15683977
C	-7.75456218	-8.18645240	-21.21761848
C	-7.56705786	-9.02034711	-22.34778472
H	-8.50724372	-7.41087460	-21.19009796
C	-6.57307650	-9.93741141	-22.22192786
H	-8.17358558	-8.93325323	-23.24116124
H	-6.26613486	-10.67816332	-22.94499273
F	-6.20139585	-9.57031994	-17.71064162
F	-7.44994218	-5.68938387	-19.97823242
F	-6.71156914	-5.57161131	-15.37164564
Se	-7.09533411	-2.98185249	-19.09279912
Se	-4.89726006	-7.55515565	-13.93889382
Se	-5.76194974	-9.83483552	-20.56638562
Cl	-3.04655410	-7.02643382	-11.50799059
C	6.18516138	10.94410536	12.19410931
C	5.73850545	12.24823461	11.99333383

C	5.21642275	12.51002217	10.72640247
C	5.13406743	11.58541108	9.68711743
C	5.62073875	10.31557124	9.99509579
C	6.15968892	9.94043047	11.22970319
C	4.56920167	11.92743715	8.38461493
C	4.75553890	13.11262036	7.72395792
C	4.06028283	13.22508186	6.49584172
H	5.38982459	13.90192011	8.10970417
C	3.29827579	12.14541672	6.17147240
H	4.12735833	14.10278277	5.86365526
H	2.67099177	11.96697045	5.31040650
C	5.80826437	13.25561163	13.05052399
C	6.74771005	13.35478992	14.03991090
C	6.55038643	14.39768551	14.97865802
H	7.58786548	12.67681135	14.09728455
C	5.44101863	15.15263373	14.76841509
H	7.23516759	14.57890725	15.79830201
H	5.10364673	16.00085404	15.34500147
C	6.65310393	8.58608015	11.47797299
C	7.17058341	7.70872481	10.56459620
C	7.52279519	6.43002588	11.06352642
H	7.29737344	7.97467325	9.52523955
C	7.28635770	6.24647390	12.38763252
H	7.94574383	5.65852398	10.43166969
H	7.48295635	5.36238143	12.97540382
F	6.66070703	10.62460791	13.40527787
F	5.56314179	9.39307494	9.03968697
F	4.74547318	13.73981229	10.50874863
Se	3.39896238	10.79944955	7.42185467
Se	4.51477236	14.59414173	13.27194488
Se	6.58042203	7.76520682	13.16476828
Cl	1.43486782	9.54364704	5.37753511
C	0.02497439	-15.11313121	5.07038231
C	-0.44444384	-14.74178554	3.81199032
C	-0.65824786	-15.80205843	2.93204594
C	-0.43736384	-17.15009967	3.23112511
C	0.03770432	-17.40146745	4.51534308
C	0.27482844	-16.42351752	5.47864547
C	-0.68705991	-18.20936632	2.25390093
C	-1.59463801	-18.19972912	1.23018042
C	-1.59207170	-19.33967146	0.38840829
H	-2.26809659	-17.37005644	1.07155097
C	-0.67469020	-20.28729197	0.70977653
H	-2.27074422	-19.44190898	-0.44962200
H	-0.50247925	-21.23166490	0.21556121
C	-0.67934778	-13.34668777	3.44992646
C	-1.22028931	-12.39286783	4.27057152
C	-1.29992799	-11.09725925	3.70545730
H	-1.56474469	-12.61394178	5.27386081
C	-0.80804265	-10.99596727	2.44080884
H	-1.71790436	-10.25111799	4.23824098
H	-0.74013819	-10.14069777	1.78455749
C	0.76256360	-16.76303375	6.81437333
C	0.50293642	-17.90166479	7.52668933
C	1.15079969	-18.00754911	8.78242645
H	-0.15746607	-18.67047675	7.15038554
C	1.95358570	-16.95920475	9.10078874
H	1.01209112	-18.85888413	9.43784344
H	2.52861311	-16.82168553	10.00421627
F	0.27519199	-14.14590188	5.95548626
F	0.29801752	-18.67529667	4.83899063
F	-1.10332649	-15.50356371	1.71552271
Se	0.30301102	-19.80347383	2.19935873
Se	-0.18693244	-12.59940071	1.78625205
Se	1.93943096	-15.66914268	7.77987691
C	0.74933061	-4.05785331	-5.75162215
C	0.51220648	-5.03580325	-6.71492454
C	0.76206053	-6.34618955	-6.30666138
C	1.23147876	-6.71753522	-5.04826939
C	1.44528279	-5.65726233	-4.16832501
C	1.22439877	-4.30922108	-4.46740418
C	1.46638270	-8.11263300	-4.68620553
C	2.00732422	-9.06645292	-5.50685058
C	2.08696291	-10.36206150	-4.94173637
H	2.35177962	-8.84537898	-6.51013988
C	1.59507757	-10.46335349	-3.67708791
H	2.50493929	-11.20820277	-5.47452005

H	1.52717310	-11.31862300	-3.02083655
C	0.02447131	-4.69628700	-8.05065240
C	0.28409849	-3.55765597	-8.76296840
C	-0.36376477	-3.45177165	-10.01870552
H	0.94450099	-2.78884402	-8.38666461
C	-1.16655078	-4.50011601	-10.33706781
H	-0.22505620	-2.60043663	-10.67412252
H	-1.74157819	-4.63763523	-11.24049534
C	1.47409483	-3.24995444	-3.49018000
C	2.38167293	-3.25959164	-2.46645949
C	2.37910662	-2.11964931	-1.62468736
H	3.05513151	-4.08926432	-2.30783004
C	1.46172512	-1.17202879	-1.94605560
H	3.05777915	-2.01741178	-0.78665707
H	1.28951418	-0.22765586	-1.45184028
F	0.48901739	-2.78402409	-6.07526970
F	1.89036141	-5.95575705	-2.95180178
F	0.51184292	-7.31341887	-7.19176532
Se	0.97396737	-8.85992005	-3.02253112
Se	-1.15239605	-5.79017808	-9.01615599
Se	0.48402390	-1.65584693	-3.43563780
Cl	0.39351746	-10.72966038	-0.61813953
C	-2.51885045	8.51979271	0.80074194
C	-2.98826867	8.89113837	-0.45765005
C	-3.20207270	7.83086549	-1.33759442
C	-2.98118869	6.48282424	-1.03851525
C	-2.50612052	6.23145646	0.24570271
C	-2.26899639	7.20940640	1.20900510
C	-3.23088475	5.42355759	-2.01573944
C	-4.13846285	5.43319479	-3.03945995
C	-4.13589654	4.29325246	-3.88123208
H	-4.81192143	6.26286747	-3.19808940
C	-3.21851504	3.34563194	-3.55986383
H	-4.81456906	4.19101494	-4.71926237
H	-3.04630410	2.40125901	-4.05407916
C	-3.22317261	10.28623615	-0.81971391
C	-3.76411414	11.24005608	0.00093114
C	-3.84375283	12.53566466	-0.56418307
H	-4.10856954	11.01898213	1.00422044
C	-3.35186749	12.63695665	-1.82883153
H	-4.26172920	13.38180593	-0.03139939
H	-3.28396302	13.49222615	-2.48508289
C	-1.78126123	6.86989016	2.54473297
C	-2.04088841	5.73125912	3.25704896
C	-1.39302514	5.62537481	4.51278608
H	-2.70129091	4.96244717	2.88074517
C	-0.59023914	6.67371916	4.83114837
H	-1.53173371	4.77403978	5.16820308
H	-0.01521173	6.81123838	5.73457590
F	-2.26863284	9.48702203	1.68584588
F	-2.24580731	4.95762724	0.56935026
F	-3.64715133	8.12936020	-2.55411766
Se	-2.24081382	3.82945009	-2.07028164
Se	-2.73075729	11.03352321	-2.48338832
Se	-0.60439387	7.96378123	3.51023655
C	-1.79449424	19.57507060	-10.02126252
C	-2.03161836	18.59712067	-10.98456491
C	-1.78176431	17.28673437	-10.57630175
C	-1.31234608	16.91538869	-9.31790976
C	-1.09854206	17.97566158	-8.43796538
C	-1.31942607	19.32370283	-8.73704455
C	-1.07744214	15.52029092	-8.95584590
C	-0.53650061	14.56647099	-9.77649096
C	-0.45686193	13.27086241	-9.21137674
H	-0.19204522	14.78754494	-10.77978025
C	-0.94874727	13.16957043	-7.94672828
H	-0.03888556	12.42472114	-9.74416042
H	-1.01665173	12.31430092	-7.29047692
C	-2.51935352	18.93663691	-12.32029277
C	-2.25972634	20.07526794	-13.03260877
C	-2.90758961	20.18115226	-14.28834589
H	-1.59932385	20.84407990	-12.65630498
C	-3.71037562	19.13280790	-14.60670818
H	-2.76888104	21.03248728	-14.94376288
H	-4.28540303	18.99528869	-15.51013571
C	-1.06973001	20.38296947	-7.75982037
C	-0.16215191	20.37333227	-6.73609986

C	-0.16471822	21.51327461	-5.89432773
H	0.51130667	19.54365959	-6.57747041
C	-1.08209971	22.46089513	-6.21569597
H	0.51395430	21.61551213	-5.05629744
H	-1.25431066	23.40526806	-5.72148065
F	-2.05480744	20.84889983	-10.34491006
F	-0.65346343	17.67716686	-7.22144215
F	-2.03198191	16.31950503	-11.46140570
Se	-1.56985748	14.77300387	-7.29217149
Se	-3.69622088	17.84274584	-13.28579635
Se	-2.05980094	21.97707698	-7.70527817
Cl	-2.15030738	12.90326354	-4.88777991
Cl	-0.87839496	1.08680158	-2.75295972