

INTERACTION BETWEEN ANIONS AND SUBSTITUTED MOLECULAR BOWLS

Patxi García-Novo^(a), Alba Campo-Cacharrón^(a), Enrique M. Cabaleiro-Lago^(a), Jesús Rodríguez-Otero^(b)

(a) Departamento de Química Física, Facultade de Ciencias, Universidade de Santiago de Compostela, Campus de Lugo. Avda. Alfonso X El Sabio s/n 27002 Lugo, Galicia (Spain). e-mail: caba.lago@usc.es

(b) Departamento de Química Física, Facultade de Química, Universidade de Santiago de Compostela, Avda. das Ciencias, s/n 15706 Santiago de Compostela, Galicia (Spain).

Coran-cl5cl-side

C 0.6967734 -0.7413337 0.9027572
C 0.8735805 0.6745261 0.9043938
C -0.4163398 1.2833342 0.8957094
C -1.3952163 0.2426364 0.8929073
C -0.7068943 -1.0070811 0.8999834
C 1.6552952 -1.6032327 0.3462516
C 1.9977727 1.3054823 0.3518799
C -2.6815854 0.3884243 0.3524439
C -0.6784549 2.5511857 0.3555353
C -1.2388503 -2.1860863 0.3539384
C 2.9291234 -1.0091140 -0.0310556
C 1.1104085 -2.9150030 -0.0083458
C -0.2679752 -3.1957955 -0.0160576
C 3.0701158 0.3878802 -0.0098875
C 1.8061158 2.6976525 -0.0194713
C -2.6436420 -2.0634716 -0.0059935
C -3.3445523 -0.8489660 -0.0192361
C -3.0002342 1.7609401 -0.0067439
C -2.0580641 2.8001956 -0.0181683
C 0.5311229 3.2769349 -0.0049298
Cl 0.3572882 4.9604653 -0.5944435
Cl -4.6527977 2.1161535 -0.6013275
Cl -3.4923923 -3.5233664 -0.5993478
Cl 2.2288108 -4.1512794 -0.5847794
Cl 4.5968670 1.0991487 -0.5855779
H -2.3532667 3.7820809 -0.4020163
H 2.6517140 3.2758100 -0.4059712
H 3.7746229 -1.6349885 -0.4108597
H -0.6031815 -4.1654834 -0.3977535
H -4.3698250 -0.8294825 -0.4024985
Cl 5.6306155 -2.7311392 -1.0650647

Coran-cl5cl-out1

C 1.0185051 -0.7185009 0.7173591
C 1.0294105 0.7079764 0.7118175
C -0.3209941 1.1590779 0.7321088
C -1.1777042 0.0123551 0.7841951
C -0.3388191 -1.1481889 0.7423904
C 2.0755577 -1.4743909 0.1925310
C 2.0755593 1.4749696 0.1811132
C -2.4494751 0.0004062 0.1855924
C -0.7277473 2.3821268 0.1867643
C -0.7265931 -2.3802629 0.2053306
C 3.2652474 -0.7186762 -0.1695335
C 1.6861489 -2.8288772 -0.1564891
C 0.3564196 -3.2721163 -0.1659602
C 3.2471024 0.6803176 -0.1632766
C 1.7261337 2.8323598 -0.1892762
C -2.1398518 -2.4346695 -0.1475391
C -2.9636252 -1.3054335 -0.1814059
C -2.9282856 1.3206547 -0.1794866
C -2.1332945 2.4733977 -0.1762078
C 0.3851363 3.2433042 -0.1776302
Cl 0.0130641 4.8909957 -0.7815796
Cl -4.6061094 1.4681174 -0.7967841
Cl -2.8103445 -3.9985061 -0.7165988
Cl 2.9579161 -3.9530532 -0.7403078
Cl 4.7123360 1.5445480 -0.7336587
H 2.4927877 3.5171181 -0.5655868
H 4.1588048 -1.2400285 -0.5279415

H 0.1334080 -4.2767787 -0.5398816
H -3.9847567 -1.4027895 -0.5639182
H -2.5502252 3.4167102 -0.5411074
Cl -1.4756951 0.0279690 3.5746527

Coran-cl5cl-out2

C 1.1345892 -0.6863318 0.7567688
C 1.1652381 0.7424619 0.7302162
C -0.1821773 1.2098306 0.7628497
C -1.0431108 0.0757338 0.8149087
C -0.2269123 -1.0974866 0.8144732
C 2.1698661 -1.4587416 0.2034798
C 2.2051638 1.4904410 0.1593084
C -2.3529113 0.0715260 0.3199305
C -0.5908672 2.4386071 0.2180079
C -0.6549844 -2.3251338 0.2806417
C 3.3497110 -0.7227566 -0.2078895
C 1.7476997 -2.8096418 -0.1294140
C 0.4130576 -3.2346248 -0.1043062
C 3.3542001 0.6802356 -0.2129041
C 1.8597467 2.8502020 -0.2161915
C -2.0658053 -2.3618204 -0.0435764
C -2.9105814 -1.2386253 0.0135952
C -2.8211680 1.3910696 -0.0713259
C -1.9949145 2.5273884 -0.1256451
C 0.5256184 3.2820785 -0.1772941
Cl 0.1651158 4.9306141 -0.7830635
Cl -4.4908048 1.5553258 -0.6614331
Cl -2.7558506 -3.9034191 -0.6319506
Cl 2.9888494 -3.9560326 -0.7353614
Cl 4.8088244 1.5167878 -0.8484911
H 2.6257483 3.5204640 -0.6191847
H 4.2186099 -1.2581059 -0.6045170
H 0.1675419 -4.2378138 -0.4681466
H -3.9434755 -1.3217335 -0.3270668
H -2.4047080 3.4609711 -0.5235739
Cl -4.4564684 -1.0877621 2.4166936

Coran-cl5cl-in

C 0.7900125 -0.9213832 0.9678062
C 1.1204148 0.4666235 0.9678062
C -0.0975581 1.2097724 0.9678062
C -1.1807090 0.2810570 0.9678062
C -0.6321602 -1.0360696 0.9678062
C 1.6387695 -1.8808848 0.4005794
C 2.2952354 0.9773370 0.4005794
C -2.4313487 0.5584232 0.4005794
C -0.2202360 2.4849123 0.4005794
C -1.2824201 -2.1397878 0.4005794
C 2.9552444 -1.4137873 0.0154618
C 0.9585014 -3.1099449 0.0320324
C -0.4313709 -3.2474887 0.0154618
C 3.2539266 -0.0494368 0.0320324
C 2.2578124 2.3737201 0.0154618
C -2.6615401 -1.8726148 0.0320324
C -3.2218462 -0.5932711 0.0154618
C -2.6034237 1.9526053 0.0320324
C -1.5598396 2.8808270 0.0154618
C 1.0525358 3.0793913 0.0320324
Cl 1.0552708 4.7635454 -0.5775427
H -1.7385307 3.8788843 -0.3957921
Cl -4.2043043 2.4756386 -0.5775427

H	-4.2262737	-0.4547998	-0.3957921	C	0.3827847	3.2446700	-0.1837885
Cl	-3.6536737	-3.2335166	-0.5775427	Cl	0.0140058	4.8932314	-0.7857740
H	-0.8734501	-4.1599660	-0.3957921	Cl	-4.6113020	1.4726733	-0.8150982
Cl	1.9462097	-4.4740618	-0.5775427	Cl	-2.8127250	-3.9987574	-0.7330951
H	3.6864519	-2.1162006	-0.3957921	Cl	2.9587158	-3.9548505	-0.7270373
Cl	4.8564975	0.4683943	-0.5775427	Cl	4.7110981	1.5444740	-0.7208758
H	3.1518026	2.8520821	-0.3957921	H	2.4928315	3.5185940	-0.5579255
Cl	0.0000000	0.0000000	-2.2114201	H	4.1570794	-1.2397202	-0.5163858
Coran-cl5br-side				H	0.1336602	-4.2791807	-0.5431057
C	0.6922812	-0.7357641	0.9056149	H	-3.9914399	-1.4061076	-0.5801885
C	0.8684008	0.6803429	0.9057944	H	-2.5510789	3.4178399	-0.5600788
C	-0.4216810	1.2877365	0.8984985	Br	-1.3720375	0.0210214	3.7774719
C	-1.3992189	0.2459657	0.8982205	Coran-cl5br-out2			
C	-0.7104307	-1.0031421	0.9030277	C	1.1371706	-0.6885431	0.7515303
C	1.6512285	-1.5984914	0.3532552	C	1.1660709	0.7402346	0.7287559
C	1.9928980	1.3132732	0.3565399	C	-0.1819859	1.2064808	0.7600319
C	-2.6877018	0.3900174	0.3620253	C	-1.0417237	0.0716766	0.8067319
C	-0.6853275	2.5549884	0.3570878	C	-0.2243232	-1.1010599	0.8036770
C	-1.2412310	-2.1833738	0.3577106	C	2.1742013	-1.4585961	0.1976240
C	2.9240623	-1.0004928	-0.0182952	C	2.2053689	1.4907306	0.1603755
C	1.1092696	-2.9108819	-0.0017250	C	-2.3508411	0.0670700	0.3098342
C	-0.2690462	-3.1921912	-0.0122159	C	-0.5910407	2.4355927	0.2161006
C	3.0668292	0.3968777	-0.0016627	C	-0.6489370	-2.3285994	0.2678052
C	1.8005970	2.7051271	-0.0149847	C	3.3541042	-0.7203273	-0.2093381
C	-2.6478150	-2.0625946	0.0036644	C	1.7545958	-2.8094873	-0.1385702
C	-3.3510584	-0.8491535	-0.0041970	C	0.4202422	-3.2364667	-0.1168334
C	-3.0073662	1.7613239	0.0000012	C	3.3564402	0.6829111	-0.2113210
C	-2.0650361	2.8016027	-0.0160256	C	1.8593574	2.8508413	-0.2135190
C	0.5240748	3.2821427	-0.0023869	C	-2.0601976	-2.3669420	-0.0575067
Cl	0.3484340	4.9633171	-0.5946317	C	-2.9031244	-1.2429588	-0.0051296
Cl	-4.6595021	2.1136252	-0.5960947	C	-2.8202749	1.3874221	-0.0797762
Cl	-3.4961400	-3.5229887	-0.5882034	C	-1.9946527	2.5239550	-0.1302249
Cl	2.2339018	-4.1426078	-0.5773854	C	0.5244843	3.2812331	-0.1760806
Cl	4.5946182	1.1028162	-0.5764308	Cl	0.1631072	4.9303817	-0.7788193
H	-2.3610903	3.7813764	-0.4038340	Cl	-4.4890341	1.5498951	-0.6711206
H	2.6455809	3.2848972	-0.4005951	Cl	-2.7501769	-3.9098669	-0.6393436
H	3.7599317	-1.6232943	-0.4010168	Cl	2.9988233	-3.9534808	-0.7413400
H	-0.6028486	-4.1627236	-0.3929005	Cl	4.8107650	1.5234426	-0.8412050
H	-4.3791129	-0.8316353	-0.3799853	H	2.6257278	3.5223889	-0.6136721
Br	5.7727755	-2.8480551	-1.2907052	H	4.2247165	-1.2542445	-0.6041437
Coran-cl5br-out1				H	0.1762328	-4.2396656	-0.4814721
C	1.0118287	-0.7180350	0.7143583	H	-3.9390656	-1.3286870	-0.3372189
C	1.0231743	0.7078322	0.7091321	H	-2.4039392	3.4589073	-0.5258844
C	-0.3274403	1.1594664	0.7202132	Br	-4.5520063	-1.0839192	2.5698171
C	-1.1822668	0.0129054	0.7549407	Coran-cl5br-in			
C	-0.3460107	-1.1478942	0.7295584	C	0.7900729	-0.9215845	0.9769120
C	2.0713713	-1.4743377	0.1952672	C	1.1206249	0.4666187	0.9769120
C	2.0713953	1.4752844	0.1836885	C	-0.0974886	1.2099707	0.9769120
C	-2.4557162	0.0009042	0.1641032	C	-1.1808761	0.2811843	0.9769120
C	-0.7316535	2.3828417	0.1731740	C	-0.6323330	-1.0361892	0.9769120
C	-0.7312086	-2.3806318	0.1916039	C	1.6377604	-1.8796367	0.4049018
C	3.2620400	-0.7186307	-0.1614959	C	2.2937366	0.9767630	0.4049018
C	1.6837591	-2.8297372	-0.1540666	C	-2.4297988	0.5580066	0.4049018
C	0.3538693	-3.2732099	-0.1712164	C	-0.2201533	2.4833095	0.4049018
C	3.2441762	0.6807301	-0.1555499	C	-1.2815449	-2.1384424	0.4049018
C	1.7238337	2.8332473	-0.1876566	C	2.9539868	-1.4130272	0.0191237
C	-2.1436306	-2.4346394	-0.1654725	C	0.9587136	-3.1093971	0.0363756
C	-2.9695381	-1.3065288	-0.2003258	C	-0.4310366	-3.2460578	0.0191237
C	-2.9338470	1.3227915	-0.1998200	C	3.2534711	-0.0490658	0.0363756
C	-2.1359441	2.4736767	-0.1949578	C	2.2567008	2.3727589	0.0191237

C	-2.6609536	-1.8726473	0.0363756	C	-2.2632361	-0.0003216	-0.1722540
C	-3.2203820	-0.5931469	0.0191237	C	-0.5336938	2.3780647	-0.2731919
C	-2.6032733	1.9520374	0.0363756	C	-0.5431933	-2.3873683	-0.1843078
C	-1.5592690	2.8794728	0.0191237	C	3.4367750	-0.7406308	-0.7284201
C	1.0520422	3.0790728	0.0363756	C	1.8540107	-2.8507065	-0.6172209
Cl	1.0529601	4.7618670	-0.5741633	C	0.5263476	-3.2939452	-0.5675257
H	-1.7365175	3.8772019	-0.3936267	C	3.4232191	0.6597007	-0.7421821
Cl	-4.2034221	2.4729224	-0.5741633	C	1.9050262	2.8187125	-0.7353247
H	-4.2240515	-0.4534050	-0.3936267	C	-1.9695074	-2.4400282	-0.4716448
Cl	-3.6508178	-3.2335169	-0.5741633	C	-2.8001467	-1.3139779	-0.4746181
H	-0.8740899	-4.1574216	-0.3936267	C	-2.7605479	1.3230374	-0.5134616
Cl	1.9470926	-4.4713458	-0.5741633	C	-1.9517757	2.4645274	-0.5731703
H	3.6838342	-2.1160228	-0.3936267	C	0.5689461	3.2379456	-0.6791363
Cl	4.8541872	0.4700732	-0.5741633	Cl	0.1821713	4.8849609	-1.2659606
H	3.1508247	2.8496476	-0.3936267	Cl	-4.4704591	1.4779547	-1.0113807
Br	0.0000000	0.0000000	-2.3475377	Cl	-2.6685791	-4.0097973	-0.9744564
Coran-cl5bf4-side				Cl	3.1040025	-3.9877129	-1.2159087
C	-0.2464229	-0.2892715	1.0613006	Cl	4.8644852	1.5104099	-1.3833856
C	-0.5488572	1.0984456	0.9271219	H	2.6616418	3.4988149	-1.1395187
C	-1.8600717	1.2148220	0.3766698	H	4.3143825	-1.2693674	-1.1142763
C	-2.3703807	-0.1030608	0.1716425	H	0.2917518	-4.3107219	-0.8987831
C	-1.3737502	-1.0311980	0.5962429	H	-3.8450833	-1.4228308	-0.7808940
C	1.0702102	-0.7661647	1.0159659	H	-2.3827289	3.4070913	-0.9245249
C	0.4287834	2.0830002	0.7343430	B	-1.3545963	0.0762133	3.3719888
C	-3.3260355	-0.4235747	-0.8025946	F	0.0631687	0.0737772	3.0950690
C	-2.2904060	2.3065723	-0.3892540	F	-1.5779300	0.1038556	4.7804938
C	-1.2427677	-2.3245621	0.0694123	F	-1.9416369	-1.1111649	2.7988493
C	2.1198545	0.2395710	1.0412532	F	-1.9470881	1.2369731	2.7517407
C	1.1675528	-2.1872494	0.6768121	Coran-cl5bf4-out2			
C	0.0655757	-2.9317480	0.2162464	C	-2.0795119	0.9555175	1.7992784
C	1.7922441	1.5973343	0.9153060	C	-0.6563184	1.1111414	1.5700967
C	-0.0444215	3.3173428	0.1314055	C	0.2086167	2.2570661	1.7981445
C	-2.3653812	-2.7086291	-0.7761971	C	1.4334866	2.4407880	1.1432184
C	-3.3596192	-1.8177321	-1.2061816	C	-2.8100724	-0.0111251	1.1035142
C	-3.9111034	0.7485962	-1.4368550	C	-0.0579652	0.1099088	0.8063975
C	-3.4269493	2.0518870	-1.2572719	C	-0.8225717	-0.8674896	0.1088379
C	-1.3415191	3.4106814	-0.3914800	C	-2.2199607	-0.9109642	0.1220115
Cl	-1.8107129	4.9208501	-1.2291268	C	-2.8314037	-1.6104052	-0.9944024
Cl	-5.2347425	0.4967067	-2.6146756	C	2.8469958	1.6104175	-0.9205136
Cl	-2.4047307	-4.3767639	-1.4168828	C	2.8684825	0.7715790	-2.0443916
Cl	2.7562281	-2.9376604	0.7174116	C	1.9345038	-0.3352696	-2.1541121
Cl	3.1120644	2.7843116	0.8305412	C	1.4405153	-1.0354830	-3.3320510
H	-3.8574944	2.8654781	-1.8499068	C	0.2247351	-1.7310939	-3.3724538
H	0.6464018	4.1561172	-0.0031983	C	-2.0594116	-2.0321406	-2.0860413
H	3.1757006	-0.0587551	1.0718217	C	-0.6270516	-1.8009761	-2.1958218
H	0.2346962	-3.9586325	-0.1230839	C	-0.0615827	-1.3044217	-1.0148674
H	-4.1109880	-2.1641504	-1.9229236	C	1.1804801	-0.5993329	-1.0041511
B	5.7252517	-1.0453835	0.9722457	C	1.1802090	0.2710373	0.1254589
F	7.0243374	-0.4557668	1.0258430	C	1.9133431	1.4618644	0.1861520
F	4.9777899	-0.6951843	2.1625978	H	-2.5970735	1.6346379	2.4822278
F	5.8273845	-2.4754860	0.8803410	H	-3.9181968	-1.7392164	-1.0309529
F	5.0020909	-0.5411147	-0.1746243	H	-0.1172554	-2.1513941	-4.3237324
Coran-cl5bf4-out1				H	3.5390677	1.0109339	-2.8757411
C	1.2295158	-0.7210610	0.2438577	H	1.9871152	3.3711055	1.3009410
C	1.2440933	0.7049645	0.2170170	Cl	-4.5822588	-0.0739936	1.3404918
C	-0.1063765	1.1574545	0.2559984	Cl	-2.9022487	-2.7801978	-3.4804055
C	-0.9515778	0.0153260	0.2987982	Cl	2.3778296	-0.8907574	-4.8526067
C	-0.1295676	-1.1443193	0.2989400	Cl	3.9428427	3.0259686	-0.9153907
C	2.2611195	-1.4866598	-0.3083602	Cl	-0.3788039	3.5615717	2.8529133
C	2.2672516	1.4611703	-0.3629947				

B	0.3328336	-0.7512206	3.9809593
F	0.7089235	-1.4578991	5.1614172
F	-0.4990737	-1.5844316	3.1471417
F	1.5076339	-0.3654149	3.2375830
F	-0.4066232	0.4400308	4.3312842
Coran-cl5bf4-in			
C	1.1487912	-0.3550486	1.3352852
C	0.7346610	1.0105594	1.3607810
C	-0.6909488	1.0381529	1.2907475
C	-1.1560875	-0.3088804	1.2262777
C	-0.0192665	-1.1700474	1.2549424
C	2.3923518	-0.7430602	0.8200764
C	1.5187792	2.0621771	0.8679772
C	-2.3501078	-0.6846238	0.5987146
C	-1.4151464	2.0946245	0.7227994
C	0.0010422	-2.4387741	0.6635716
C	3.3092171	0.3361182	0.5090136
C	2.4408657	-2.1373255	0.4124253
C	1.3112430	-2.9540195	0.3225761
C	2.8787048	1.6660673	0.5453128
C	0.7990272	3.2593466	0.4816523
C	-1.3057055	-2.8919179	0.2165709
C	-2.4302275	-2.0652790	0.1678679
C	-3.1849079	0.4431400	0.2204783
C	-2.7510630	1.7710513	0.2638759
C	-0.5980217	3.2591380	0.4259052
Cl	-1.4149335	4.7329826	-0.1790509
H	-3.3891783	2.5538629	-0.1569372
Cl	-4.7954875	0.1079898	-0.4697273
H	-3.3398388	-2.4315550	-0.3163576
Cl	-1.4444582	-4.5419419	-0.4480916
H	1.4054291	-3.9464329	-0.1276729
Cl	4.0056702	-2.7968275	-0.1527103
H	4.3157052	0.1109942	0.1424915
Cl	4.0296230	2.9370973	0.0284090
H	1.3468348	4.1390145	0.1301570
B	-0.2706595	-0.4120796	-2.4441178
F	0.1861111	-1.7591889	-2.2250840
F	0.3204023	0.4465378	-1.4411541
F	-1.7024210	-0.3669358	-2.3047826
F	0.1144765	0.0347386	-3.7428105

Coran-f5cl-side				F	4.3434013	1.3488471	-0.6540006
C	0.1413032	-0.0224293	3.3010125	F	2.6585821	-3.6653683	-0.6587072
C	-0.9769513	0.3464070	2.4551495	F	-2.6276176	-3.6232023	-0.6489916
C	-2.3695977	-0.0535190	2.5372564	Cl	-1.4520670	0.0123164	3.6369037
C	-3.1678966	-0.0344985	1.3897454	Coran-f5cl-out2			
C	1.4764970	-0.0356612	2.8931647	C	1.1537854	-0.7143798	0.7442355
C	-0.5700897	0.8990060	1.2299250	C	1.1623284	0.7138321	0.7462413
C	0.7851735	0.9145310	0.7815757	C	-0.1937882	1.1613549	0.7922103
C	1.8289028	0.3624338	1.5408894	C	-1.0401854	0.0154504	0.8248093
C	2.9906770	0.0025829	0.7484971	C	-0.2058626	-1.1448830	0.7910866
C	-3.2135964	-0.0553532	-1.2331948	C	2.1926560	-1.4671234	0.1678503
C	-2.3635278	-0.0316630	-2.3429322	C	2.1903572	1.4838519	0.1765651
C	-0.9641021	0.3431513	-2.3109720	C	-2.3533537	0.0043592	0.3319432
C	0.1176458	-0.0424540	-3.1931533	C	-0.6167798	2.3904078	0.2555363
C	1.4432178	-0.0161963	-2.7359980	C	-0.6142484	-2.3705718	0.2417105
C	3.0347710	-0.0324058	-0.6491319	C	3.3623202	-0.7111254	-0.2466706
C	1.8420405	0.3534120	-1.3839723	C	1.7765885	-2.8015759	-0.1988432
C	0.7823251	0.9102155	-0.6453774	C	0.4524785	-3.2545896	-0.1860946
C	-0.5793180	0.8996654	-1.0797517	C	3.3334711	0.6848517	-0.2193215
C	-1.4161736	0.8929307	0.0777611	C	1.8286862	2.8353746	-0.2010110
C	-2.7067031	0.3381485	0.0685373	C	-2.0289073	-2.4009590	-0.0825601
F	2.4037676	-0.4849372	-3.5801569	C	-2.8767089	-1.2969595	-0.0494120
F	-2.8607566	-0.5236082	-3.5376532	C	-2.8211120	1.3220891	-0.0598139
F	-4.4592339	-0.5291804	1.4951915	C	-2.0189668	2.4673137	-0.1073720
F	-0.1582231	-0.5159370	4.5620162	C	0.4869780	3.2344262	-0.1436001
F	4.0794461	-0.4576119	1.4536793	H	2.5640971	3.5270415	-0.6252586
H	-0.0775790	-0.4531977	-4.1892604	H	4.2406006	-1.2086487	-0.6720694
H	3.9494913	-0.4281350	-1.1642645	H	0.2355111	-4.2470237	-0.5962807
H	2.2295682	-0.4460450	3.5749209	H	-3.9213243	-1.4027200	-0.3519826
H	-2.7896148	-0.4662605	3.4609166	H	-2.4499998	3.3873522	-0.5154464
H	-4.2213128	-0.4670877	-1.3529493	F	0.1800437	4.4958150	-0.6334964
Cl	5.8023058	-1.0824087	-2.1798325	F	4.4347153	1.3616362	-0.7282897
Coran-f5cl-out1				F	2.7451376	-3.6506818	-0.7221443
C	1.0198467	-0.7185927	0.7280912	F	-2.5377953	-3.6061927	-0.5478037
C	1.0286230	0.7093958	0.7235971	F	-4.0830689	1.4226179	-0.5807572
C	-0.3241131	1.1586409	0.7383254	Cl	-4.5774197	-0.2303443	2.3955913
C	-1.1775242	0.0101356	0.7780862	Coran-f5cl-in			
C	-0.3385456	-1.1499384	0.7462041	C	0.2651521	1.1852930	0.9815479
C	2.0741619	-1.4732204	0.1918031	C	1.2092171	0.1141011	0.9815479
C	2.0733853	1.4744261	0.1827638	C	0.4821852	-1.1147746	0.9815479
C	-2.4484122	-0.0000260	0.1792724	C	-0.9112103	-0.8030697	0.9815479
C	-0.7290410	2.3802341	0.1826812	C	-1.0453441	0.6184503	0.9815479
C	-0.7265088	-2.3785187	0.1978538	C	0.5602989	2.4292870	0.4039251
C	3.2585315	-0.7211037	-0.1926360	C	2.4835311	0.2178150	0.4039251
C	1.6724527	-2.8139533	-0.1733360	C	-1.8811904	-1.6359990	0.4039251
C	0.3516845	-3.2674618	-0.1944132	C	0.9746077	-2.2946699	0.4039251
C	3.2273139	0.6731933	-0.1768067	C	-2.1372474	1.2835669	0.4039251
C	1.7258704	2.8262685	-0.2105707	C	1.9333543	2.6369802	-0.0056137
C	-2.1299609	-2.4160464	-0.1706342	C	-0.6182453	3.1722588	0.0166960
C	-2.9628103	-1.3005462	-0.2098871	C	-1.9104779	2.6536009	-0.0056137
C	-2.9102978	1.3159710	-0.1973551	C	2.8259491	1.5682681	0.0166960
C	-2.1263199	2.4717395	-0.2057628	C	3.1053566	-1.0238575	-0.0056137
C	0.3858356	3.2237918	-0.1919488	C	-3.2080457	0.3922957	0.0166960
H	2.4748383	3.5165771	-0.6127436	C	-3.1140946	-0.9969647	-0.0056137
H	4.1522253	-1.2230168	-0.5805651	C	-1.3644360	-2.9298067	0.0166960
H	0.1464084	-4.2652715	-0.5971450	C	-0.0141384	-3.2697590	-0.0056137
H	-3.9742967	-1.4129144	-0.6157129	C	2.3647779	-2.2030158	0.0166960
H	-2.5527965	3.3991899	-0.6007855	F	-4.3591571	0.9706600	-0.4953757
F	-4.1986802	1.4138927	-0.7054844	F	-2.2702062	-3.8458543	-0.4953757
F	0.0871625	4.4840929	-0.6916717	F	2.9560925	-3.3475287	-0.4953757

F	4.0971718	1.7769678	-0.4953757	C	0.3851355	3.2256143	-0.1992927
F	-0.4239011	4.4457552	-0.4953757	H	2.4767857	3.5163536	-0.6101764
H	-3.9285193	-1.5728078	-0.4569408	H	4.1502922	-1.2236975	-0.5709986
H	0.2818499	-4.2222682	-0.4569408	H	0.1471931	-4.2672451	-0.5976157
H	4.1027121	-1.0366975	-0.4569408	H	-3.9777377	-1.4160307	-0.6315258
H	2.2537657	3.5815539	-0.4569408	H	-2.5522304	3.4009288	-0.6187273
H	-2.7098083	3.2502196	-0.4569408	F	-4.2010627	1.4180393	-0.7259128
Cl	0.0000000	0.0000000	-2.2209808	F	0.0892759	4.4858243	-0.7008716
Coran-f5br-side				F	4.3427850	1.3488139	-0.6462332
C	0.1352376	-0.0226021	3.3057970	F	2.6592560	-3.6658604	-0.6495080
C	-0.9834766	0.3440507	2.4590239	F	-2.6288694	-3.6228037	-0.6617936
C	-2.3758217	-0.0551808	2.5416333	Br	-1.3893513	0.0054205	3.8383492
C	-3.1742021	-0.0360160	1.3936771	Coran-f5br-out2			
C	1.4707310	-0.0347407	2.8988830	C	1.1581098	-0.7114169	0.7472411
C	-0.5763054	0.8961033	1.2336041	C	1.1704921	0.7171628	0.7433397
C	0.7778149	0.9117289	0.7856319	C	-0.1840568	1.1686606	0.7878385
C	1.8227952	0.3621184	1.5464155	C	-1.0335331	0.0250590	0.8235917
C	2.9845336	0.0026813	0.7547277	C	-0.2023672	-1.1381088	0.7957953
C	-3.2198099	-0.0568827	-1.2296565	C	2.1945121	-1.4684043	0.1713123
C	-2.3701651	-0.0331025	-2.3397968	C	2.1991155	1.4820713	0.1683701
C	-0.9705614	0.3411257	-2.3078018	C	-2.3456594	0.0153829	0.3275785
C	0.1117752	-0.0436480	-3.1899783	C	-0.6044036	2.3973717	0.2478747
C	1.4373830	-0.0166551	-2.7333056	C	-0.6146244	-2.3637278	0.2485192
C	3.0253231	-0.0298910	-0.6434247	C	3.3639454	-0.7171945	-0.2499951
C	1.8345737	0.3533048	-1.3818798	C	1.7744281	-2.8026653	-0.1917950
C	0.7751953	0.9075116	-0.6415182	C	0.4497923	-3.2526330	-0.1759582
C	-0.5860134	0.8968230	-1.0758637	C	3.3389327	0.6788845	-0.2282078
C	-1.4220667	0.8898906	0.0815670	C	1.8406280	2.8330110	-0.2146586
C	-2.7126532	0.3357121	0.0724251	C	-2.0274596	-2.3915736	-0.0789371
F	2.3999804	-0.4852708	-3.5757181	C	-2.8738122	-1.2848699	-0.0485385
F	-2.8683658	-0.5229760	-3.5346062	C	-2.8112035	1.3336516	-0.0625741
F	-4.4654853	-0.5301591	1.4992879	C	-2.0065286	2.4768926	-0.1130716
F	-0.1635881	-0.5151667	4.5667793	C	0.5007612	3.2369244	-0.1567019
F	4.0749006	-0.4595267	1.4543963	H	2.5769667	3.5188914	-0.6465624
H	-0.0828692	-0.4546049	-4.1860636	H	4.2384476	-1.2187240	-0.6785700
H	3.9326169	-0.4231250	-1.1547260	H	0.2298948	-4.2450925	-0.5842516
H	2.2237990	-0.4430407	3.5816422	H	-3.9162655	-1.3891029	-0.3592247
H	-2.7963031	-0.4669829	3.4654347	H	-2.4360493	3.3965701	-0.5232301
H	-4.2281771	-0.4670450	-1.3494457	F	0.1959166	4.4956906	-0.6534551
Br	5.9871964	-1.1350812	-2.2967957	F	4.4384541	1.3510891	-0.7460118
Coran-f5br-out1				F	2.7394636	-3.6541212	-0.7161184
C	1.0145791	-0.7169698	0.7252277	F	-2.5374007	-3.5936373	-0.5481837
C	1.0236553	0.7101034	0.7196770	F	-4.0765645	1.4367414	-0.5758655
C	-0.3290061	1.1598717	0.7265469	Br	-4.7394423	-0.3368929	2.4908129
C	-1.1812006	0.0116180	0.7539786	Coran-f5br-in			
C	-0.3441245	-1.1486053	0.7361166	C	0.2649370	1.1855679	0.9905700
C	2.0710537	-1.4723668	0.1946162	C	1.2094122	0.1143905	0.9905700
C	2.0706517	1.4751192	0.1837105	C	0.4825208	-1.1148707	0.9905700
C	-2.4534762	0.0010483	0.1599184	C	-0.9111979	-0.8034185	0.9905700
C	-0.7314587	2.3818086	0.1695871	C	-1.0456721	0.6183307	0.9905700
C	-0.7295400	-2.3784244	0.1879868	C	0.5597877	2.4287746	0.4103455
C	3.2566286	-0.7209288	-0.1858614	C	2.4828859	0.2181429	0.4103455
C	1.6710891	-2.8140681	-0.1697283	C	-1.8804757	-1.6358850	0.4103455
C	0.3502663	-3.2681486	-0.1969486	C	0.9747201	-2.2939549	0.4103455
C	3.2256650	0.6738250	-0.1709694	C	-2.1369180	1.2829224	0.4103455
C	1.7251118	2.8271697	-0.2109798	C	1.9323918	2.6366025	-0.0004724
C	-2.1321332	-2.4160949	-0.1837712	C	-0.6184254	3.1716466	0.0217444
C	-2.9669044	-1.3012317	-0.2257693	C	-1.9104161	2.6525688	-0.0004724
C	-2.9141487	1.3183554	-0.2165228	C	2.8253112	1.5682502	0.0217444
C	-2.1278109	2.4728028	-0.2227414	C	3.1046999	-1.0230588	-0.0004724

C	-3.2075191	0.3919352	0.0217444	C	-2.2454658	0.0016684	-0.1638252
C	-3.1130939	-0.9972248	-0.0004724	C	-0.5192149	2.3812149	-0.1942115
C	-1.3639304	-2.9294173	0.0217444	C	-0.5270809	-2.3811323	-0.2608318
C	-0.0135817	-3.2688876	-0.0004724	C	3.4419858	-0.7214286	-0.7939403
C	2.3645637	-2.2024147	0.0217444	C	1.8529188	-2.8159074	-0.7334057
F	-4.3555349	0.9702564	-0.4948357	C	0.5337204	-3.2712131	-0.7011742
F	-2.2687030	-3.8425342	-0.4948357	C	3.4157058	0.6739416	-0.7525086
F	2.9533994	-3.3450731	-0.4948357	C	1.9173843	2.8327833	-0.6768302
F	4.0940042	1.7751653	-0.4948357	C	-1.9457552	-2.4083483	-0.5571791
F	-0.4231657	4.4421856	-0.4948357	C	-2.7835116	-1.2938516	-0.5304235
H	-3.9251637	-1.5728337	-0.4560645	C	-2.7272402	1.3314644	-0.4735254
H	0.2829115	-4.2190849	-0.4560645	C	-1.9322864	2.4780083	-0.5093769
H	4.1000126	-1.0347041	-0.4560645	C	0.5823312	3.2357724	-0.5909709
H	2.2510357	3.5796026	-0.4560645	H	2.6518275	3.5318882	-1.0906686
H	-2.7087961	3.2470202	-0.4560645	H	4.3153519	-1.2174884	-1.2304643
Br	0.0000000	0.0000000	-2.3555635	H	0.3137377	-4.2698631	-1.0936095
Coran-f5bf4-side				H	-3.8205892	-1.4074761	-0.8625053
C	-1.9240954	-3.0872335	-0.0122824	H	-2.3774933	3.4165083	-0.8552754
C	-2.6686162	-1.8562913	0.1692685	F	-4.0426893	1.4495989	-0.8856031
C	-3.9065667	-1.4225367	-0.4535442	F	0.2694126	4.5101378	-1.0374233
C	-4.1901640	-0.0585840	-0.5604892	F	4.5102282	1.3539802	-1.2677777
C	-0.5502829	-3.2228285	0.1988515	F	2.8172428	-3.6622549	-1.2639681
C	-1.9111304	-0.8498417	0.7873022	F	-2.4723970	-3.6053116	-1.0182961
C	-0.5075876	-0.9537659	1.0295494	B	-1.4340514	-0.0185578	3.3866887
C	0.2294778	-2.0861171	0.6541216	F	-2.0113135	-1.1909115	2.7749596
C	1.6475859	-1.8209580	0.4882006	F	-0.0119840	-0.0150025	3.1399465
C	-3.2117344	2.3784283	-0.5717721	F	-1.6861286	-0.0254862	4.7927776
C	-2.0141697	3.0794811	-0.3974963	F	-2.0155622	1.1581759	2.7863962
C	-0.8120850	2.5352539	0.2038057	Coran-f5bf4-out2			
C	0.5740254	2.9160347	0.0151932	C	1.4919419	-0.7464188	0.2984180
C	1.5975051	1.9875876	0.2527528	C	1.4731086	0.6824596	0.3278326
C	2.2252072	-0.5489093	0.4731924	C	0.1107608	1.1027150	0.3913229
C	1.3745279	0.6098434	0.6680005	C	-0.7100051	-0.0604871	0.3947388
C	0.0410344	0.3632788	1.0350182	C	0.1400687	-1.2027930	0.3440185
C	-1.0261625	1.2835080	0.8019475	C	2.5354900	-1.4672590	-0.2997262
C	-2.2326768	0.5350622	0.6481780	C	2.4796239	1.4802245	-0.2362207
C	-3.3152591	1.0062771	-0.1106409	C	-2.0118445	-0.0842189	-0.1095838
F	2.8717015	2.3650573	-0.0400653	C	-0.3421209	2.3301399	-0.1119995
F	-1.9288788	4.3434693	-0.9507639	C	-0.2491379	-2.4303034	-0.2068677
F	-5.3296289	0.3094747	-1.2564826	C	3.6869628	-0.6839515	-0.7158791
F	-2.6065253	-4.1632300	-0.5544549	C	2.1422161	-2.8093904	-0.6789822
F	2.4390805	-2.9046615	0.1980225	C	0.8314302	-3.2908000	-0.6554919
H	0.8459774	3.8892374	-0.4075001	C	3.6317221	0.7104958	-0.6635911
H	3.2893558	-0.4461186	0.2205144	C	2.0885423	2.8346096	-0.5813291
H	-0.0654469	-4.1630851	-0.0848311	C	-1.6656168	-2.4838445	-0.5132829
H	-4.5855563	-2.1377300	-0.9301007	C	-2.5233326	-1.3864767	-0.4829176
H	-4.0175871	2.8518916	-1.1427268	C	-2.5223811	1.2327394	-0.4267031
B	5.9492316	-0.1410494	-0.0753632	C	-1.7500475	2.3957522	-0.4476700
F	4.9375240	-0.3453952	-1.0973175	C	0.7433012	3.2075286	-0.5005657
F	5.2769135	-0.0607921	1.2049978	H	2.8079606	3.5492986	-0.9945766
F	6.8547338	-1.2482663	-0.0738018	H	4.5699009	-1.1583412	-1.1573848
F	6.6452860	1.0804415	-0.3330007	H	0.6319698	-4.2871282	-1.0649029
Coran-f5bf4-out1				H	-3.5623705	-1.5137970	-0.8010425
C	1.2495276	-0.7304053	0.2243986	H	-2.2092825	3.3245046	-0.8006474
C	1.2613269	0.6972814	0.2437025	F	0.4072890	4.4736742	-0.9503909
C	-0.0906108	1.1459868	0.3047274	F	4.7122225	1.4163867	-1.1726511
C	-0.9341864	0.0008036	0.3141804	F	3.1241284	-3.6296008	-1.2183773
C	-0.1101019	-1.1576974	0.2729045	F	-2.1635890	-3.6907944	-0.9795768
C	2.2747289	-1.4769716	-0.3693606	F	-3.8177322	1.3198526	-0.8745950
C	2.2803470	1.4700524	-0.3279747	B	-2.8179351	0.1729206	2.9889473

F	-3.8967621	0.0896990	2.0300963
F	-1.9929626	-1.0023822	2.8650992
F	-3.3486496	0.2643894	4.3117018
F	-2.0246629	1.3404771	2.6925698
Coran-f5bf4-in			
C	-0.4414345	1.1056610	1.3838535
C	0.9647707	0.8528527	1.3591259
C	1.1569220	-0.5604869	1.2760950
C	-0.1295849	-1.1806620	1.2513384
C	-1.1175093	-0.1507443	1.3179677
C	-0.9878983	2.2949022	0.8772428
C	1.8961865	1.7586821	0.8282699
C	-0.3798370	-2.3998126	0.6039551
C	2.2697335	-1.1471474	0.6524337
C	-2.3905364	-0.2755200	0.7426397
C	-0.0422351	3.3316413	0.5174202
C	-2.3747428	2.1656947	0.4863490
C	-3.0626083	0.9585749	0.3980074
C	1.3221505	3.0487035	0.5152972
C	3.1494104	1.1940616	0.3712637
C	-2.6813005	-1.6136403	0.2750050
C	-1.7434221	-2.6381442	0.1843913
C	0.8234013	-3.0702779	0.1622755
C	2.0935472	-2.4976043	0.1623904
C	3.2988066	-0.1901996	0.3097181
F	-3.9399639	-1.8405004	-0.2414415
F	0.6778983	-4.3136665	-0.4164239
F	4.4682583	-0.6879556	-0.2419787
F	2.1851011	4.0303368	0.0526573
F	-3.0114338	3.3103663	0.0336737
H	-2.0175931	-3.5546366	-0.3458972
H	2.9096913	-3.0330813	-0.3329052
H	3.9413467	1.8275999	-0.0413245
H	-0.3798971	4.2983008	0.1295737
H	-4.0527662	0.9497857	-0.0674374
B	-0.4815722	-0.3947190	-2.4516773
F	0.2447562	0.3143281	-1.4219179
F	-0.1011941	0.1048498	-3.7338046
F	-0.1742010	-1.7979211	-2.3546691
F	-1.8923054	-0.2000049	-2.2407734

Coran-cn5cl-out1

C 1.0489830 -0.7053808 0.8250617
C 1.0588375 0.7214776 0.7988066
C -0.2867694 1.1727268 0.8888217
C -1.1471533 0.0260539 1.0414511
C -0.3022242 -1.1353643 0.9321129
C 2.0725821 -1.4734463 0.2603862
C 2.0814742 1.4689701 0.2051240
C -2.4279224 0.0135870 0.4436536
C -0.7074841 2.3834090 0.3377438
C -0.7231963 -2.3656634 0.4216369
C 3.2424521 -0.7361383 -0.1714078
C 1.6820396 -2.8484766 -0.0616709
C 0.3298650 -3.2637041 0.0060363
C 3.2573428 0.6758673 -0.1928137
C 1.7269234 2.8142034 -0.1735117
C -2.1590794 -2.4463200 0.1142415
C -2.9571943 -1.2741697 0.0931534
C -2.9427004 1.3334649 0.0663193
C -2.1228806 2.4815540 0.0321958
C 0.3820586 3.2567495 -0.1118477
H 2.4811579 3.4810127 -0.6071384
H 4.1088457 -1.2757911 -0.5719554
H 0.0731739 -4.2664671 -0.3559188
H -3.9845626 -1.3526770 -0.2821955
H -2.5412756 3.4234518 -0.3390496
C 4.4095310 1.3593934 -0.7132868
N 5.3361443 1.9526059 -1.1328744
C 0.0591112 4.5656413 -0.6131652
N -0.2335443 5.6320228 -1.0166265
C -4.3022754 1.4395707 -0.3924231
N -5.4161535 1.4950983 -0.7688282
C -2.7088833 -3.6961771 -0.3189472
N -3.1212343 -4.7425233 -0.6732649
C 2.6768901 -3.7534892 -0.5683344
N 3.5203832 -4.4661715 -0.9776339
Cl -1.4631853 0.1050977 3.5755247

Coran-cn5cl-out2

C 1.1061320 -0.6773614 0.9059917
C 1.1333869 0.7532945 0.8643279
C -0.2140860 1.2156589 0.9028292
C -1.0687307 0.0792363 0.9869600
C -0.2481868 -1.0945124 0.9934257
C 2.1338242 -1.4495528 0.3398508
C 2.1684359 1.4887729 0.2782073
C -2.3777814 0.0794848 0.5074290
C -0.6218972 2.4359829 0.3460546
C -0.6909239 -2.3138791 0.4448748
C 3.3027757 -0.7279684 -0.0900752
C 1.7234346 -2.8189948 -0.0027177
C 0.3696225 -3.2201129 0.0398663
C 3.3375386 0.6926966 -0.1099643
C 1.8265932 2.8418848 -0.1082332
C -2.1016387 -2.3843480 0.1236927
C -2.9802422 -1.2460249 0.2992537
C -2.8632784 1.3826972 0.0717979
C -2.0170385 2.5241752 0.0018720
C 0.4895210 3.3018227 -0.0743607
H 2.5977261 3.5004119 -0.5248928
H 4.1581264 -1.2743667 -0.5052684

H 0.1085159 -4.2170754 -0.3353558
H -3.9628258 -1.2977882 -0.1753868
H -2.4219641 3.4508543 -0.4206547
C 0.1948994 4.6209479 -0.5673413
N -0.0747819 5.6976807 -0.9591350
C 4.4922582 1.3661529 -0.6325166
N 5.4235075 1.9546173 -1.0503017
C 2.7165952 -3.7299454 -0.5049585
N 3.5622297 -4.4424317 -0.9089642
C -2.6288177 -3.5937332 -0.4257208
N -3.0149169 -4.6059312 -0.8925301
C -4.2081191 1.5070697 -0.4263570
N -5.2979164 1.6115403 -0.8567579
Cl -4.0505011 -1.4106185 2.4591583

Coran-cn5cl-in

C 0.2384095 -1.1919414 1.1084344
C 1.2072762 -0.1415892 1.1084344
C 0.5077282 1.1044344 1.1084344
C -0.8934829 0.8241672 1.1084344
C -1.0599310 -0.5950711 1.1084344
C 0.4966771 -2.4304132 0.5125973
C 2.4649420 -0.2786710 0.5125973
C -1.8303812 1.6743061 0.5125973
C 1.0267408 2.2581850 0.5125973
C -2.1579786 -1.2234069 0.5125973
C 1.8597666 -2.6749338 0.1061127
C -0.6925118 -3.1899021 0.1215933
C -1.9693137 -2.5953432 0.1061127
C 2.8197793 -1.6443518 0.1215933
C 3.1187127 0.9421432 0.1061127
C -3.2477751 -0.3271161 0.1215933
C -3.0768694 1.0709235 0.1061127
C -1.3147236 2.9877333 0.1215933
C 0.0677038 3.2572103 0.1061127
C 2.4352313 2.1736368 0.1215933
H 0.4166988 4.2040879 -0.3206595
H -3.8695582 1.6954387 -0.3206595
H -2.8082173 -3.1562491 -0.3206595
H 2.1339844 -3.6461080 -0.3206595
H 4.1270922 0.9028305 -0.3206595
C 4.1436171 -1.9045160 -0.3741971
N 5.2441810 -2.0891992 -0.7483619
C -0.5308543 -4.5293418 -0.3741971
N -0.3664055 -5.6331106 -0.7483619
C -4.4717030 -0.8947712 -0.3741971
N -5.4706321 -1.3922546 -0.7483619
C -2.2328102 3.9763428 -0.3741971
N -3.0146310 4.7726499 -0.7483619
C 3.0917504 3.3522862 -0.3741971
N 3.6074876 4.3419144 -0.7483619
Cl 0.0000000 0.0000000 -2.0240439

Coran-cn5br-out1

C 1.0458683 -0.7047782 0.8141465
C 1.0550858 0.7208878 0.7872574
C -0.2914337 1.1719539 0.8678155
C -1.1481604 0.0250990 0.9970321
C -0.3061866 -1.1355920 0.9116251
C 2.0733102 -1.4750678 0.2594769
C 2.0822614 1.4707410 0.2042418
C -2.4361466 0.0124880 0.4248402

C	-0.7102306	2.3854215	0.3201136	C	-2.6305185	-3.6233023	-0.4095636
C	-0.7255623	-2.3686581	0.4068708	N	-3.0118377	-4.6544319	-0.8353694
C	3.2450901	-0.7365201	-0.1650640	C	-4.2146438	1.5146424	-0.4381615
C	1.6837542	-2.8509530	-0.0603180	N	-5.3079560	1.6221752	-0.8583973
C	0.3303024	-3.2671831	0.0004795	Br	-4.1639534	-1.3376179	2.6445245
C	3.2596988	0.6766593	-0.1866445	Coran-cn5br-in			
C	1.7288605	2.8178392	-0.1719561	C	0.2386374	-1.1912898	1.1150505
C	-2.1631429	-2.4480627	0.1036580	C	1.2067270	-0.1411712	1.1150505
C	-2.9668542	-1.2792355	0.0857723	C	0.5071609	1.1040412	1.1150505
C	-2.9508467	1.3353474	0.0552279	C	-0.8932843	0.8235062	1.1150505
C	-2.1268012	2.4816040	0.0186714	C	-1.0592409	-0.5950864	1.1150505
C	0.3828416	3.2603037	-0.1174664	C	0.4959872	-2.4300489	0.5160964
H	2.4851112	3.4879219	-0.5979027	C	2.4643823	-0.2792145	0.5160964
H	4.1147531	-1.2745711	-0.5603049	C	-1.8296090	1.6744169	0.5160964
H	0.0790829	-4.2724075	-0.3581487	C	1.0270848	2.2574848	0.5160964
H	-3.9983716	-1.3634446	-0.2766973	C	-2.1578453	-1.2226383	0.5160964
H	-2.5482482	3.4251436	-0.3469860	C	1.8592665	-2.6750371	0.1096831
C	4.4137338	1.3602636	-0.7041326	C	-0.6931183	-3.1904764	0.1267371
N	5.3397521	1.9543502	-1.1238091	C	-1.9695665	-2.5948994	0.1096831
C	0.0627874	4.5705129	-0.6160715	C	2.8201381	-1.6451061	0.1267371
N	-0.2300283	5.6367060	-1.0203871	C	3.1186564	0.9416356	0.1096831
C	-4.3126001	1.4453743	-0.3949322	C	-3.2485087	-0.3267167	0.1267371
N	-5.4277569	1.5017754	-0.7672334	C	-3.0765255	1.0713010	0.1096831
C	-2.7122799	-3.6993141	-0.3277361	C	-1.3145705	2.9885544	0.1267371
N	-3.1230556	-4.7453630	-0.6836685	C	0.0681691	3.2569999	0.1096831
C	2.6811703	-3.7562414	-0.5610855	C	2.4360595	2.1737449	0.1267371
N	3.5272235	-4.4670205	-0.9678361	H	0.4174169	4.2036574	-0.3173764
Br	-1.4112784	0.1122273	3.7682739	H	-3.8689269	1.6959886	-0.3173764
Coran-cn5br-out2				H	-2.8085452	-3.1554788	-0.3173764
C	1.1057207	-0.6800272	0.8832073	H	2.1331505	-3.6461818	-0.3173764
C	1.1294462	0.7493900	0.8505068	H	4.1269047	0.9020145	-0.3173764
C	-0.2190257	1.2098893	0.8828055	C	4.1434115	-1.9048689	-0.3702781
C	-1.0713222	0.0723665	0.9477306	N	5.2436379	-2.0889383	-0.7461702
C	-0.2492595	-1.0991538	0.9522168	C	-0.5312534	-4.5292554	-0.3702781
C	2.1379394	-1.4510277	0.3268712	N	-0.3663251	-5.6325135	-0.7461702
C	2.1686255	1.4912015	0.2809384	C	-4.4717442	-0.8943649	-0.3702781
C	-2.3796475	0.0713650	0.4657885	N	-5.4700393	-1.3921465	-0.7461702
C	-0.6241097	2.4360573	0.3378296	C	-2.2324365	3.9765075	-0.3702781
C	-0.6836105	-2.3231873	0.4158765	N	-3.0143451	4.7721196	-0.7461702
C	3.3103277	-0.7244159	-0.0887901	C	3.0920226	3.3519817	-0.3702781
C	1.7343991	-2.8226234	-0.0127917	N	3.6070716	4.3414786	-0.7461702
C	0.3803649	-3.2294745	0.0244521	Br	0.0000000	0.0000000	-2.1684189
C	3.3417732	0.6961603	-0.1008967	Coran-cn5bf4-out1			
C	1.8278180	2.8480122	-0.0945634	C	1.1889557	-0.7095281	0.4303553
C	-2.1002517	-2.3934214	0.0948733	C	1.1986370	0.7165605	0.4028260
C	-2.9629979	-1.2500379	0.2239646	C	-0.1530169	1.1640610	0.4308871
C	-2.8674320	1.3842061	0.0502953	C	-0.9939318	0.0190897	0.4659770
C	-2.0201113	2.5247426	-0.0079315	C	-0.1684689	-1.1373094	0.4755730
C	0.4888349	3.3062613	-0.0654651	C	2.2156989	-1.4792740	-0.1148354
H	2.6000731	3.5133012	-0.4983256	C	2.2253896	1.4637423	-0.1733329
H	4.1719270	-1.2667986	-0.4959099	C	-2.2998986	0.0094394	-0.0092678
H	0.1262601	-4.2310245	-0.3428536	C	-0.5696595	2.3820679	-0.1004649
H	-3.9688274	-1.3173100	-0.1966010	C	-0.5853937	-2.3755088	-0.0058884
H	-2.4263794	3.4563348	-0.4183368	C	3.3920023	-0.7429067	-0.5320131
C	0.1971905	4.6293880	-0.5490368	C	1.8259844	-2.8613180	-0.4349072
N	-0.0685578	5.7085552	-0.9364875	C	0.4766208	-3.2842417	-0.3835001
C	4.5009298	1.3735541	-0.6093001	C	3.4046312	0.6711036	-0.5564859
N	5.4340853	1.9665591	-1.0157686	C	1.8730789	2.8169655	-0.5520907
C	2.7343343	-3.7315032	-0.5047950	C	-2.0220835	-2.4503296	-0.3062130
N	3.5856804	-4.4412906	-0.9016752	C	-2.8405974	-1.2980987	-0.3084490

C	-2.8182645	1.3366697	-0.3610279	F	0.7667157	-1.5747897	5.1947453
C	-1.9818018	2.4745479	-0.4083828	F	-0.4576067	-1.6928727	3.1903128
C	0.5318514	3.2650277	-0.5114187	F	1.5545746	-0.4826282	3.2668995
H	2.6379187	3.4878106	-0.9599935	F	-0.3466934	0.3293461	4.3745093
H	4.2647900	-1.2811031	-0.9199771	Coran-cn5bf4-in			
H	0.2339238	-4.2986161	-0.7213030	C	1.1298368	-0.3716087	1.3715250
H	-3.8853934	-1.3991242	-0.6234768	C	0.7121261	0.9926734	1.3975580
H	-2.4028790	3.4205757	-0.7672651	C	-0.7132606	1.0157858	1.3278200
C	4.5605809	1.3541855	-1.0717391	C	-1.1753982	-0.3324234	1.2698421
N	5.4880403	1.9462176	-1.4894806	C	-0.0360054	-1.1905049	1.2971414
C	0.2225712	4.5843065	-0.9944980	C	2.3640554	-0.7650393	0.8483717
N	-0.0622481	5.6558870	-1.3887813	C	1.4976344	2.0350861	0.8986735
C	-4.1887087	1.4579924	-0.7799437	C	-2.3697898	-0.7015598	0.6483732
N	-5.3099748	1.5206890	-1.1313643	C	-1.4300407	2.0702704	0.7569814
C	-2.5753169	-3.7116372	-0.7180587	C	-0.0238321	-2.4559808	0.7078243
N	-2.9858201	-4.7600781	-1.0610252	C	3.2810065	0.3038890	0.5270797
C	2.8322060	-3.7684473	-0.9160090	C	2.4330952	-2.1714764	0.4378698
N	3.6844436	-4.4792503	-1.3082832	C	1.2787063	-2.9773922	0.3628134
B	-1.2878690	0.0581193	3.5009142	C	2.8724508	1.6547284	0.5597775
F	0.1280412	0.0706294	3.1952187	C	0.7858532	3.2289288	0.5052760
F	-1.4896486	0.0850833	4.9028470	C	-1.3345058	-2.9292240	0.2530348
F	-1.8666023	-1.1355639	2.9266833	C	-2.4563781	-2.0774957	0.2149774
F	-1.8979629	1.2113563	2.8777699	C	-3.2265317	0.4222148	0.2602762
Coran-cn5bf4-out2				C	-2.7652982	1.7536657	0.3031863
C	-2.0367145	0.8804290	1.9447849	C	-0.6237558	3.2544467	0.4439716
C	-0.6176592	1.0344585	1.7160552	H	-3.3990162	2.5428836	-0.1165771
C	0.2410722	2.1954559	1.9613573	H	-3.3740066	-2.4387599	-0.2614775
C	1.4764806	2.3609753	1.2976784	H	1.3632502	-3.9759493	-0.0795477
C	-2.7901011	-0.0934819	1.2552600	H	4.2836754	0.0675399	0.1531872
C	-0.0211764	0.0316608	0.9596337	H	1.3429293	4.1016979	0.1463040
C	-0.7753442	-0.9518089	0.2625255	C	3.7935546	2.6798039	0.1490723
C	-2.1693987	-0.9971133	0.2756680	N	4.5276893	3.5472161	-0.1568830
C	-2.7777425	-1.6994793	-0.8326168	C	3.6942411	-2.6998650	-0.0058992
C	2.9038791	1.5490272	-0.7634908	N	4.7504939	-3.1030334	-0.3324630
C	2.9126697	0.6826695	-1.8834802	C	-1.4444399	-4.2639278	-0.2697992
C	1.9856082	-0.4245718	-1.9837211	N	-1.5072161	-5.3747717	-0.6523287
C	1.5097208	-1.1302554	-3.1840040	C	-4.5303823	0.1465228	-0.2788483
C	0.2800355	-1.8289981	-3.2003370	N	-5.6068795	-0.1089983	-0.6789355
C	-2.0139502	-2.1386597	-1.9417371	C	-1.2856788	4.4389664	-0.0329610
C	-0.5674520	-1.8941244	-2.0266493	N	-1.8599566	5.4007421	-0.3937155
C	-0.0044308	-1.3912469	-0.8520859	B	-0.1895964	-0.3445981	-2.3368740
C	1.2343724	-0.6808123	-0.8353150	F	0.3116475	-1.6669503	-2.0626349
C	1.2221325	0.1943626	0.2897874	F	0.4229750	0.5759159	-1.3980268
C	1.9537018	1.3807669	0.3441172	F	-1.6134528	-0.3280613	-2.1192954
H	-2.5541384	1.5714749	2.6180969	F	0.1204301	0.0442321	-3.6624319
H	-3.8668427	-1.8222333	-0.8679336				
H	-0.0694556	-2.2511183	-4.1500201				
H	3.5773652	0.9178186	-2.7228515				
H	2.0334832	3.2922862	1.4495234				
C	-0.2460103	3.2574913	2.7994199				
N	-0.6764288	4.1375237	3.4501243				
C	3.7740387	2.6951906	-0.7673510				
N	4.4730542	3.6414821	-0.7478206				
C	2.2657387	-1.0119682	-4.4017600				
N	2.9101464	-0.8941024	-5.3796319				
C	-2.6795632	-2.7391680	-3.0659704				
N	-3.1854344	-3.2320835	-4.0074105				
C	-4.2169155	-0.1418016	1.4236373				
N	-5.3884525	-0.2094313	1.5130529				
B	0.3864610	-0.8690752	4.0268880				

Coran-cl10cl-out1			Cl	4.9658433	-1.5311457	-0.3651827	
C	1.0072360	-0.7096659	0.3918335	Cl	4.9634522	1.5402161	-0.3610253
C	1.0077339	0.7097164	0.3885787	Cl	3.0675476	4.1343761	-0.4032334
C	-0.3387088	1.1490639	0.4059728				
C	-1.1818011	0.0007712	0.4540579	Cl	-3.4279259	-0.0146045	2.8340972
C	-0.3397691	-1.1476205	0.4094417	Coran-cl10cl-in			
C	2.1072217	-1.5057044	0.0686247	C	-0.9767448	0.7096466	0.6182761
C	2.1074130	1.5033795	0.0578993	C	-0.9767448	-0.7096466	0.6182761
C	-2.5154104	0.0008655	0.0345779	C	0.3730833	-1.1482324	0.6182761
C	-0.7528559	2.4294212	0.0437506	C	1.2073230	0.0000000	0.6182761
C	-0.7537330	-2.4298989	0.0535486	C	0.3730833	1.1482324	0.6182761
C	3.3338830	-0.7126518	-0.0899968	C	-2.0663633	1.5013008	0.2587290
C	1.7334073	-2.9023978	-0.1514195	C	-2.0663633	-1.5013008	0.2587290
C	0.3749722	-3.3370626	-0.1664020	C	2.5541654	0.0000000	0.2587290
C	3.3340386	0.7089527	-0.0945857	C	0.7892805	-2.4291557	0.2587290
C	1.7333422	2.8972239	-0.1776629	C	0.7892805	2.4291557	0.2587290
C	-2.2073578	-2.5102746	-0.1383873	C	-3.2793578	0.7112955	0.0418604
C	-3.0339765	-1.3526923	-0.1691891	C	-1.6898595	2.8990522	0.0418604
C	-3.0365843	1.3564054	-0.1575149	C	-0.3368951	3.3386570	0.0418604
C	-2.2087378	2.5120700	-0.1329878	C	-3.2793578	-0.7112955	0.0418604
C	0.3746473	3.3319346	-0.1946327	C	-1.6898595	-2.8990522	0.0418604
Cl	0.0687393	5.0396454	-0.5648357	C	2.2349672	2.5030083	0.0418604
Cl	-2.9847591	4.0976985	-0.3135146	C	3.0711452	1.3521080	0.0418604
Cl	-4.7719099	1.6017341	-0.4295370	C	3.0711452	-1.3521080	0.0418604
Cl	-4.7634591	-1.5947171	-0.4792070	C	2.2349672	-2.5030083	0.0418604
Cl	-2.9828678	-4.0932241	-0.3453156	C	-0.3368951	-3.3386570	0.0418604
Cl	0.0707318	-5.0525962	-0.5003291	Cl	-0.0342955	-5.0637375	-0.2347416
Cl	2.9934427	-4.1163186	-0.4525746	Cl	3.0041359	-4.0764913	-0.2347416
Cl	4.8945055	-1.5387908	-0.2656174	Cl	4.8053027	-1.5973979	-0.2347416
Cl	4.8952412	1.5334264	-0.2723684	Cl	4.8053027	1.5973979	-0.2347416
Cl	2.9922951	4.1062791	-0.5021868	Cl	3.0041359	4.0764913	-0.2347416
Cl	-1.1512006	0.0247830	3.2879179	Cl	-0.0342955	5.0637375	-0.2347416
Coran-cl10cl-out2			Cl	-2.9486446	4.1168081	-0.2347416	
C	1.0916126	-0.7080676	0.3780570	Cl	-4.8264984	1.5321640	-0.2347416
C	1.0902994	0.7099608	0.3795907	Cl	-4.8264984	-1.5321640	-0.2347416
C	-0.2612945	1.1448351	0.3908365	Cl	-2.9486446	-4.1168081	-0.2347416
C	-1.0911804	-0.0013011	0.3945364	Cl	0.0000000	0.0000000	-2.4548073
C	-0.2592216	-1.1457396	0.3880317	Coran-cl10br-out1			
C	2.1899197	-1.5062902	0.0489337	C	1.0016563	-0.7086054	0.3723946
C	2.1875400	1.5100607	0.0517553	C	1.0021991	0.7093776	0.3692612
C	-2.4614462	-0.0018918	0.1346683	C	-0.3443682	1.1490921	0.3776963
C	-0.6824338	2.4362474	0.0662295	C	-1.1851379	0.0012373	0.4102122
C	-0.6783840	-2.4369552	0.0596953	C	-0.3452859	-1.1471897	0.3828245
C	3.4099128	-0.7096867	-0.1325250	C	2.1034292	-1.5069110	0.0626792
C	1.8134194	-2.9063372	-0.1443696	C	2.1043604	1.5050918	0.0545684
C	0.4516313	-3.3461025	-0.1365890	C	-2.5225663	0.0008422	0.0087287
C	3.4088209	0.7155617	-0.1310000	C	-0.7571233	2.4327319	0.0258079
C	1.8086163	2.9097979	-0.1392864	C	-0.7590060	-2.4324550	0.0382958
C	-2.1323104	-2.5083280	-0.1324747	C	3.3288284	-0.7134801	-0.0970426
C	-2.9742424	-1.3605521	-0.1032641	C	1.7300454	-2.9071805	-0.1410697
C	-2.9771851	1.3570735	-0.0956652	C	0.3710880	-3.3422964	-0.1615724
C	-2.1370631	2.5062461	-0.1220791	C	3.3292989	0.7099021	-0.1008861
C	0.4460131	3.3473042	-0.1301406	C	1.7320712	2.9042505	-0.1584085
Cl	0.1461797	5.0767912	-0.3862318	C	-2.2130775	-2.5122180	-0.1518718
Cl	-2.9037498	4.0834185	-0.3915764	C	-3.0423914	-1.3554699	-0.1809268
Cl	-4.6975503	1.5978837	-0.3855597	C	-3.0421999	1.3572549	-0.1831362
Cl	-4.6929132	-1.6022701	-0.4017216	C	-2.2117996	2.5130376	-0.1610162
Cl	-2.8956833	-4.0851846	-0.4126816	C	0.3733241	3.3401016	-0.1818191
Cl	0.1548324	-5.0760174	-0.3930497	Cl	0.0718643	5.0579771	-0.5043499
Cl	3.0746626	-4.1284458	-0.4084658	Cl	-2.9850455	4.0958859	-0.3708294

Cl	-4.7764633	1.6021371	-0.4598214	C	2.2338838	-2.5021106	0.0463014
Cl	-4.7749914	-1.5994923	-0.4686219	C	-0.3365463	-3.3372939	0.0463014
Cl	-2.9872847	-4.0947774	-0.3611016	Cl	-0.0339279	-5.0607914	-0.2357587
Cl	0.0686238	-5.0628860	-0.4684698	Cl	3.0021067	-4.0743239	-0.2357587
Cl	2.9922272	-4.1268933	-0.4047876	Cl	4.8026143	-1.5961379	-0.2357587
Cl	4.8879130	-1.5387114	-0.2889912	Cl	4.8026143	1.5961379	-0.2357587
Cl	4.8890875	1.5329761	-0.2945304	Cl	3.0021067	4.0743239	-0.2357587
Cl	2.9949133	4.1211693	-0.4315361	Cl	-0.0339279	5.0607914	-0.2357587
Br	-1.0335899	0.0155874	3.4621941	Cl	-2.9472103	4.1142085	-0.2357587
Coran-cl10br-out2				Cl	-4.8235829	1.5316032	-0.2357587
C	1.0905483	-0.7081073	0.3698197	Cl	-4.8235829	-1.5316032	-0.2357587
C	1.0893182	0.7095153	0.3725109	Cl	-2.9472103	-4.1142085	-0.2357587
C	-0.2623982	1.1441413	0.3750613	Br	0.0000000	0.0000000	-2.5979665
C	-1.0923550	-0.0013580	0.3721321	Coran-cl10bf4-out1			
C	-0.2602424	-1.1453069	0.3720617	C	1.1512645	-0.7105491	-0.1464950
C	2.1905218	-1.5068079	0.0482326	C	1.1543150	0.7051508	-0.1441723
C	2.1876525	1.5109993	0.0527609	C	-0.1897478	1.1432151	-0.1252081
C	-2.4603153	-0.0021765	0.1023326	C	-1.0215565	0.0018748	-0.1236808
C	-0.6830342	2.4367219	0.0537600	C	-0.1947661	-1.1431567	-0.1288408
C	-0.6785215	-2.4376164	0.0461687	C	2.2486887	-1.5150265	-0.4257401
C	3.4111299	-0.7094522	-0.1258275	C	2.2553642	1.5054479	-0.4206229
C	1.8143018	-2.9071221	-0.1460764	C	-2.3895499	0.0052688	-0.3495451
C	0.4524502	-3.3473589	-0.1444033	C	-0.6151281	2.4422989	-0.3659321
C	3.4097963	0.7164005	-0.1240060	C	-0.6259080	-2.4394430	-0.3742013
C	1.8088523	2.9111379	-0.1384235	C	3.4744524	-0.7206885	-0.5922137
C	-2.1324251	-2.5103239	-0.1443019	C	1.8635130	-2.9252549	-0.5715948
C	-2.9749654	-1.3616401	-0.1208874	C	0.5043996	-3.3616458	-0.5468435
C	-2.9777217	1.3566595	-0.1151359	C	3.4775928	0.7061518	-0.5898661
C	-2.1372390	2.5075838	-0.1351028	C	1.8764977	2.9179777	-0.5608859
C	0.4461686	3.3488326	-0.1347866	C	-2.0869523	-2.5128119	-0.4859758
Cl	0.1464889	5.0776911	-0.3908434	C	-2.9210060	-1.3560551	-0.4714329
Cl	-2.9050836	4.0849333	-0.3941091	C	-2.9148590	1.3692474	-0.4681164
Cl	-4.6986454	1.5984159	-0.4040235	C	-2.0757224	2.5223950	-0.4785759
Cl	-4.6948658	-1.6046654	-0.4139215	C	0.5193166	3.3602599	-0.5342774
Cl	-2.8970659	-4.0880593	-0.4091604	Cl	0.2172565	5.0953327	-0.7257578
Cl	0.1561315	-5.0761830	-0.4042330	Cl	-2.8509727	4.1064634	-0.6380783
Cl	3.0763086	-4.1287359	-0.4056095	Cl	-4.6593266	1.6211913	-0.6169658
Cl	4.9679710	-1.5305088	-0.3502269	Cl	-4.6667521	-1.5999302	-0.6187663
Cl	4.9650882	1.5409817	-0.3458099	Cl	-2.8692900	-4.0930633	-0.6488014
Cl	3.0685105	4.1358094	-0.3955433	Cl	0.1945566	-5.0943746	-0.7465193
Br	-3.4364978	-0.0142501	3.0200547	Cl	3.1221600	-4.1536890	-0.7984128
Coran-cl10br-in				Cl	5.0269359	-1.5483435	-0.8110168
C	-0.9769248	0.7097774	0.6322788	Cl	5.0336350	1.5277447	-0.8061940
C	-0.9769248	-0.7097774	0.6322788	Cl	3.1406813	4.1416169	-0.7824261
C	0.3731521	-1.1484439	0.6322788	B	-1.0398409	0.0001060	3.0299436
C	1.2075454	0.0000000	0.6322788	F	-1.6666128	1.1752268	2.4712623
C	0.3731521	1.1484439	0.6322788	F	-1.1655273	-0.0003284	4.4455829
C	-2.0654886	1.5006653	0.2662215	F	0.3551621	-0.0011767	2.6523810
C	-2.0654886	-1.5006653	0.2662215	F	-1.6696184	-1.1729625	2.4703639
C	2.5530843	0.0000000	0.2662215	Coran-cl10bf4-out2			
C	0.7889464	-2.4281274	0.2662215	C	1.3304301	-0.6979440	0.0166877
C	0.7889464	2.4281274	0.2662215	C	1.2969205	0.7207195	0.0452347
C	-3.2779536	0.7112060	0.0463014	C	-0.0578160	1.1262457	-0.0288293
C	-1.6893405	2.8977444	0.0463014	C	-0.8587390	-0.0362564	-0.1122438
C	-0.3365463	3.3372939	0.0463014	C	-0.0035976	-1.1624849	-0.0801713
C	-3.2779536	-0.7112060	0.0463014	C	2.4641486	-1.4651454	-0.2402901
C	-1.6893405	-2.8977444	0.0463014	C	2.3931032	1.5502409	-0.1794622
C	2.2338838	2.5021106	0.0463014	C	-2.1955115	-0.0593497	-0.4813633
C	3.0699566	1.3513550	0.0463014	C	-0.4922493	2.4135440	-0.3258705
C	3.0699566	-1.3513550	0.0463014				

C	-0.3775008	-2.4563413	-0.4254872	F	0.2625593	1.3412726	-1.9599682
C	3.6760668	-0.6389580	-0.3252396	F	-1.1107634	-0.5590150	-1.9844085
C	2.1297894	-2.8744317	-0.4731512	F	1.2196903	-0.7961115	-1.9791457
C	0.7842600	-3.3432752	-0.5565722				
C	3.6423380	0.7861208	-0.2982482				
C	1.9924012	2.9503853	-0.3556237				
C	-1.8197535	-2.5606407	-0.6743253				
C	-2.6812595	-1.4259002	-0.7003025				
C	-2.7457258	1.2902518	-0.6380176				
C	-1.9373114	2.4614114	-0.5680961				
C	0.6260372	3.3583274	-0.4207766				
Cl	0.2979662	5.0842094	-0.6431317				
Cl	-2.7336187	4.0272758	-0.7848460				
Cl	-4.4701498	1.5004410	-0.9357294				
Cl	-4.3909486	-1.7019848	-1.0270527				
Cl	-2.5415264	-4.1522127	-0.9622546				
Cl	0.5370784	-5.0728684	-0.8475025				
Cl	3.4324245	-4.0619303	-0.6706764				
Cl	5.2600986	-1.4225634	-0.4682632				
Cl	5.1872558	1.6482753	-0.4146707				
Cl	3.2373517	4.2051048	-0.5035862				
B	-2.2010914	0.0017877	2.8308437				
F	-1.2356586	-1.0371819	2.5531978				
F	-3.3965003	-0.2631088	2.0692821				
F	-1.6545750	1.2699937	2.4049876				
F	-2.4943925	0.0381620	4.2216802				
Coran-cl10bf4-in							
C	0.9314483	-0.7205331	0.9946913				
C	0.9463168	0.6988912	0.9883543				
C	-0.3989545	1.1530854	0.9519853				
C	-1.2451750	0.0143289	0.9281801				
C	-0.4225239	-1.1434641	0.9485931				
C	2.0217882	-1.5238963	0.6622072				
C	2.0512421	1.4749905	0.6414458				
C	-2.5770360	0.0284036	0.5157282				
C	-0.7877389	2.4357265	0.5672589				
C	-0.8399697	-2.4149550	0.5575362				
C	3.2489258	-0.7490786	0.4765328				
C	1.6379821	-2.9154500	0.4246179				
C	0.2812540	-3.3376798	0.3718643				
C	3.2624563	0.6723571	0.4626789				
C	1.6988740	2.8790604	0.4209612				
C	-2.2816368	-2.4757056	0.3070789				
C	-3.1051123	-1.3184495	0.2902274				
C	-3.0707989	1.3834408	0.2702865				
C	-2.2223025	2.5251805	0.2947427				
C	0.3539421	3.3347963	0.3889215				
Cl	0.0787243	5.0624828	0.1128017				
Cl	-2.9595993	4.1016888	-0.0362672				
Cl	-4.7859180	1.6444508	-0.0896168				
Cl	-4.8340807	-1.5449902	-0.0219316				
Cl	-3.0575100	-4.0397721	0.0070933				
Cl	-0.0322553	-5.0525097	0.0543773				
Cl	2.8893557	-4.1433255	0.1747591				
Cl	4.7927649	-1.5861134	0.2479012				
Cl	4.8207352	1.4753724	0.2064914				
Cl	2.9782303	4.0789556	0.1737680				
B	0.1253445	0.0007688	-2.4751995				
F	0.1289076	0.0163131	-3.8962735				

Coran-fl0cl-out1

C 1.0256443 -0.6765188 -0.7131665
C 1.0256443 -0.6765188 0.7131665
C -0.3274792 -0.6969607 1.1527060
C -1.1751267 -0.7471697 0.0000000
C -0.3274792 -0.6969607 -1.1527060
C 2.0868108 -0.1729343 -1.4824440
C 2.0868108 -0.1729343 1.4824440
C -2.4593133 -0.1712776 0.0000000
C -0.7307585 -0.1850387 2.3935099
C -0.7307585 -0.1850387 -2.3935099
C 3.2578362 0.1727115 -0.7010847

C 1.7080406 0.1790083 -2.8304931
C 0.3692269 0.1758476 -3.2594885
C 3.2578362 0.1727115 0.7010847
C 1.7080406 0.1790083 2.8304931
C -2.1358024 0.1604638 -2.4563593
C -2.9480893 0.1811684 -1.3126482
C -2.9480893 0.1811684 1.3126482
C -2.1358024 0.1604638 2.4563593
C 0.3692269 0.1758476 3.2594885
F -4.2304492 0.6437010 1.4524672
F 0.1087930 0.6264768 4.5279825
F 4.3945194 0.5958291 1.3424255
F 2.6633392 0.6257785 -3.7092868
F -2.6747576 0.5925693 -3.6436499
F -2.6747576 0.5925693 3.6436499
F 2.6633392 0.6257785 3.7092868
F 4.3945194 0.5958291 -1.3424255
F 0.1087930 0.6264768 -4.5279825
F -4.2304492 0.6437010 -1.4524672
Cl -1.4950377 -3.5124134 0.0000000

Coran-fl0cl-out2

C 1.1263482 -0.7091746 -0.7123880
C 1.1263482 -0.7091746 0.7123880
C -0.2326252 -0.7401400 1.1496198
C -1.0704832 -0.7656164 0.0000000
C -0.2326252 -0.7401400 -1.1496198
C 2.1778444 -0.1801094 -1.4832125
C 2.1778444 -0.1801094 1.4832125
C -2.4066042 -0.3262678 0.0000000
C -0.6438834 -0.2244216 2.3921318
C -0.6438834 -0.2244216 -2.3921318
C 3.3413788 0.1831367 -0.7021482
C 1.7908267 0.1749499 -2.8261879
C 0.4481098 0.1569239 -3.2538653
C 3.3413788 0.1831367 0.7021482
C 1.7908267 0.1749499 2.8261879
C -2.0507934 0.1155829 -2.4404610
C -2.8809681 0.0768500 -1.3119575
C -2.8809681 0.0768500 1.3119575
C -2.0507934 0.1155829 2.4404610
C 0.4481098 0.1569239 3.2538653
F 0.1844968 0.6203643 4.5165982
F 4.4680771 0.6354206 1.3406701
F 2.7370633 0.6424556 -3.7048650
F -2.5847067 0.5751759 -3.6179850
F -4.1507511 0.5386180 1.4498127
F -2.5847067 0.5751759 3.6179850

F 2.7370633 0.6424556 3.7048650
F 4.4680771 0.6354206 -1.3406701
F 0.1844968 0.6203643 -4.5165982
F -4.1507511 0.5386180 -1.4498127
Cl -3.9783603 -2.6332849 0.0000000

Coran-fl0cl-in

C 0.9812733 -0.7129368 0.9282898
C 0.9812733 0.7129368 0.9282898
C -0.3748131 1.1535560 0.9282898
C -1.2129205 0.0000000 0.9282898
C -0.3748131 -1.1535560 0.9282898
C 2.0289034 -1.4740846 0.3877735
C 2.0289034 1.4740846 0.3877735
C -2.5078625 0.0000000 0.3877735
C -0.7749721 2.3851190 0.3877735
C -0.7749721 -2.3851190 0.3877735
C 3.1887903 -0.7005661 0.0148277
C 1.6516684 -2.8162329 0.0148277
C 0.3191124 -3.2492066 0.0148277
C 3.1887903 0.7005661 0.0148277
C 1.6516684 2.8162329 0.0148277
C -2.1680031 -2.4410938 0.0148277
C -2.9915680 -1.3075540 0.0148277
C -2.9915680 1.3075540 0.0148277
C -2.1680031 2.4410938 0.0148277
C 0.3191124 3.2492066 0.0148277
F 0.0554307 4.5081325 -0.4535445
F -2.6946582 3.6145745 -0.4535445
F -4.2703598 1.4458073 -0.4535445
F -4.2703598 -1.4458073 -0.4535445
F -2.6946582 -3.6145745 -0.4535445
F 0.0554307 -4.5081325 -0.4535445
F 2.6049695 -3.6797371 -0.4535445
F 4.3046178 -1.3403719 -0.4535445
F 4.3046178 1.3403719 -0.4535445
F 2.6049695 3.6797371 -0.4535445
Cl 0.0000000 0.0000000 -2.1919620

Coran-fl0br-out1

C 1.0198707 -0.6700517 -0.7125614
C 1.0198707 -0.6700517 0.7125614
C -0.3330708 -0.6837120 1.1527894
C -1.1783060 -0.7179873 0.0000000
C -0.3330708 -0.6837120 -1.1527894
C 2.0839852 -0.1748776 -1.4830445
C 2.0839852 -0.1748776 1.4830445
C -2.4653343 -0.1524327 0.0000000
C -0.7340774 -0.1724163 2.3947194
C -0.7340774 -0.1724163 -2.3947194
C 3.2558997 0.1655670 -0.7015102
C 1.7070363 0.1756048 -2.8322199
C 0.3677289 0.1799282 -3.2616083
C 3.2558997 0.1655670 0.7015102
C 1.7070363 0.1756048 2.8322199
C -2.1390360 0.1750935 -2.4572268
C -2.9534749 0.1971937 -1.3144032
C -2.9534749 0.1971937 1.3144032
C -2.1390360 0.1750935 2.4572268
C 0.3677289 0.1799282 3.2616083
F -4.2357308 0.6584636 1.4560577
F 0.1099606 0.6304506 4.5302468

F	4.3928999	0.5876864	1.3420576	C	-2.1674529	2.4407058	0.0201034
F	2.6646125	0.6152145	-3.7117748	C	0.3188954	3.2485693	0.0201034
F	-2.6770492	0.6063560	-3.6443600	F	0.0543588	4.5048465	-0.4528986
F	-2.6770492	0.6063560	3.6443600	F	-2.6918595	3.6125461	-0.4528986
F	2.6646125	0.6152145	3.7117748	F	-4.2675658	1.4437724	-0.4528986
F	4.3928999	0.5876864	-1.3420576	F	-4.2675658	-1.4437724	-0.4528986
F	0.1099606	0.6304506	-4.5302468	F	-2.6918595	-3.6125461	-0.4528986
F	-4.2357308	0.6584636	-1.4560577	F	0.0543588	-4.5048465	-0.4528986
Br	-1.4119000	-3.7135145	0.0000000	F	2.6039051	-3.6764487	-0.4528986
Coran-fl0br-out2				F	4.3011614	-1.3403758	-0.4528986
C	1.1278683	-0.7059211	-0.7124878	F	4.3011614	1.3403758	-0.4528986
C	1.1278683	-0.7059211	0.7124878	F	2.6039051	3.6764487	-0.4528986
C	-0.2309383	-0.7315430	1.1498094	Br	0.0000000	0.0000000	-2.3304818
C	-1.0683567	-0.7529969	0.0000000	Coran-fl0bf4-out1			
C	-0.2309383	-0.7315430	-1.1498094	C	1.2503386	-0.1965626	-0.7127312
C	2.1805661	-0.1797278	-1.4834548	C	1.2503386	-0.1965626	0.7127312
C	2.1805661	-0.1797278	1.4834548	C	-0.1032120	-0.2436089	1.1501144
C	-2.4007318	-0.3039972	0.0000000	C	-0.9353261	-0.2603620	0.0000000
C	-0.6415123	-0.2168127	2.3926891	C	-0.1032120	-0.2436089	-1.1501144
C	-0.6415123	-0.2168127	-2.3926891	C	2.2895336	0.3415991	-1.4826657
C	3.3444759	0.1815102	-0.7023297	C	2.2895336	0.3415991	1.4826657
C	1.7944479	0.1750828	-2.8271705	C	-2.2609085	0.1766034	0.0000000
C	0.4516532	0.1595877	-3.2556919	C	-0.5292907	0.2286241	2.3962614
C	3.3444759	0.1815102	0.7023297	C	-0.5292907	0.2286241	-2.3962614
C	1.7944479	0.1750828	2.8271705	C	3.4456703	0.7329874	-0.7025229
C	-2.0479229	0.1241434	-2.4423693	C	1.8955979	0.6687552	-2.8372528
C	-2.8783382	0.0904219	-1.3125223	C	0.5595185	0.6122263	-3.2704497
C	-2.8783382	0.0904219	1.3125223	C	3.4456703	0.7329874	0.7025229
C	-2.0479229	0.1241434	2.4423693	C	1.8955979	0.6687552	2.8372528
C	0.4516532	0.1595877	3.2556919	C	-1.9474456	0.5066124	-2.4564105
F	0.1888261	0.6223291	4.5184986	C	-2.7697940	0.4799983	-1.3179713
F	4.4713568	0.6332395	1.3403687	C	-2.7697940	0.4799983	1.3179713
F	2.7416843	0.6399044	-3.7055467	C	-1.9474456	0.5066124	2.4564105
F	-2.5823081	0.5791510	-3.6207098	C	0.5595185	0.6122263	3.2704497
F	-4.1476778	0.5533981	1.4508142	F	-4.0767429	0.8489144	1.4679988
F	-2.5823081	0.5791510	3.6207098	F	0.2872327	1.0290706	4.5454742
F	2.7416843	0.6399044	3.7055467	F	4.5615502	1.2065511	1.3413422
F	4.4713568	0.6332395	-1.3403687	F	2.8361110	1.1353361	-3.7188150
F	0.1888261	0.6223291	-4.5184986	F	-2.5056466	0.9033071	-3.6420649
F	-4.1476778	0.5533981	-1.4508142	F	-2.5056466	0.9033071	3.6420649
Br	-4.0749224	-2.7912554	0.0000000	F	2.8361110	1.1353361	3.7188150
Coran-fl0br-in				F	4.5615502	1.2065511	-1.3413422
C	0.9814610	-0.7130732	0.9376584	F	0.2872327	1.0290706	-4.5454742
C	0.9814610	0.7130732	0.9376584	F	-4.0767429	0.8489144	-1.4679988
C	-0.3748847	1.1537766	0.9376584	B	-1.4404056	-3.3005000	0.0000000
C	-1.2131525	0.0000000	0.9376584	F	-2.0115361	-2.6820675	-1.1747771
C	-0.3748847	-1.1537766	0.9376584	F	-1.7084680	-4.6979349	0.0000000
C	2.0283121	-1.4736550	0.3940610	F	-2.0115361	-2.6820675	1.1747771
C	2.0283121	1.4736550	0.3940610	F	-0.0155614	-3.0641189	0.0000000
C	-2.5071317	0.0000000	0.3940610	Coran-fl0bf4-out2			
C	-0.7747463	2.3844239	0.3940610	C	1.3881425	-0.6817770	0.3423269
C	-0.7747463	-2.3844239	0.3940610	C	1.4212944	0.7446783	0.3127346
C	3.1881171	-0.7005756	0.0201034	C	0.0760841	1.2118411	0.2771626
C	1.6514693	-2.8155898	0.0201034	C	-0.7836219	0.0795673	0.2784922
C	0.3188954	-3.2485693	0.0201034	C	0.0233253	-1.0890113	0.3267171
C	3.1881171	0.7005756	0.0201034	C	2.4390103	-1.4851624	-0.1250889
C	1.6514693	2.8155898	0.0201034	C	2.5059803	1.4799607	-0.1875165
C	-2.1674529	-2.4407058	0.0201034	C	-2.0754436	0.0969897	-0.2512969
C	-2.9910289	-1.3071507	0.0201034	C	-0.2942160	2.4557252	-0.2514762
C	-2.9910289	1.3071507	0.0201034	C	-0.4026837	-2.3330318	-0.1570199

C	3.6308986	-0.7378426	-0.4697685	F	-0.7519504	1.1504267	-1.9198714
C	2.0330858	-2.8341453	-0.4531854				
C	0.6849876	-3.2350875	-0.4663220				
C	3.6631862	0.6663023	-0.4991114				
C	2.1610662	2.8318238	-0.5704757				
C	-1.8002122	-2.3676666	-0.5234431				
C	-2.5970990	-1.2124486	-0.5666724				
C	-2.5385343	1.4160916	-0.6168399				
C	-1.6911638	2.5367185	-0.6189922				
C	0.8331758	3.2939248	-0.5985308				
F	0.6138566	4.5614031	-1.0662011				
F	4.8169486	1.2700705	-0.9258822				
F	2.9766056	-3.7437265	-0.8560687				
F	-2.3559180	-3.5472239	-0.9363262				
F	-3.8079481	1.5810009	-1.0780113				
F	-2.1949812	3.7236571	-1.0815350				
F	3.1443650	3.6800084	-1.0101965				
F	4.7555333	-1.4101074	-0.8703948				
F	0.4088819	-4.5076662	-0.8854770				
F	-3.8732304	-1.3372580	-1.0200135				
B	-2.6367753	-0.2218098	2.9246809				
F	-1.6346710	0.8157979	2.8870475				
F	-2.0392159	-1.4638332	2.4899453				
F	-3.1543892	-0.3621802	4.2422097				
F	-3.6963033	0.1244876	2.0050353				
Coran-fl0bf4-in							
C	0.9601116	-0.7163635	1.2296781				
C	0.9526132	0.7084238	1.2359134				
C	-0.4043494	1.1413134	1.2108570				
C	-1.2342300	-0.0164135	1.1854652				
C	-0.3918715	-1.1651719	1.2041215				
C	2.0283536	-1.4722426	0.7258092				
C	2.0143878	1.4816692	0.7455169				
C	-2.5250372	-0.0212839	0.6374887				
C	-0.8048366	2.3814344	0.6937994				
C	-0.7789363	-2.4077187	0.6825900				
C	3.1997070	-0.6887068	0.4088265				
C	1.6627211	-2.8184238	0.3513995				
C	0.3309104	-3.2623746	0.3323122				
C	3.1937509	0.7138666	0.4200830				
C	1.6331223	2.8244915	0.3757383				
C	-2.1689855	-2.4696562	0.2959646				
C	-2.9969989	-1.3368109	0.2720182				
C	-3.0128425	1.2915186	0.2832784				
C	-2.1970927	2.4327122	0.3129978				
C	0.2955935	3.2511565	0.3513993				
F	0.0383693	4.5131153	-0.1077089				
F	-2.7262214	3.6067435	-0.1444909				
F	-4.2853412	1.4288682	-0.1988781				
F	-4.2679148	-1.4856698	-0.2118716				
F	-2.6858108	-3.6466504	-0.1690758				
F	0.0874475	-4.5249958	-0.1324053				
F	2.6282443	-3.6794599	-0.0936160				
F	4.3337916	-1.3187268	-0.0236856				
F	4.3217389	1.3601103	-0.0026529				
F	2.5892051	3.7000655	-0.0599530				
B	0.0423104	0.0377495	-2.3782503				
F	1.3742476	0.1717226	-1.8415129				
F	-0.5377971	-1.1796566	-1.8701411				
F	0.0820910	0.0131789	-3.7980155				

Coran-cn10cl-out1

C	1.0234752	-0.7032119	-0.7116192
C	1.0234752	-0.7032119	0.7116192
C	-0.3181974	-0.7988820	1.1524345
C	-1.1754628	-0.9611932	0.0000000
C	-0.3181974	-0.7988820	-1.1524345
C	2.0829301	-0.2316922	-1.4866310
C	2.0829301	-0.2316922	1.4866310
C	-2.4718404	-0.3815154	0.0000000
C	-0.7386075	-0.3507862	2.4000733
C	-0.7386075	-0.3507862	-2.4000733
C	3.2969406	0.0689086	-0.7162858
C	1.7255176	0.0383892	-2.8735299
C	0.3541683	-0.0089648	-3.3101010
C	3.2969406	0.0689086	0.7162858
C	1.7255176	0.0383892	2.8735299
C	-2.1843493	-0.1188113	-2.5044833
C	-3.0031903	-0.0922770	-1.3224438
C	-3.0031903	-0.0922770	1.3224438
C	-2.1843493	-0.1188113	2.5044833
C	0.3541683	-0.0089648	3.3101010
C	0.0881771	0.3487175	4.6759392
N	-0.0832455	0.6373988	5.8025276
C	2.7254239	0.4163010	3.8329131
N	3.5263524	0.7158280	4.6392865
C	4.5239359	0.4004791	1.3850485
N	5.5459373	0.6597866	1.9049183
C	4.5239359	0.4004791	-1.3850485
N	5.5459373	0.6597866	-1.9049183
C	2.7254239	0.4163010	-3.8329131
N	3.5263524	0.7158280	-4.6392865
C	0.0881771	0.3487175	-4.6759392
N	-0.0832455	0.6373988	-5.8025276
C	-2.7973283	0.1580008	-3.7685074
N	-3.3240224	0.3701880	-4.7990546
C	-4.3834065	0.2703234	-1.4985426
N	-5.5062059	0.5612021	-1.6869830
C	-4.3834065	0.2703234	1.4985426
N	-5.5062059	0.5612021	1.6869830
C	-2.7973283	0.1580008	3.7685074
N	-3.3240224	0.3701880	4.7990546
Cl	-1.4612491	-3.3381019	0.0000000

Coran-cn10cl-out2

C	-2.1284382	1.4502565	2.0168873
C	-0.6533087	1.4481105	1.9473986
C	0.3084223	2.5678122	2.0037585
C	1.6100838	2.4875516	1.4122084
C	-2.9222642	0.4084391	1.4377207
C	-0.1339996	0.3076424	1.3279688
C	-0.9206531	-0.7305665	0.7725202
C	-2.3147227	-0.7166595	0.7120479
C	-2.8787585	-1.6864870	-0.2193499
C	3.1529368	1.0810894	-0.2547727
C	3.1840860	-0.0503066	-1.1562120
C	2.1071561	-1.0356127	-1.1704383
C	1.7152511	-2.0421947	-2.1625582
C	0.4080690	-2.6418687	-2.1548641
C	-2.0501929	-2.4516156	-1.1258310
C	-0.6011194	-2.2784104	-1.1544199
C	-0.1059576	-1.4726176	-0.1296064

C	1.1824854	-0.8805210	-0.1383355
C	1.1596707	0.2258286	0.7582945
C	2.0582522	1.2908239	0.6851801
C	-0.0651511	3.8132977	2.6125005
N	-0.3357303	4.8646920	3.0620290
C	2.4668018	3.6353538	1.5151479
N	3.1596719	4.5799260	1.6124289
C	4.2327078	2.0238946	-0.3514656
N	5.1444567	2.7592618	-0.4487723
C	4.2846871	-0.1519219	-2.0707886
N	5.2030868	-0.2216899	-2.8019976
C	2.6239052	-2.4377128	-3.2025461
N	3.3519429	-2.7943337	-4.0536760
C	0.1044727	-3.5938545	-3.1873206
N	-0.1069768	-4.3829492	-4.0321303
C	-2.6996841	-3.3561096	-2.0303279
N	-3.2524926	-4.1011899	-2.7529082
C	-4.2985605	-1.8899569	-0.3014048
N	-5.4517023	-2.1018264	-0.3860076
C	-4.3501005	0.5105651	1.5511458
N	-5.5169109	0.6043018	1.6570539
C	-2.8227542	2.5496408	2.6256407
N	-3.4383979	3.4436109	3.0755840
Cl	-0.4170742	0.9662959	4.4980248

Coran-cn10cl-in

C	-3.0538998	-1.3306150	0.1455609
C	-2.5254438	0.0000000	0.4384406
C	-3.0538998	1.3306150	0.1455609
C	-2.2091970	2.4932487	0.1455609
C	-2.2091970	-2.4932487	0.1455609
C	-1.2090265	0.0000000	0.8903314
C	-0.3736097	-1.1498526	0.8903314
C	-0.7804050	-2.4018397	0.4384406
C	0.3217831	-3.3156140	0.1455609
C	0.3217831	3.3156140	0.1455609
C	1.6885410	2.8715274	0.1455609
C	2.0431269	1.4844186	0.4384406
C	3.2527727	0.7185472	0.1455609
C	3.2527727	-0.7185472	0.1455609
C	1.6885410	-2.8715274	0.1455609
C	2.0431269	-1.4844186	0.4384406
C	0.9781230	-0.7106480	0.8903314
C	0.9781230	0.7106480	0.8903314
C	-0.3736097	1.1498526	0.8903314
C	-0.7804050	2.4018397	0.4384406
C	-4.4400416	-1.5136149	-0.1807791
N	-5.5759804	-1.6991273	-0.4198039
C	-2.8115816	-3.7549977	-0.1807791
N	-3.3390388	-4.7780132	-0.4198039
C	0.0674850	-4.6904632	-0.1807791
N	-0.1071066	-5.8281317	-0.4198039
C	2.7023885	-3.8343312	-0.1807791
N	3.5123409	-4.6521019	-0.4198039
C	4.4817496	-1.3852507	-0.1807791
N	5.5097848	-1.9028562	-0.4198039
C	4.4817496	1.3852507	-0.1807791
N	5.5097848	1.9028562	-0.4198039
C	2.7023885	3.8343312	-0.1807791
N	3.5123409	4.6521019	-0.4198039
C	0.0674850	4.6904632	-0.1807791

N	-0.1071066	5.8281317	-0.4198039	C	1.3624711	1.1586059	2.8808820
C	-2.8115816	3.7549977	-0.1807791	C	1.8072533	1.1868717	1.4904909
N	-3.3390388	4.7780132	-0.4198039	C	2.5484524	2.1903803	0.7191470
C	-4.4400416	1.5136149	-0.1807791	C	2.5484524	2.1903803	-0.7191470
N	-5.5759804	1.6991273	-0.4198039	C	1.3624711	1.1586059	-2.8808820
Cl	0.0000000	0.0000000	-2.1163545	C	1.8072533	1.1868717	-1.4904909
Coran-cn10br-out1				C	1.2883530	0.1544844	-0.7093290
C	1.0221090	-0.6876741	-0.7107546	C	1.2883530	0.1544844	0.7093290
C	1.0221090	-0.6876741	0.7107546	C	0.2805441	-0.7506684	1.1458629
C	-0.3215179	-0.7711085	1.1516531	C	-0.3114074	-0.6944620	2.4080475
C	-1.1731179	-0.8978294	0.0000000	C	-3.4707643	-2.6504517	1.5179596
C	-0.3215179	-0.7711085	-1.1516531	N	-4.5364533	-3.1065754	1.7103082
C	2.0845943	-0.2286017	-1.4885937	C	-2.2554925	-1.5633210	3.7548671
C	2.0845943	-0.2286017	1.4885937	N	-2.8191719	-1.6791842	4.7800040
C	-2.4792707	-0.3628032	0.0000000	C	-0.0744510	0.3272264	4.6971983
C	-0.7404027	-0.3299761	2.4028993	N	-0.3628687	0.4136756	5.8335173
C	-0.7404027	-0.3299761	-2.4028993	C	1.9065392	2.0727980	3.8435862
C	3.2988614	0.0655907	-0.7171812	N	2.3473549	2.8035770	4.6527498
C	1.7274545	0.0382660	-2.8770110	C	3.2753769	3.2351332	1.3850246
C	0.3542814	-0.0009861	-3.3141087	N	3.8935066	4.0906012	1.9025829
C	3.2988614	0.0655907	0.7171812	C	3.2753769	3.2351332	-1.3850246
C	1.7274545	0.0382660	2.8770110	N	3.8935066	4.0906012	-1.9025829
C	-2.1874761	-0.1018749	-2.5048929	C	1.9065392	2.0727980	-3.8435862
C	-3.0128088	-0.0849433	-1.3262848	N	2.3473549	2.8035770	-4.6527498
C	-3.0128088	-0.0849433	1.3262848	C	-0.0744510	0.3272264	-4.6971983
C	-2.1874761	-0.1018749	2.5048929	N	-0.3628687	0.4136756	-5.8335173
C	0.3542814	-0.0009861	3.3141087	C	-2.2554925	-1.5633210	-3.7548671
C	0.0902058	0.3518268	4.6815170	N	-2.8191719	-1.6791842	-4.7800040
N	-0.0823839	0.6370423	5.8086699	C	-3.4707643	-2.6504517	-1.5179596
C	2.7295280	0.4052292	3.8377700	N	-4.5364533	-3.1065754	-1.7103082
N	3.5323693	0.6963911	4.6456161	Br	-0.9651529	-4.6968766	0.0000000
C	4.5270618	0.3948815	1.3850894	Coran-cn10br-in			
N	5.5495895	0.6533306	1.9041966	C	-3.0550444	-1.3308407	0.1509425
C	4.5270618	0.3948815	-1.3850894	C	-2.5266872	0.0000000	0.4425901
N	5.5495895	0.6533306	-1.9041966	C	-3.0550444	1.3308407	0.1509425
C	2.7295280	0.4052292	-3.8377700	C	-2.2097653	2.4942675	0.1509425
N	3.5323693	0.6963911	-4.6456161	C	-2.2097653	-2.4942675	0.1509425
C	0.0902058	0.3518268	-4.6815170	C	-1.2089061	0.0000000	0.8920074
N	-0.0823839	0.6370423	-5.8086699	C	-0.3735725	-1.1497380	0.8920074
C	-2.7998003	0.1786123	-3.7689649	C	-0.7807893	-2.4030223	0.4425901
N	-3.3262100	0.3954491	-4.7985834	C	0.3216441	-3.3167722	0.1509425
C	-4.3970726	0.2580589	-1.5045514	C	0.3216441	3.3167722	0.1509425
N	-5.5243269	0.5332066	-1.6916341	C	1.6893343	2.8723827	0.1509425
C	-4.3970726	0.2580589	1.5045514	C	2.0441329	1.4851495	0.4425901
N	-5.5243269	0.5332066	1.6916341	C	3.2538313	0.7190373	0.1509425
C	-2.7998003	0.1786123	3.7689649	C	3.2538313	-0.7190373	0.1509425
N	-3.3262100	0.3954491	4.7985834	C	1.6893343	-2.8723827	0.1509425
Br	-1.3994782	-3.5430019	0.0000000	C	2.0441329	-1.4851495	0.4425901
Coran-cn10br-out2				C	0.9780255	-0.7105772	0.8920074
C	-2.1893143	-2.0266358	-1.3404904	C	0.9780255	0.7105772	0.8920074
C	-1.5837509	-1.9324668	0.0000000	C	-0.3735725	1.1497380	0.8920074
C	-2.1893143	-2.0266358	1.3404904	C	-0.7807893	2.4030223	0.4425901
C	-1.5762076	-1.4376779	2.4964508	C	-4.4407544	-1.5140816	-0.1761466
C	-1.5762076	-1.4376779	-2.4964508	N	-5.5767221	-1.7005363	-0.4143110
C	-0.3336792	-1.3130060	0.0000000	C	-2.8122457	-3.7555315	-0.1761466
C	0.2805441	-0.7506684	-1.1458629	N	-3.3406080	-4.7782832	-0.4143110
C	-0.3114074	-0.6944620	-2.4080475	C	0.0677086	-4.6912854	-0.1761466
C	0.3305251	0.2442945	-3.3215428	N	-0.1059958	-5.8292725	-0.4143110
C	0.3305251	0.2442945	3.3215428	C	2.7026910	-3.8351277	-0.1761466
				N	3.5121128	-4.6536778	-0.4143110

C	4.4826006	-1.3852922	-0.1761466	C	1.2501411	-0.7088460	0.4150176
N	5.5112131	-1.9021522	-0.4143110	C	1.2147530	0.7129079	0.4460978
C	4.4826006	1.3852922	-0.1761466	C	-0.1427246	1.1173503	0.3812555
N	5.5112131	1.9021522	-0.4143110	C	-0.9413780	-0.0480560	0.2947245
C	2.7026910	3.8351277	-0.1761466	C	-0.0860640	-1.1753037	0.3272151
N	3.5121128	4.6536778	-0.4143110	C	2.3620655	-1.4539826	0.0436954
C	0.0677086	4.6912854	-0.1761466	C	2.2889323	1.5275565	0.1095113
N	-0.1059958	5.8292725	-0.4143110	C	-2.2448889	-0.0692857	-0.1675436
C	-2.8122457	3.7555315	-0.1761466	C	-0.5646364	2.3774643	-0.0183620
N	-3.3406080	4.7782832	-0.4143110	C	-0.4465187	-2.4373206	-0.1222370
C	-4.4407544	1.5140816	-0.1761466	C	3.5766381	-0.6476450	-0.1326935
N	-5.5767221	1.7005363	-0.4143110	C	2.0537655	-2.8532753	-0.2686335
Br	0.0000000	0.0000000	-2.2796392	C	0.6956646	-3.3269782	-0.3455489
Coran-cn10bf4-out1							
C	1.1366330	-0.7128126	0.3058217	C	3.5410181	0.7898298	-0.1014009
C	1.1396858	0.7075398	0.3072734	C	1.9120104	2.9215753	-0.1433399
C	-0.2078471	1.1465200	0.3270212	C	-1.8748049	-2.5602801	-0.4380704
C	-1.0400077	0.0021568	0.3214756	C	-2.7414691	-1.4163930	-0.4558495
C	-0.2128291	-1.1458270	0.3238793	C	-2.8073186	1.2629583	-0.3961819
C	2.2001541	-1.4946418	-0.1185334	C	-1.9968766	2.4450073	-0.3278137
C	2.2067202	1.4862724	-0.1141754	C	0.5316233	3.3303282	-0.2018354
C	-2.3763031	0.0057009	-0.0375971	C	4.8417442	-1.2792087	-0.3839713
C	-0.6256289	2.4114270	-0.0548172	N	5.8910687	-1.7717150	-0.5787691
C	-0.6361374	-2.4074957	-0.0624159	C	4.7736012	1.4926576	-0.3239544
C	3.4207304	-0.7254242	-0.3941518	N	5.7978662	2.0428542	-0.4966798
C	1.8359194	-2.8952207	-0.3662346	C	2.9189436	3.9160184	-0.3845854
C	0.4662742	-3.3351646	-0.3367101	N	3.7283373	4.7468184	-0.5760025
C	3.4238949	0.7125782	-0.3919603	C	0.2631544	4.7093305	-0.5023671
C	1.8485680	2.8890884	-0.3579327	N	0.0800877	5.8446937	-0.7446708
C	-2.0851496	-2.5009494	-0.2673912	C	-2.6175654	3.7070176	-0.6138045
C	-2.9245852	-1.3347101	-0.2530394	N	-3.1395901	4.7331093	-0.8507635
C	-2.9187273	1.3492172	-0.2487669	C	-4.1898555	1.4194281	-0.7456771
C	-2.0742585	2.5118227	-0.2596468	N	-5.3132552	1.5808689	-1.0505089
C	0.4808149	3.3349692	-0.3266194	C	-4.1150879	-1.6254076	-0.8151094
C	0.2249955	4.7178981	-0.6195438	N	-5.2283551	-1.8308831	-1.1290132
N	0.0452275	5.8542952	-0.8589770	C	-2.4332986	-3.8373170	-0.7814843
C	2.8625832	3.8538851	-0.6794163	N	-2.9041366	-4.8765828	-1.0638269
N	3.6784325	4.6597170	-0.9372093	C	0.4944729	-4.7037125	-0.7031030
C	4.6553946	1.3791585	-0.7113478	N	0.3655205	-5.8358437	-0.9916655
N	5.6759275	1.9028112	-0.9673803	C	3.1080611	-3.7861767	-0.5506992
C	4.6493295	-1.3964770	-0.7158046	N	3.9564088	-4.5678323	-0.7761996
N	5.6675413	-1.9238732	-0.9731843	B	-2.3820351	0.0270863	3.0603555
C	2.8458153	-3.8636634	-0.6904966	F	-1.4607686	-1.0645431	2.8041415
N	3.6582408	-4.6723450	-0.9497566	F	-3.5298726	-0.1457706	2.1985914
C	0.2044785	-4.7151560	-0.6331188	F	-1.7268490	1.2664552	2.6880255
N	0.0196677	-5.8512124	-0.8758352	F	-2.7584883	0.0507663	4.4142956
C	-2.7005854	-3.7697573	-0.5362702	Coran-cn10bf4-in			
N	-3.2209719	-4.8003914	-0.7566024	C	-2.0695067	1.4543335	2.1970107
C	-4.3262804	-1.5171494	-0.5050812	C	-0.6118992	1.4573360	2.0816541
N	-5.4690667	-1.6918762	-0.7169230	C	0.3498798	2.5569883	2.1381160
C	-4.3195797	1.5387033	-0.5001558	C	1.6652889	2.4312081	1.5829467
N	-5.4615715	1.7189142	-0.7115283	C	-2.8586253	0.3698438	1.6922188
C	-2.6840329	3.7841470	-0.5243635	C	-0.0741619	0.2535126	1.6384153
N	-3.1999472	4.8176518	-0.7417053	C	-0.8567236	-0.8256000	1.1455779
B	-1.1790120	-0.0059237	3.3513631	C	-2.2431744	-0.7893932	1.0462430
F	-1.7803137	1.1712179	2.7566111	C	-2.8067434	-1.8175210	0.1705276
F	-1.3552454	-0.0086636	4.7470001	C	3.2209424	0.9286010	0.0257532
F	0.2314981	-0.0103369	3.0074450	C	3.2545331	-0.2489284	-0.7882806
F	-1.7874689	-1.1756008	2.7507732	C	2.1776075	-1.2387676	-0.7452902
Coran-cn10bf4-out2							
C	1.7828234	-2.2688573	-1.7042173	C	1.7828234	-2.2688573	-1.7042173
C	0.4780866	-2.8646665	-1.6718334	C	0.4780866	-2.8646665	-1.6718334

C	-1.9729932	-2.6330855	-0.6603201
C	-0.5187511	-2.4695879	-0.6786880
C	-0.0279687	-1.6305367	0.3159628
C	1.2641536	-1.0411277	0.2848107
C	1.2333072	0.1267325	1.0963474
C	2.1111563	1.1941462	0.9422354
C	4.3021991	1.8641858	-0.1057371
N	5.2190760	2.5924703	-0.2062467
C	4.3677972	-0.4153933	-1.6791096
N	5.3104754	-0.5453861	-2.3687849
C	2.6854554	-2.6936455	-2.7372919
N	3.4141955	-3.0865415	-3.5713384
C	0.1658934	-3.8437750	-2.6748918
N	-0.0486306	-4.6670471	-3.4857721
C	-2.6124719	-3.5986013	-1.5087011
N	-3.1590148	-4.4088715	-2.1612431
C	-4.2265847	-2.0182728	0.0955624
N	-5.3812508	-2.2290857	0.0404159
C	-4.2861767	0.4697578	1.8133561
N	-5.4486318	0.5641856	1.9576695
C	-2.7599107	2.5654253	2.7888896
N	-3.3487268	3.4425744	3.3034964
C	-0.0109873	3.8173231	2.7237286
N	-0.2632590	4.8461967	3.2325371
C	2.5304301	3.5757673	1.6487878
N	3.2279576	4.5162209	1.7483130
B	-0.6428076	1.2774859	-1.8170579
F	-1.3321881	0.0061529	-1.8041187
F	0.7798607	1.0156606	-1.8097265
F	-0.9715110	1.9712782	-0.5913687
F	-1.0089891	2.0369953	-2.9399285

Coran-cl-side

Cl	4.7697759	-1.2716390	-3.4503749
C	0.1619025	-0.0441503	3.3747586
C	-0.9378939	0.3357206	2.4988258
C	-2.3393511	-0.0577540	2.5675698
C	-3.1658510	-0.0634957	1.4314020
C	1.4966328	-0.0319153	2.9340386
C	-0.5444092	0.8953355	1.2739985
C	0.8144387	0.9174848	0.8311986
C	1.8633082	0.3614105	1.5803436
C	3.0419093	-0.0151081	0.8077844
C	-3.1630012	-0.0642935	-1.1976923
C	-2.3302883	-0.0618768	-2.3301077
C	-0.9291685	0.3322026	-2.2626601
C	0.1724025	-0.0498981	-3.1391907
C	1.5088226	-0.0413710	-2.7077429
C	3.0444403	-0.0211934	-0.5964599
C	1.8560609	0.3604730	-1.3499651
C	0.8143041	0.9218364	-0.5977895
C	-0.5445775	0.9029951	-1.0392232
C	-1.3853863	0.8872020	0.1166031
C	-2.6702272	0.3237049	0.1169168
H	-0.0524964	-0.4654149	-4.1318765
H	3.8998507	-0.4268869	-1.1625842
H	2.2711830	-0.4356622	3.6015255
H	-2.7397270	-0.4597856	3.5091540
H	-4.1804947	-0.4699949	-1.2942058
H	-2.7265027	-0.4710313	-3.2704817
H	2.3140718	-0.4495957	-3.3412679
H	3.9209754	-0.4152152	1.3327746
H	-0.0590774	-0.4526460	4.3712303
H	-4.1829875	-0.4703535	1.5251695

Coran-cl-out

Cl	-1.4069945	0.0223944	3.7761975
C	1.0223135	-0.7148320	0.7162415
C	1.0267488	0.7132739	0.7126239
C	-0.3295149	1.1579908	0.7232731
C	-1.1765240	0.0058863	0.7513266
C	-0.3367737	-1.1519484	0.7310492
C	2.0652599	-1.4779704	0.1727885
C	2.0744207	1.4656773	0.1637257
C	-2.4468470	0.0083126	0.1570120
C	-0.7199333	2.3791209	0.1603985
C	-0.7348767	-2.3742185	0.1768242
C	3.2476811	-0.7126542	-0.2056165
C	1.6959216	-2.8343054	-0.2053804
C	0.3561680	-3.2584603	-0.2056074
C	3.2520426	0.6908247	-0.2100351
C	1.7141082	2.8223857	-0.2217543
C	-2.1420463	-2.4456649	-0.2066584
C	-2.9524910	-1.3019015	-0.2231274
C	-2.9440371	1.3183384	-0.2323944
C	-2.1248138	2.4569532	-0.2252836
C	0.3769186	3.2545485	-0.2258153
H	2.4885285	3.4962939	-0.6156287
H	4.1314825	-1.2421375	-0.5904530
H	0.1234380	-4.2580700	-0.6009644
H	-3.9741081	-1.3885625	-0.6207558
H	-2.5268295	3.4026366	-0.6154147
H	-3.9650527	1.4082354	-0.6315093
H	0.1503349	4.2537335	-0.6256882
H	4.1389079	1.2123498	-0.5986649
H	2.4650927	-3.5149604	-0.5980336
H	-2.5496745	-3.3920939	-0.5876362

Coran-cl-in

Cl	0.0000000	0.0000000	-2.3552502
C	-0.9830178	0.7142043	0.9689035

C	-0.9830178	-0.7142043	0.9689035
C	0.3754794	-1.1556068	0.9689035
C	1.2150769	0.0000000	0.9689035
C	0.3754794	1.1556068	0.9689035
C	-2.0172717	1.4656337	0.3937970
C	-2.0172717	-1.4656337	0.3937970
C	2.4934850	0.0000000	0.3937970
C	0.7705292	-2.3714451	0.3937970
C	0.7705292	2.3714451	0.3937970
C	-3.1876949	0.7005803	-0.0037532
C	-1.6513434	2.8151868	-0.0037532
C	-0.3187604	3.2481693	-0.0037532
C	-3.1876949	-0.7005803	-0.0037532
C	-1.6513434	-2.8151868	-0.0037532
C	2.1671086	2.4404615	-0.0037532
C	2.9906901	1.3068987	-0.0037532
C	2.9906901	-1.3068987	-0.0037532
C	2.1671086	-2.4404615	-0.0037532
C	-0.3187604	-3.2481693	-0.0037532
H	2.5545431	-3.3718643	-0.4402333
H	-2.4174363	-3.4714782	-0.4402333
H	-4.0486009	1.2263728	-0.4402333
H	-0.0847366	4.2294183	-0.4402333
H	3.9962308	1.3875514	-0.4402333
H	-4.0486009	-1.2263728	-0.4402333
H	-0.0847366	-4.2294183	-0.4402333
H	3.9962308	-1.3875514	-0.4402333
H	2.5545431	3.3718643	-0.4402333
H	-2.4174363	3.4714782	-0.4402333

Coran-br-side

Br	4.8997554	-1.3981181	-3.5440740
C	0.1559232	-0.0408289	3.3773279
C	-0.9420601	0.3427237	2.5007675
C	-2.3444038	-0.0475784	2.5692201
C	-3.1700511	-0.0511489	1.4327554
C	1.4907294	-0.0324766	2.9375574
C	-0.5470055	0.9022853	1.2763666
C	0.8123231	0.9209125	0.8347060
C	1.8587531	0.3607550	1.5841430
C	3.0365632	-0.0189766	0.8126724
C	-3.1650317	-0.0564681	-1.1950258
C	-2.3328935	-0.0538732	-2.3274834
C	-0.9323599	0.3414034	-2.2601154
C	0.1674143	-0.0436685	-3.1365739
C	1.5031646	-0.0401226	-2.7036637
C	3.0393144	-0.0243219	-0.5913331
C	1.8533810	0.3602836	-1.3465915
C	0.8133345	0.9256114	-0.5945339
C	-0.5454872	0.9112715	-1.0368364
C	-1.3870563	0.8970857	0.1185244
C	-2.6724079	0.3341768	0.1185732
H	-0.0579138	-0.4584024	-4.1290949
H	3.8972600	-0.4331228	-1.1492083
H	2.2641106	-0.4385471	3.6049399
H	-2.7458922	-0.4485302	3.5107901
H	-4.1809470	-0.4658224	-1.2897686
H	-2.7282212	-0.4652883	-3.2671694
H	2.3010182	-0.4525761	-3.3419753
H	3.9142689	-0.4220809	1.3372293
H	-0.0671605	-0.4501694	4.3729699
H	-4.1887830	-0.4543630	1.5254835

Coran-br-out

Br	-1.4264880	0.0240100	3.9322842
C	1.0229991	-0.7162765	0.7068640
C	1.0285343	0.7119979	0.7025920
C	-0.3270960	1.1580438	0.7137703
C	-1.1746471	0.0064214	0.7373993

C	-0.3360741	-1.1517149	0.7205554	C	-4.1827906	-0.3251527	-0.5168612
C	2.0666361	-1.4800633	0.1664556	C	-1.1258798	-0.2453290	3.3107809
C	2.0774567	1.4645866	0.1565353	C	-2.0258454	0.7781839	0.8760812
C	-2.4464918	0.0096273	0.1474836	C	-0.6567969	0.9225629	1.2602939
C	-0.7173434	2.3807905	0.1547053	C	-0.1291269	0.3314513	2.4181427
C	-0.7351757	-2.3749892	0.1685228	C	1.3121300	0.1147603	2.3969246
C	3.2499147	-0.7151372	-0.2096855	C	-2.7575499	0.0222923	-2.6987772
C	1.6964179	-2.8370416	-0.2089970	C	-1.4524319	0.2172935	-3.1811176
C	0.3561065	-3.2601912	-0.2107655	C	-0.3667065	0.6664192	-2.3189667
C	3.2552304	0.6885478	-0.2142439	C	1.0679815	0.4570188	-2.4715129
C	1.7172102	2.8216602	-0.2276229	C	1.9452200	0.4681993	-1.3745300
C	-2.1415392	-2.4455608	-0.2129459	C	2.0756023	0.2858468	1.2304765
C	-2.9525608	-1.3007190	-0.2308388	C	1.4558863	0.7017318	-0.0215733
C	-2.9434922	1.3218299	-0.2368149	C	0.1177234	1.1090539	0.0742307
C	-2.1231274	2.4599653	-0.2268369	C	-0.7724329	1.0852423	-1.0427774
C	0.3802644	3.2555475	-0.2302688	C	-2.0974670	0.8794832	-0.5484820
H	2.4913666	3.4959449	-0.6210391	C	-3.1028816	0.2571426	-1.3028801
H	4.1347038	-1.2444360	-0.5924375	H	1.4681166	0.1721318	-3.4544519
H	0.1237508	-4.2603306	-0.6040985	H	3.1382663	0.0054169	1.2265786
H	-3.9745523	-1.3876851	-0.6270176	H	-0.8006799	-0.6862063	4.2635620
H	-2.5266952	3.4073462	-0.6119505	H	-4.9088999	-0.9682607	1.4104717
H	-3.9654689	1.4149941	-0.6318453	H	-3.5063409	-0.4178600	-3.3725598
H	0.1551672	4.2558867	-0.6279214	H	-1.2271638	-0.0805245	-4.2148519
H	4.1441556	1.2086866	-0.5995712	H	3.0003004	0.1950213	-1.5163558
H	2.4655844	-3.5203028	-0.5971581	H	1.8068378	-0.3007273	3.2858294
H	-2.5522868	-3.3922229	-0.5916501	H	-3.1534651	-0.9220154	3.6112177
Br	0.0000000	0.0000000	-2.4930043	H	-5.0320727	-0.7946471	-1.0333074
Coran-br-in				Coran-bf4-out			
C	-0.9832812	0.7143956	0.9778526	B	-1.3834403	0.0747305	3.4311987
C	-0.9832812	-0.7143956	0.9778526	F	0.0285084	0.0683541	3.1421735
C	0.3755800	-1.1559163	0.9778526	F	-1.5865484	0.1024120	4.8516947
C	1.2154023	0.0000000	0.9778526	F	-1.9860174	-1.1106058	2.8754081
C	0.3755800	1.1559163	0.9778526	F	-1.9847033	1.2382372	2.8297559
C	-2.0167010	1.4652190	0.3998579	C	1.2379432	-0.7182866	0.2232387
C	-2.0167010	-1.4652190	0.3998579	C	1.2467849	0.7092006	0.1962001
C	2.4927795	0.0000000	0.3998579	C	-0.1069192	1.1572185	0.2381011
C	0.7703112	-2.3707742	0.3998579	C	-0.9490497	0.0104817	0.2873549
C	0.7703112	2.3707742	0.3998579	C	-0.1210710	-1.1476261	0.2820657
C	-3.1865446	0.7004366	0.0003577	C	2.2578037	-1.4938116	-0.3391692
C	-1.6508513	2.8141372	0.0003577	C	2.2754894	1.4509638	-0.3948848
C	-0.3185416	3.2470308	0.0003577	C	-2.2558504	0.0096732	-0.2009547
C	-3.1865446	-0.7004366	0.0003577	C	-0.5182595	2.3771356	-0.3063387
C	-1.6508513	-2.8141372	0.0003577	C	-0.5475898	-2.3815233	-0.2174643
C	2.1662624	2.4396691	0.0003577	C	3.4295503	-0.7383808	-0.7684146
C	2.9896751	1.3063388	0.0003577	C	1.8682331	-2.8595184	-0.6706437
C	2.9896751	-1.3063388	0.0003577	C	0.5294790	-3.2812867	-0.6114260
C	2.1662624	-2.4396691	0.0003577	C	3.4379971	0.6659277	-0.7949129
C	-0.3185416	-3.2470308	0.0003577	C	1.9026973	2.8085904	-0.7762339
H	2.5520323	-3.3697182	-0.4399082	C	-1.9699235	-2.4513534	-0.5284698
H	-2.4161711	-3.4684271	-0.4399082	C	-2.7841236	-1.3088188	-0.5192652
H	-4.0453082	1.2261124	-0.4399082	C	-2.7678392	1.3219821	-0.5674676
H	-0.0839668	4.2262063	-0.4399082	C	-1.9398309	2.4534570	-0.6183054
H	3.9934138	1.3858268	-0.4399082	C	0.5692960	3.2489427	-0.7328403
H	-4.0453082	-1.2261124	-0.4399082	H	2.6659076	3.4812628	-1.1934647
H	-0.0839668	-4.2262063	-0.4399082	H	4.3002850	-1.2753583	-1.1715048
H	3.9934138	-1.3858268	-0.4399082	H	0.2855535	-4.2946218	-0.9617033
H	2.5520323	3.3697182	-0.4399082	H	-3.8295927	-1.4067833	-0.8435032
H	-2.4161711	3.4684271	-0.4399082	H	-2.3625934	3.4001964	-0.9832562
Coran-bf4-side				H	0.3363938	4.2518382	-1.1187329
B	5.9017736	-0.6382064	-0.3503154	H	4.3154538	1.1766048	-1.2172724
F	5.0567604	-0.2839259	-1.4732372	H	2.6219904	-3.5561048	-1.0650492
F	7.0729713	0.1817420	-0.3613615	H	-2.4038014	-3.4045155	-0.8621562
F	6.2524288	-2.0221252	-0.4392484	H	-3.8124550	1.4211874	-0.8940180
F	5.1670041	-0.4068194	0.8775612	Coran-bf4-in			
C	-2.4734850	-0.3817465	2.9373768	B	-0.5170731	-0.8548313	-2.6283357
C	-2.9547229	0.0475983	1.6311121	F	-0.0851982	-2.2285207	-2.5384539
C	-4.1122146	-0.4250246	0.8827287	F	0.0008447	-0.1181527	-1.5046094

F	-1.9583860	-0.8067335	-2.6066055
F	-0.0318042	-0.2752995	-3.8468549
C	1.1643666	-0.3369276	1.3825934
C	0.7436599	1.0294247	1.4041361
C	-0.6840608	1.0524037	1.3302392
C	-1.1461071	-0.2991638	1.2665620
C	-0.0028965	-1.1585462	1.2996937
C	2.4022966	-0.7290772	0.8506001
C	1.5415218	2.0732587	0.9111591
C	-2.3252291	-0.6513641	0.5926377
C	-1.3855908	2.1183694	0.7463111
C	0.0099637	-2.4068005	0.6594405
C	3.3143711	0.3594637	0.5378977
C	2.4694934	-2.1039236	0.3843003
C	1.3232163	-2.9023952	0.2875260
C	2.9046298	1.7000043	0.5683449
C	0.8170016	3.2697179	0.5129625
C	-1.2705784	-2.8610635	0.1484812
C	-2.3879010	-2.0213001	0.1163112
C	-3.1524121	0.4620697	0.1627495
C	-2.7077454	1.7876793	0.2415542
C	-0.5826581	3.2897030	0.4329699
H	-3.3179427	2.5769049	-0.2191252
H	-3.2750369	-2.3505562	-0.4381154
H	1.3993290	-3.8723518	-0.2205719
H	4.3148634	0.1237724	0.1484385
H	1.3786877	4.1410762	0.1476652
H	3.5976041	2.4719515	0.2048897
H	-1.0723486	4.1756865	0.0046304
H	-4.0884042	0.2523039	-0.3710072
H	-1.3195437	-3.8196123	-0.3819236
H	3.4120555	-2.4814538	-0.0358337

Table S1. Complexation energies (kJ/mol) obtained for the complexes formed with pentasubstituted bowls in different solvents. BLYP-D/aug-cc-pVDZ. Energies corrected with the BSSE obtained from gas-phase calculations.

5

		Water	Ethanol	THF	CHCl ₃	Vacuum
Coran...Cl	side	11.64	9.95	3.76	-1.11	-56.07
	out1	30.59	30.86	30.49	29.19	-9.87
	in	34.63	33.52	29.26	25.69	-20.32
Coran...Br	side	7.62	6.21	1.03	-3.09	-50.52
	out1	22.76	23.29	23.82	23.22	-8.46
	in	24.77	23.98	20.74	17.90	-21.29
Coran...BF ₄	side	-1.37	-2.66	-7.17	-10.60	-45.81
	out1	8.24	8.32	7.94	7.17	-11.04
	in	4.90	3.52	-1.07	-4.43	-37.40
Cl5...Cl	side	22.6	20.8	14.0	8.6	-57.3
	out1	36.5	34.2	25.6	18.7	-63.7
	out2	34.7	32.4	24.0	17.1	-66.0
Cl5...Br	side	16.5	15.1	9.9	5.6	-51.0
	out1	25.3	23.6	16.9	11.3	-59.9
	in	25.7	24.0	17.2	11.5	-61.8
Cl5...BF ₄	side	1.4	0.0	-5.0	-8.8	-49.9
	out1	0.5	-1.2	-7.0	-11.4	-55.7
	out2	2.1	0.4	-5.5	-9.9	-55.0
F5...Cl	side	-9.0	-11.4	-19.4	-25.1	-78.0
	out1	18.5	16.7	10.5	5.5	-52.5
	out2	34.6	32.7	25.6	19.9	-52.3
F5...Br	side	29.4	27.5	20.5	14.8	-58.0
	out1	27.3	24.5	15.0	7.7	-66.7
	in	13.0	11.7	6.9	3.0	-45.7
F5...BF ₄	side	23.9	22.5	17.2	12.6	-49.1
	out1	22.1	20.7	15.0	10.3	-53.9
	in	17.4	15.1	6.9	0.7	-65.6
CN5...Cl	side	0.8	-0.4	-4.6	-7.7	-41.8
	out1	2.2	0.7	-4.5	-8.4	-48.5
	out2	3.0	1.5	-3.8	-7.8	-49.1
CN5...Br	side	-8.4	-10.7	-18.5	-24.1	-74.7
	out1	52.4	44.7	20.0	2.7	-145.6
	out2	41.8	34.6	11.6	-4.6	-145.2
CN5...BF ₄	side	51.2	43.6	19.1	1.9	-145.7
	out1	20.0	13.5	-7.4	-21.9	-147.1
	in	35.2	29.0	8.4	-6.3	-137.4
CN5...Br	side	29.5	23.3	3.1	-11.3	-138.9
	out1	35.0	28.7	8.3	-6.4	-137.4
	in	10.4	4.5	-14.5	-27.8	-144.5
CN5...BF ₄	side	-5.8	-10.6	-25.8	-36.0	-117.3
	out1	-4.3	-8.9	-23.5	-33.4	-114.0
	in	-18.6	-24.1	-41.3	-52.9	-144.4

Table S2. Complexation energies (kJ/mol) obtained for the complexes formed with decasubstituted bowls in different solvents. BLYP-D/aug-cc-pVDZ. Energies corrected with the BSSE obtained from gas-phase calculations.

5

		Water	Ethanol	THF	CHCl ₃	Vacuum
Cl10···Cl	out1	32.4	28.8	16.6	7.4	-90.7
	out2	34.9	31.9	21.1	12.7	-82.2
	in	20.6	17.1	5.1	-3.7	-93.2
Cl10···Br	out1	21.7	18.8	8.6	0.7	-86.5
	out2	24.5	22.1	13.5	6.5	-77.0
	in	10.5	7.5	-2.7	-10.3	-89.7
Cl10···BF ₄	out1	-5.5	-8.3	-17.5	-24.1	-83.4
	out2	-4.5	-7.2	-15.8	-22.0	-79.3
	in	-16.1	-19.2	-29.4	-36.7	-101.2
F10···Cl	out1	35.7	31.9	18.9	9.3	-89.1
	out2	34.1	30.5	18.3	9.0	-89.9
	in	19.7	15.4	1.0	-9.5	-107.9
F10···Br	out1	24.8	21.6	10.7	2.5	-84.6
	out2	24.5	21.7	11.5	3.7	-83.8
	in	9.7	5.9	-6.8	-16.1	-105.3
F10···BF ₄	out1	-3.0	-6.0	-15.7	-22.5	-82.5
	out2	-2.4	-5.3	-14.6	-21.2	-80.6
	in	-16.5	-20.1	-31.9	-40.1	-111.0
CN10···Cl	out1	25.5	13.2	-24.6	-49.6	-238.1
	out2	24.3	13.8	-19.4	-42.0	-222.1
	in	9.8	-1.0	-34.0	-56.0	-229.2
CN10···Br	out1	14.0	2.6	-32.3	-55.5	-230.7
	out2	15.2	5.5	-25.3	-46.4	-215.3
	in	3.1	-7.0	-38.0	-58.7	-223.6
CN10···BF ₄	out1	-15.5	-24.3	-51.0	-68.3	-190.3
	out2	-13.9	-22.2	-47.6	-64.1	-183.5
	in	-30.7	-40.3	-69.3	-88.1	-222.6