Supporting Information

Anion/π Interactions Revisited: Are There Really Attractive Interactions between Anions and the π–Systems of Substituted Benzenes?

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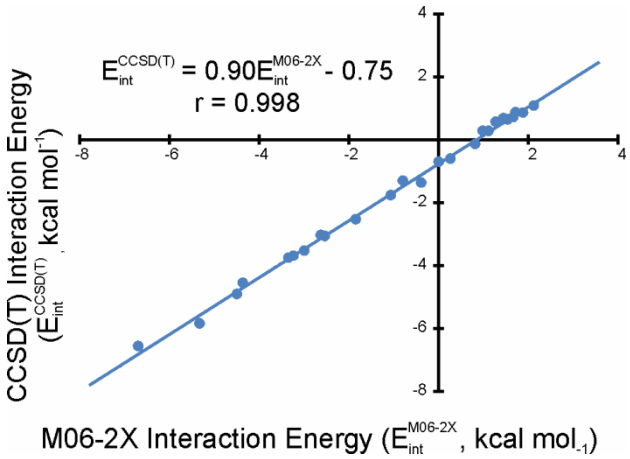

Figure S1. Esimated CCSD(T)/AVTZ interaction energies versus M06–2X/6–31+G(d) interaction energies, in kcal mol^{-1}.

Table S1. Additive M06–2X/6–31+G(d) interaction energies [$E_{int}^{additive}$, in kcal mol^{-1}. See eq (1) in main text] for $Cl^{-\cdots}C_6H_{6-n}X_n$ complexes. Estimated CCSD(T)/AVTZ//M06–2X/6–31+G(d) additive interaction energies for the monosubstituted systems are provided in parentheses.

	n					
	1		2	3	4	6
H	1.7	(0.9)				
CH_2OH	1.7	(0.7)	1.7	1.6		
NHOH	0.2	(–0.5)	–2.2	–3.6		
$N(CH_3)_2$	–0.9	(–1.8)	–4.8	–6.5		
$NHCH_3$	–0.5	(–1.2)	–4.1	–5.3		
OCH_3	–0.5	(–1.0)	–2.9	–5.5		
OH	–0.4	(–0.7)	–2.6	–4.8		
CH_3	1.2	(0.4)	0.5	–0.1	–0.3	–1.6
NH_2	–0.8	(–1.0)	–4.1	–5.7	–0.9	–4.2
SCH_3	0.1	(–0.3)	–1.8	–3.8		
SH	–0.3	(–0.6)	–2.6	–5.1		
CCH	0.1	(–0.5)	–1.7	–3.8	–6.1	–11.1
SiH_3	0.5	(–0.5)	–0.8	–2.2		
F	–2.7	(–2.8)	–7.9	–13.2	–19.3	–31.9
$COOCH_3$	–0.8	(–1.5)	–3.6	–6.5		
COOH	–1.6	(–2.3)	–5.2	–9.0		
$COCH_3$	–2.0	(–2.6)	–6.0	–10.2		
OCF_3	–4.5	(–4.7)	–11.6	–19.1		
BF_2	–2.3	(–2.7)	–6.3	–10.5		
CHO	–2.5	(–2.9)	–7.0	–11.7		
CF_3	–3.9	(–4.2)	–10.2	–16.8		
NO	–3.8	(–3.8)	–10.0	–16.7		
SiF_3	–4.0	(–4.3)	–9.8	–15.6		
CN	–6.3	(–6.7)	–13.2	–25.0	–30.0	–56.8
NO_2	–7.1	(–6.9)	–18.7	–27.6		

Table S2. Absolute energies (hartree) for C_6H_5X and $Cl^-\cdots C_6H_5X$, ESP (kcal mol^{-1}), and Q_{zz} component of the arene quadrupole moment (Buckinghams).

	C_6H_5X	$Cl^-\cdots C_6H_5X$	ESP	Q_{zz}
H	–232.144420	–692.377006	–6.9	–8.6
BF_2	–456.161696	–916.401788	–3.3	–3.3
CCH	–308.266166	–768.501475	–6.8	–11.5
CF_3	–569.101316	–1029.341964	–3.1	–8.2
CH_2OH	–346.626584	–806.858523	–8.1	–11.4
CH_3	–271.441420	–731.674965	–7.3	–8.2
CHO	–345.431563	–805.672042	–3.2	–3.8
CN	–324.362323	–784.606131	–1.2	–1.8
$COCH_3$	–384.734790	–844.974148	–4.4	–5.0
$COOCH_3$	–459.946137	–920.183162	–5.6	–8.9
COOH	–420.662289	–880.900556	–4.6	–7.7
F	–331.357687	–791.594270	–4.9	–6.2
$N(CH_3)_2$	–366.052394	–826.285067	–8.4	–11.0
NH_2	–287.479896	–747.713646	–6.8	–11.5
$NHCH_3$	–326.766511	–786.999366	–7.5	–11.4
NHOH	–362.617436	–822.849760	–7.9	–10.6
NO	–361.396213	–821.638488	–2.1	–3.2
NO_2	–436.579762	–896.825744	0.1	–2.0
OCF_3	–644.297749	–1104.537256	–4.0	–8.2
OH	–307.341603	–767.574898	–7.2	–9.0
OCH_3	–346.625421	–806.858432	–7.8	–9.4
SCH_3	–669.591880	–1129.825902	–7.6	–10.7
SH	–630.296401	–1090.531306	–6.9	–10.2
SiF_3	–820.662272	–1280.904758	–2.3	–8.6
SiH_3	–522.790737	–983.026668	–6.4	–7.8

Table S3. Absolute energies (hartree) for $C_6H_4X_2$ and $Cl^{-}\cdots C_6H_4X_2$, ESP (kcal mol^{-1}), and Q_{zz} component of the arene quadrupole moment (Buckinghams).

	$C_6H_4X_2$	$Cl^{-}\cdots C_6H_4X_2$	ESP	Q_{zz}
BF_2	–680.17658	–1140.42398	0.6	7.4
CCH	–384.38769	–844.625452	–6.2	–13.8
CF_3	–906.05542	–1366.30433	1.5	0.4
CH_2OH	–461.10845	–921.339783	–9.4	–16.9
CH_3	–310.73819	–770.972945	–7.3	–8.0
CHO	–458.7163	–918.964376	0.9	4.5
CN	–416.57597	–876.831116	5.4	11.2
$COCH_3$	–537.32361	–997.569386	–1.3	2.7
$COOCH_3$	–687.74631	–1147.98731	–4.1	–7.3
COOH	–609.17812	–1069.42169	–2.1	–4.3
F	–430.56863	–890.809612	–2.4	–2.2
$N(CH_3)_2$	–499.95663	–960.191489	–9.1	–16.6
NH_2	–342.81132	–803.047598	–5.9	–14.3
$NHCH_3$	–421.38443	–881.619656	–7.7	–15.5
NHOH	–493.08838	–953.321696	–8.5	–12.5
NO	–490.64419	–950.89598	3.4	6.9
NO_2	–641.00859	–1101.26808	8.4	14.0
OCF_3	–1056.4483	–1516.69493	–0.3	0.1
OH	–382.53552	–842.769809	–6.9	–9.0
OCH_3	–461.10386	–921.337712	–7.8	–10.2
SCH_3	–1107.0388	–1567.27438	–8.2	–11.9
SH	–1028.4475	–1488.6849	–6.4	–10.1
SiF_3	–1409.1772	–1869.42903	2.9	2.3
SiH_3	–813.43695	–1273.67615	–5.7	–5.8

Table S4. Absolute energies (hartree) for $C_6H_3X_3$ and $Cl^-\cdots C_6H_3X_3$, ESP (kcal mol^{-1}), and Q_{zz} component of the arene quadrupole moment (Buckinghams).

	$C_6H_3X_3$	$Cl^-\cdots C_6H_3X_3$	ESP	Q_{zz}
BF_2	–904.19296	–1364.44805	5.1	15.0
CCH	–460.50724	–920.74736	–5.6	–17.0
CF_3	–1243.0069	–1703.26401	6.2	4.1
CH_2OH	–575.59206	–1035.82291	–10.8	–19.7
CH_3	–350.03535	–810.271348	–7.5	–7.6
CHO	–572.00168	–1032.25763	5.3	11.4
CN	–508.78473	–969.051429	12.2	19.8
$COCH_3$	–689.9151	–1150.16745	1.9	7.4
$COOCH_3$	–915.54645	–1375.79165	–2.3	–8.4
COOH	–797.69337	–1257.94249	0.8	–3.0
F	–529.78035	–990.025709	0.3	0.6
$N(CH_3)_2$	–633.86733	–1094.10108	–11.0	–21.0
NH_2	–398.15155	–858.387304	–6.6	–18.9
$NHCH_3$	–516.01153	–976.245282	–9.2	–20.7
NHOH	–623.56576	–1083.7979	–10.2	–15.9
NO	–619.88981	–1080.15183	9.6	14.0
NO_2	–845.432	–1305.70551	16.7	23.8
OCF_3	–1468.5984	–1928.85128	2.9	3.5
OH	–457.73783	–917.972437	–7.0	–9.9
OCH_3	–575.5893	–1035.82306	–9.0	–12.6
SCH_3	–1544.4875	–2004.72394	–9.1	–15.6
SH	–1426.5998	–1886.83905	–6.5	–11.8
SiF_3	–1997.6908	–2457.95183	7.9	6.4
SiH_3	–1104.0836	–1564.32601	–4.7	–4.6

Table S5. Absolute energies (hartree) for $C_6H_2X_4$ and $Cl^-\cdots C_6H_2X_4$, ESP (kcal mol^{-1}), and Q_{zz} component of the arene quadrupole moment (Buckinghams).

	$C_6H_2X_4$	$Cl^-\cdots C_6H_2X_4$	ESP	Q_{zz}
CCH	–536.62689	–996.867697	–5.8	–21.4
CH_3	–389.33365	–849.56917	–8.0	–7.2
CN	–600.98727	–1061.26282	17.8	26.0
F	–628.97592	–1089.22589	3.3	3.7
NH_2	–453.48441	–913.714989	–10.5	–15.2

Table S6. Absolute energies (hartree) for $C_6H_2X_4$ and $Cl^-\cdots C_6H_2X_4$, ESP (kcal mol^{-1}), and Q_{zz} component of the arene quadrupole moment (Buckinghams).

	$C_6H_2X_4$	$Cl^-\cdots C_6H_2X_4$	ESP	Q_{zz}
CCH	–688.86251	–1149.10463	–6.3	–30.6
CH_3	–467.91471	–928.151546	–8.6	–6.3
CN	–785.38471	–1245.67727	28.2	37.1
F	–827.36665	–1287.62609	9.4	9.1
NH_2	–564.1445	–1024.37741	–10.5	–13.3

Optimized Cartesian coordinates (Angstrom)

15
Cl^-···C6H5BF2

C	1.75532853	1.73197405	0.00000000
C	1.42924486	1.12006945	-1.20980600
C	1.42924486	1.12006945	1.20980600
C	0.44076362	-0.73484162	0.00000000
C	0.77499601	-0.10764574	1.20800000
C	0.77499601	-0.10764574	-1.20800000
H	0.51983257	-0.58646667	-2.14609300
H	1.68459783	1.59924603	-2.14674300
H	1.68459783	1.59924603	2.14674300
H	0.51983257	-0.58646667	2.14609300
F	-0.61521130	-2.71640639	-1.13455100
F	-0.61521130	-2.71640639	1.13455100
B	-0.28617421	-2.09895961	0.00000000
H	2.26486768	2.68813770	0.00000000
Cl	-1.98802926	2.14967868	0.00000000

15
Cl^-···C6H5CCH

C	0.14866529	-1.13567711	0.00000000
C	0.59785875	-0.59208852	1.21067500
C	0.59785875	-0.59208852	-1.21067500
C	1.92819742	1.01781230	0.00000000
C	1.48356489	0.47974309	-1.20665700
C	1.48356489	0.47974309	1.20665700
H	0.24756991	-1.01598832	-2.14301400
H	0.24756991	-1.01598832	2.14301400
H	1.82707094	0.89543474	-2.14584400
H	1.82707094	0.89543474	2.14584400
C	-0.76571418	-2.24220757	0.00000000
C	-1.53505487	-3.17322026	0.00000000
H	-2.21389743	-3.99471724	0.00000000
H	2.61813337	1.85273386	0.00000000
Cl	-1.65806843	2.17241127	0.00000000

16
Cl^-···C6H5CF3

C	1.84892313	1.87204269	0.00000000
C	1.49041732	1.27666931	-1.20768600
C	1.49041732	1.27666931	1.20768600
C	0.41703644	-0.50385216	0.00000000
C	0.77256965	0.08434931	1.21154400
C	0.77256965	0.08434931	-1.21154400
H	1.76585897	1.74061530	2.14615600
H	1.76585897	1.74061530	-2.14615600
C	-0.30997113	-1.81498253	0.00000000
F	-1.09530787	-1.95958059	1.08558200
F	0.54493122	-2.86217007	0.00000000
F	-1.09530787	-1.95958059	-1.08558200
H	0.48561118	-0.38229525	2.14479900
H	0.48561118	-0.38229525	-2.14479900
H	2.40527413	2.80105635	0.00000000
Cl	-1.82287224	2.46251843	0.00000000

17
Cl^-···C6H5CH2OH

C	2.07498866	0.85069420	0.36722796
C	1.37687149	0.18784761	1.37218163
C	1.79781194	0.56196599	-0.96899143
C	0.12656584	-1.05016384	-0.28239641
C	0.82900143	-0.38315264	-1.28919568
C	0.40492278	-0.76032826	1.05122581
H	2.33542171	1.07217952	-1.75884046
H	1.58689303	0.40702504	2.41203038
C	-0.91715051	-2.06897470	-0.66933402
H	-1.68121393	-1.58368104	-1.28670411
H	-0.44585378	-2.85635887	-1.26796099
H	0.61609511	-0.60514872	-2.33029789
H	-0.14045772	-1.27827877	1.82789508
H	2.82875247	1.58607786	0.61994527
O	-1.50154308	-2.61899399	0.50111891
H	-2.16621751	-3.26792332	0.24685653
Cl	-1.47524379	2.55592530	0.00257752

16
Cl^-···C6H5CH3

C	1.95672908	-0.34588745	0.00722630
C	1.29660089	-0.58050064	-1.19692758
C	1.28066163	-0.54438671	1.20903010
C	-0.71867938	-1.20809740	0.00244455
C	-0.04474061	-0.97323453	1.20351284
C	-0.02884342	-1.00925309	-1.19610025
H	1.78567676	-0.36984697	2.15155539
H	1.81409162	-0.43422743	-2.13749494
C	-2.16414024	-1.64010549	-0.00064780
H	-2.40250391	-2.22212720	0.89100220
H	-2.82750335	-0.77103408	-0.01808728
H	-2.39078767	-2.24867296	-0.87750589
H	-0.56386510	-1.12919542	2.14322292
H	-0.53550561	-1.19345018	-2.13749995
H	2.98848503	-0.01625978	0.00911422
Cl	-0.43138915	2.71727094	-0.01150210

15
Cl⁻···C6H5CHO

C	0.15583924	-1.07049228	-0.21795767
C	0.44438413	-0.70585365	1.10047099
C	0.74027879	-0.38517539	-1.28364717
C	1.90300118	1.03071503	0.27813642
C	1.61632073	0.66836869	-1.03625064
C	1.31818437	0.34497676	1.34598764
H	0.50808966	-0.67799466	-2.30235388
H	-0.02369556	-1.25538616	1.90769072
H	2.07208980	1.20290757	-1.86018376
H	1.54726496	0.63406153	2.36408868
C	-0.77370352	-2.18860967	-0.49675816
O	-1.33051406	-2.84384090	0.35631371
H	-0.94134820	-2.40480137	-1.56703487
H	2.58415899	1.84993465	0.47377846
Cl	-1.61931039	2.19049580	-0.00037550

14
Cl⁻···C6H5CN

C	1.84571519	1.09569317	0.00000000
C	1.42786852	0.54151975	1.20898600
C	1.42786852	0.54151975	-1.20898600
C	0.17410573	-1.12129591	0.00000000
C	0.59092292	-0.56848788	-1.21523800
C	0.59092292	-0.56848788	1.21523800
C	-0.69270356	-2.27091057	0.00000000
N	-1.38877854	-3.19408711	0.00000000
H	1.75356182	0.97347382	2.14648100
H	1.75356182	0.97347382	-2.14648100
H	0.25855056	-1.00930010	-2.14582200
H	0.25855056	-1.00930010	2.14582200
H	2.49762136	1.96029037	0.00000000
Cl	-1.70521163	2.03368643	0.00000000

18
Cl⁻···C6H5COCH3

C	0.39789800	-0.75716013	0.04046105
C	0.77900471	-0.12734319	1.22959218
C	0.72329836	-0.17102259	-1.18564277
C	1.79929701	1.65479616	-0.03463136
C	1.42278426	1.03285430	-1.22254447
C	1.47666015	1.07339272	1.19235220
H	0.43558543	-0.64581436	-2.11499101
H	0.51720725	-0.59788426	2.16833417
H	1.67243346	1.48280205	-2.17523427
H	1.76973951	1.55754816	2.11550713
C	-0.35292200	-2.05051254	0.13219038
O	-0.62066721	-2.53440424	1.21551428
C	-0.77079165	-2.74163264	-1.14622736
H	0.10226040	-2.98390937	-1.75648875
H	-1.42452927	-2.09621486	-1.73732792
H	-1.29896068	-3.65569133	-0.88518053
H	2.34320953	2.59092780	-0.06380032
Cl	-1.88252829	2.18489632	0.04069224

19
Cl⁻···C6H5COOCH3

C	0.59674790	-0.32088136	-0.10436719
C	0.95705802	0.45296982	-1.20906731
C	0.74294706	0.18486202	1.18896362
C	1.61091606	2.24087835	0.27029209
C	1.25088127	1.46745606	1.37267247
C	1.46402322	1.73369271	-1.02047985
H	0.46060491	-0.42344420	2.03727103
H	0.83314403	0.03589437	-2.20010164
H	1.36561302	1.86287071	2.37424104
H	1.74408272	2.33553207	-1.87599705
C	0.05919973	-1.68515169	-0.36143493
O	-0.08538194	-2.16583755	-1.46368779
O	-0.25539817	-2.34279665	0.76685947
C	-0.77840789	-3.66414427	0.57146638
H	-0.97634580	-4.04635091	1.56809340
H	-1.69263425	-3.61915351	-0.01738360
H	-0.04567600	-4.28183394	0.05557710
H	2.00595053	3.23879762	0.41689551
Cl	-2.14051121	2.26521597	-0.06072005

16
Cl⁻···C6H5COOH

C	1.83680023	1.58949871	-0.02020145
C	1.46193854	0.98177759	-1.21735953
C	1.48589767	1.01405178	1.20098345
C	0.38460458	-0.77791861	0.02559085
C	0.75928051	-0.17050829	1.22559928
C	0.73440441	-0.20426119	-1.19848780
H	1.73579032	1.43084928	-2.16353329
H	1.77836653	1.48821515	2.12913831
H	0.43789892	-0.68502197	-2.12053333
H	0.47382283	-0.63846238	2.15861265
C	-0.39043897	-2.04156538	0.10179143
O	-0.72421256	-2.58854289	1.12804333
O	-0.70340340	-2.54834355	-1.11015770
H	-1.20361132	-3.36420746	-0.94875720
H	2.40297840	2.51250219	-0.03845590
Cl	-1.87289646	2.23557465	0.00782038

13
Cl⁻···C6H5F

C	0.68644763	1.18781778	0.00000000
C	0.06074714	0.97313410	1.21658000
C	0.06074714	0.97313410	-1.21658000
C	-1.91775662	0.29429098	0.00000000
C	-1.25708627	0.52097314	-1.20644900
C	-1.25708627	0.52097314	1.20644900
F	1.96689448	1.62715105	0.00000000
H	0.59983218	1.15809921	2.13600000
H	0.59983218	1.15809921	-2.13600000
H	-1.76715665	0.34596323	-2.14537100
H	-1.76715665	0.34596323	2.14537100
H	-2.94136591	-0.05691893	0.00000000
Cl	0.54811106	-2.61279440	0.00000000

13
Cl⁻···C6H6

C	-0.98556382	0.98556382	1.08050847
C	-1.34630522	-0.36074140	1.08050847
C	0.36074140	1.34630522	1.08050847
C	0.98556382	-0.98556382	1.08050847
C	1.34630522	0.36074140	1.08050847
C	-0.36074140	-1.34630522	1.08050847
H	-1.75154749	1.75154749	1.08050847
H	-2.39265837	-0.64111088	1.08050847
H	-0.64111088	-2.39265837	1.08050847
H	1.75154749	-1.75154749	1.08050847
H	2.39265837	0.64111088	1.08050847
H	0.64111088	2.39265837	1.08050847
Cl	0.00000000	0.00000000	-2.66949153

21
Cl⁻···C6H5NCH3_2

C	0.42933225	-0.84621748	0.00000000
C	0.84155937	-0.24240876	1.20480800
C	0.84155937	-0.24240876	-1.20480800
C	2.06440253	1.47001125	0.00000000
C	1.64797040	0.89041203	-1.19537800
C	1.64797040	0.89041203	1.19537800
H	0.53856359	-0.65352489	2.15666650
H	1.94805706	1.32462824	2.14181049
H	1.94805706	1.32462824	-2.14181049
H	0.53856359	-0.65352489	-2.15666650
N	-0.34587239	-1.99919219	0.00000000
C	-1.00725621	-2.37416484	-1.23492797
H	-1.59310683	-3.27409960	-1.05913546
H	-0.27409087	-2.60632470	-2.00861246
H	-1.67461421	-1.58672541	-1.61084497
C	-1.00725621	-2.37416484	1.23492797
H	-0.27409087	-2.60632470	2.00861246
H	-1.59310683	-3.27409960	1.05913546
H	-1.67461421	-1.58672541	1.61084497
H	2.68968142	2.35335094	0.00000000
Cl	-1.81811080	2.48260373	0.00000000

15
Cl⁻···C6H5NH2

C	0.77905109	1.18973755	0.00000000
C	0.08868170	1.01102680	-1.20529550
C	0.08868170	1.01102680	1.20529550
C	-1.94197058	0.47749163	0.00000000
C	-1.25632578	0.65796805	1.19985750
C	-1.25632578	0.65796805	-1.19985750
H	0.60973140	1.15637048	2.14520650
H	-1.77067190	0.52160613	2.14355150
H	-1.77067190	0.52160613	-2.14355150
H	0.60973140	1.15637048	-2.14520650
H	2.63086284	1.36299740	0.83449000
H	2.63086284	1.36299740	-0.83449000
N	2.11516628	1.59662962	0.00000000
H	-2.98829671	0.20109575	0.00000000
Cl	0.36656082	-2.79357438	0.00000000

18
Cl⁻···C6H5NHCH3

C	0.07369107	-1.11398630	-0.26625791
C	0.39744505	-0.81078496	1.06364885
C	0.81915782	-0.50791417	-1.29282924
C	2.17795062	0.66415889	0.32997728
C	1.85241247	0.36763138	-0.99541060
C	1.44287810	0.06695143	1.34796944
H	0.58359462	-0.74047146	-2.32601503
H	2.41054238	0.82168484	-1.80557487
H	1.67690939	0.28452906	2.38337851
H	-0.15806009	-1.25698114	1.87750484
N	-0.93285734	-2.01296809	-0.59148683
H	-1.29981071	-1.89878207	-1.52211661
C	-1.90351938	-2.42153476	0.40232171
H	-2.66043212	-3.03425557	-0.08440116
H	-1.42429275	-3.03283350	1.16915196
H	-2.39506984	-1.57108969	0.89130790
H	2.98579587	1.34681078	0.55953420
Cl	-1.31466294	2.68853155	-0.03169877

16
C6H5NHOH

C	2.09235245	0.79690317	-0.34736119
C	1.80076603	0.48432733	0.98082083
C	1.38845837	0.15812857	-1.36354922

C	0.11957216	-1.09102245	0.25764935
C	0.40276549	-0.78389919	-1.07218688
C	0.82328520	-0.45410143	1.28585229
H	0.60942708	-0.70513921	2.31924095
H	2.33813806	0.97228203	1.78499669
H	1.60020727	0.39479213	-2.39939607
H	-0.15410273	-1.26637553	-1.86216596
N	-0.81841261	-2.08798313	0.61922437
H	-1.38262198	-1.78374642	1.40392858
O	-1.72534225	-2.37206259	-0.41941948
H	-1.59207406	-3.31256427	-0.59173002
H	2.85486490	1.52823955	-0.58315630
Cl	-1.44149473	2.53546343	0.02951273

15

Cl¯···C6H5NO2

C	0.36672165	-0.76696376	0.00000000
C	0.70145779	-0.19276922	-1.21951500
C	0.70145779	-0.19276922	1.21951500
C	1.75088051	1.60737341	0.00000000
C	1.40191015	1.00876198	-1.21000200
C	1.40191015	1.00876198	1.21000200
H	1.67450837	1.47636733	-2.14716400
H	0.41660010	-0.68140403	-2.13988900
H	0.41660010	-0.68140403	2.13988900
H	1.67450837	1.47636733	2.14716400
O	-0.65784217	-2.52446432	-1.07799600
O	-0.65784217	-2.52446432	1.07799600
N	-0.37396506	-2.03751155	0.00000000
H	2.29609055	2.54260743	0.00000000
Cl	-1.84006503	2.09924146	0.00000000

14

Cl¯···C6H5NO

C	0.10884775	-1.07943027	-0.21809534
C	0.69985954	-0.42319115	-1.29458896
C	0.39854781	-0.72899733	1.10278891
C	1.89873662	0.96618827	0.26175201
C	1.29910125	0.30009887	1.33628072
C	1.60245121	0.60837186	-1.05172077
H	-0.08191382	-1.26351867	1.91150532
H	0.44079594	-0.73382004	-2.29935404
H	1.53938469	0.58950590	2.35153421
H	2.07105998	1.12914186	-1.87679257
N	-0.80885798	-2.12998648	-0.57555069
O	-1.31831572	-2.69556071	0.35947267
H	2.60044394	1.76822409	0.45452119
Cl	-1.55332377	2.18391862	-0.01216706

17

Cl¯···C6H5OCF3

C	0.62359471	-0.02863721	-0.36837246
C	0.97537665	0.88347597	-1.35589192
C	0.74355457	0.27412134	0.98183885
C	1.59046323	2.46137930	0.36477576
C	1.23199417	1.53210191	1.33552351
C	1.45997752	2.13146466	-0.98354273
H	0.47004060	-0.43505004	1.74847578
H	0.86386361	0.60097250	-2.39433841
H	1.32928945	1.77788113	2.38533826
H	1.73525211	2.84517390	-1.74959345
C	-0.23058552	-2.23323554	-0.03936390
O	0.15039621	-1.24660026	-0.86670682
F	-1.24967947	-1.87462492	0.76263758
F	0.76652872	-2.65638513	0.75880154
F	-0.63054685	-3.26111294	-0.78274968
H	1.96791145	3.43342030	0.65445314
Cl	-2.11250003	2.45620520	0.00184186

14

Cl¯···C6H5OH

C	-0.74384370	-1.17735055	0.00385504
C	-0.08229756	-0.97881413	1.21475627
C	-0.07854419	-0.97711602	-1.20411983
C	1.92722654	-0.37458482	0.00659157
C	1.25612787	-0.57599413	-1.19597944
C	1.24880223	-0.57876253	1.20879299
H	-0.59810646	-1.13304431	-2.14406849
H	1.76820089	-0.42187314	-2.13798518
H	1.76008879	-0.42532205	2.15135218
H	-0.62316131	-1.14158350	2.13801051
O	-2.05151197	-1.57037244	0.06253135
H	-2.40322817	-1.67586732	-0.82976234
H	2.96375363	-0.06306639	0.00896951
Cl	-0.44825169	2.67055702	0.00646196

17

Cl¯···C6H5OMe

C	0.09749778	-1.05068782	-0.25839041
C	0.40035395	-0.73164230	1.06548857
C	0.77014912	-0.41063389	-1.30476023
C	2.05138921	0.87032082	0.29638097
C	1.73859450	0.54158950	-1.02534844
C	1.37896354	0.23025903	1.32945527
H	-0.10680268	-1.21362148	1.88931465
H	1.60955803	0.47356077	2.35959427
H	2.25367703	1.03143362	-1.84271265
H	0.51354473	-0.67915011	-2.32148331
O	-0.83612280	-1.97044667	-0.63109018

C	-1.54273660	-2.64407469	0.39498328
H	-2.11089675	-1.93868837	1.00664674
H	-0.86069410	-3.21663753	1.02862185
H	-2.22621804	-3.32139254	-0.10956341
H	2.80770519	1.61392893	0.51231247
Cl	-1.44448000	2.48137389	-0.02710960

17

Cl^{-}···C6H5SCH3

C	0.42469192	-0.71853951	-0.21503155
C	0.65347120	-0.29877317	1.09669639
C	0.93404513	0.04289563	-1.27559626
C	1.88676719	1.62131645	0.28615022
C	1.65760372	1.20097913	-1.02470080
C	1.38184285	0.86655882	1.33879857
H	0.27329711	-0.86502664	1.93590855
H	1.55133171	1.17977816	2.36207700
H	2.04413618	1.77764330	-1.85633024
H	0.75948243	-0.27825731	-2.29632784
S	-0.48171293	-2.17484703	-0.65744107
C	-0.95369047	-2.85318389	0.95131907
H	-1.59192620	-2.16324385	1.50270478
H	-0.07855994	-3.11777286	1.54421666
H	-1.51894329	-3.75877567	0.73501788
H	2.45110877	2.52452711	0.48092032
Cl	-1.88770053	2.37242115	-0.04911435

14

Cl^{-}···C6H5SH

C	0.09483756	-1.06884109	-0.00945885
C	0.56989404	-0.56921703	1.20624284
C	0.58729567	-0.54929701	-1.20809075
C	2.02089550	0.96004603	0.02292578
C	1.54603887	0.46062861	-1.18685318
C	1.52753731	0.43955628	1.21779632
H	0.22705867	-0.92814578	-2.15716563
H	1.92023226	0.85542018	-2.12339638
H	1.88837164	0.81903503	2.16574018
H	0.19076603	-0.96920436	2.13917185
S	-1.12650800	-2.35544556	0.05083148
H	-1.26019570	-2.49539869	-1.27610664
H	2.76599848	1.74492908	0.03514089
Cl	-1.51688806	2.38960228	0.00870230

16

Cl^{-}···C6H5SiF3

C	0.55514067	-0.16946221	0.00000000
C	0.84215853	0.47931338	1.20869900
C	0.84215853	0.47931338	-1.20869900
C	1.70186932	2.37973421	0.00000000
C	1.41472297	1.74770436	-1.20842900
C	1.41472297	1.74770436	1.20842900
Si	-0.17909343	-1.84642320	0.00000000
F	0.90477973	-3.02051410	0.00000000
F	-1.07592372	-2.07742793	1.30156500
F	-1.07592372	-2.07742793	-1.30156500
H	0.61197020	-0.00231194	-2.15222700
H	0.61197020	-0.00231194	2.15222700
H	1.63229804	2.24272421	-2.14632000
H	1.63229804	2.24272421	2.14632000
H	2.14611935	3.36734824	0.00000000
Cl	-1.97225743	2.50554335	0.00000000

16

Cl^{-}···C6H5SiH3

C	0.16478306	-1.04432016	-0.00078791
C	0.64396011	-0.50755304	1.20145508
C	0.63524078	-0.50118959	-1.20365280
C	2.00942390	1.07593021	-0.00189012
C	1.54819550	0.55119029	-1.20733163
C	1.55697751	0.54482858	1.20405218
Si	-1.08885016	-2.44045606	0.00004710
H	-2.48425980	-1.91922946	-0.00120013
H	-0.90647492	-3.27497098	1.21905001
H	-0.90581777	-3.27784159	-1.21690264
H	0.29074030	-0.90421811	-2.15019676
H	0.30631033	-0.91559988	2.14830260
H	1.90141631	0.95753299	-2.14730436
H	1.91703778	0.94618734	2.14356994
H	2.72115731	1.89243669	-0.00232827
Cl	-1.58515838	2.34992766	0.00325186

17

Cl⁻···C6H4(BF2)2

C	0.69500700	1.20965400	0.55338278
C	-0.69500700	1.20965400	0.55338278
C	-0.69500700	-1.20965400	0.55338278
C	0.69500700	-1.20965400	0.55338278
C	1.40221200	0.00000000	0.55317978
C	-1.40221200	0.00000000	0.55317978
H	1.23828400	2.14683700	0.55314578
H	-1.23828400	2.14683700	0.55314578
H	-1.23828400	-2.14683700	0.55314578
H	1.23828400	-2.14683700	0.55314578
F	-3.64749100	1.13532100	0.55236678
F	-3.64749100	-1.13532100	0.55236678
F	3.64749100	1.13532100	0.55236678
F	3.64749100	-1.13532100	0.55236678
B	-2.95365200	0.00000000	0.55265178
B	2.95365200	0.00000000	0.55265178
Cl	0.00000000	0.00000000	-2.79668522

17

Cl⁻···C6H4(CCH)2

C	-1.40053000	0.00000000	-0.69638554
C	-0.69346500	1.21011600	-0.69638554
C	-0.69346500	-1.21011600	-0.69638554
C	1.40053000	0.00000000	-0.69638554
C	0.69346500	-1.21011600	-0.69638554
C	0.69346500	1.21011600	-0.69638554
H	-1.24069100	-2.14358900	-0.69638554
H	-1.24069100	2.14358900	-0.69638554
H	1.24069100	-2.14358900	-0.69638554
H	1.24069100	2.14358900	-0.69638554
C	-2.83454200	0.00000000	-0.69638554
C	-4.04230000	0.00000000	-0.69638554
H	-5.10788400	0.00000000	-0.69638554
C	2.83454200	0.00000000	-0.69638554
C	4.04230000	0.00000000	-0.69638554
H	5.10788400	0.00000000	-0.69638554
Cl	0.00000000	0.00000000	2.70361446

19

Cl⁻···C6H4(CF3)2

C	-0.69508904	-1.21182567	0.42024826
C	0.69508904	-1.21182567	0.42024826
C	1.38072824	0.00000000	0.41944801
C	0.69508904	1.21182567	0.42024826
C	-0.69508904	1.21182567	0.42024826
C	-1.38072824	0.00000000	0.41944801
H	-1.24124175	-2.14563430	0.41144976
H	1.24124175	-2.14563430	0.41144976
H	1.24124175	2.14563430	0.41144976
H	-1.24124175	2.14563430	0.41144976
C	-2.88197481	0.00000000	0.46837051
C	2.88197481	0.00000000	0.46837051
F	-3.33392977	0.00000000	1.73991503
F	-3.40436510	-1.08550806	-0.13177050
F	-3.40436510	1.08550806	-0.13177050
F	3.33392977	0.00000000	1.73991503
F	3.40436510	-1.08550806	-0.13177050
F	3.40436510	1.08550806	-0.13177050
Cl	0.00000000	0.00000000	-2.88001836

21

Cl⁻···C6H4(CH2OH)2

C	-0.64949419	-0.30408648	1.40450600
C	-0.79632085	0.88481091	0.69844650
C	-0.50190417	-1.49916492	0.69395650
C	-0.64949419	-0.30408648	-1.40450600
C	-0.50190417	-1.49916492	-0.69395650
C	-0.79632085	0.88481091	-0.69844650
H	-0.91076016	1.81145863	1.24405400
H	-0.91076016	1.81145863	-1.24405400
H	-0.38622957	-2.43581515	-1.23078000
H	-0.38622957	-2.43581515	1.23078000
C	-0.64493966	-0.34096581	2.91270950
H	-1.45851390	-0.98765608	3.25986950
H	0.30152103	-0.77029497	3.25986950
C	-0.64493966	-0.34096581	-2.91270950
H	0.30152103	-0.77029497	-3.25986950
H	-1.45851390	-0.98765608	-3.25986950
O	-0.80738191	0.97437549	3.42081100
H	-0.80354998	0.94334721	4.38325300
O	-0.80738191	0.97437549	-3.42081100
H	-0.80354998	0.94334721	-4.38325300
Cl	2.97324013	0.14122285	0.00000000

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Cl⁻···C6H4(CH3)2

C	1.41661200	0.00000000	0.82166316
C	0.69624750	-1.19608200	0.82563516
C	0.69624750	1.19608200	0.82563516
C	-1.41661200	0.00000000	0.82166316
C	-0.69624750	1.19608200	0.82563516
C	-0.69624750	-1.19608200	0.82563516
H	1.23122825	-2.14002550	0.83458991
H	-1.23122825	-2.14002550	0.83458991
H	-1.23122825	2.14002550	0.83458991
H	1.23122825	2.14002550	0.83458991
C	2.92486750	0.00000000	0.79144266
H	3.32808075	0.88415550	1.28809416

H	3.29306700	0.00000000	-0.23826984
H	3.32808075	-0.88415550	1.28809416
C	-2.92486750	0.00000000	0.79144266
H	-3.29306700	0.00000000	-0.23826984
H	-3.32808075	0.88415550	1.28809416
H	-3.32808075	-0.88415550	1.28809416
Cl	0.00000000	0.00000000	-2.77568884

17

$Cl^{-}\cdots C_6H_4(CHO)_2$

C	-0.62454674	-0.22475460	-1.38483900
C	-0.75340879	0.98586649	-0.69245200
C	-0.49624006	-1.43015817	-0.69581200
C	-0.62454674	-0.22475460	1.38483900
C	-0.49624006	-1.43015817	0.69581200
C	-0.75340879	0.98586649	0.69245200
H	-0.39733659	-2.35932721	-1.24647000
H	-0.85101195	1.90281953	-1.25985100
H	-0.39733659	-2.35932721	1.24647000
H	-0.85101195	1.90281953	1.25985100
C	-0.62331396	-0.23633618	2.86968300
O	-0.72893584	0.75595030	3.55340800
H	-0.51731973	-1.23212090	3.33428600
C	-0.62331396	-0.23633618	-2.86968300
O	-0.72893584	0.75595030	-3.55340800
H	-0.51731973	-1.23212090	-3.33428600
Cl	2.65673085	0.12627305	0.00000000

15

$Cl^{-}\cdots C_6H_4(CN)_2$

C	1.38416400	0.00000000	-0.66569953
C	0.69363700	-1.21638300	-0.66631853
C	0.69363700	1.21638300	-0.66631853
C	-1.38416400	0.00000000	-0.66569953
C	-0.69363700	1.21638300	-0.66631853
C	-0.69363700	-1.21638300	-0.66631853
C	2.82381900	0.00000000	-0.66491153
C	-2.82381900	0.00000000	-0.66491153
N	3.97947200	0.00000000	-0.66400653
N	-3.97947200	0.00000000	-0.66400653
H	1.24420500	-2.14732900	-0.66775453
H	1.24420500	2.14732900	-0.66775453
H	-1.24420500	2.14732900	-0.66775453
H	-1.24420500	-2.14732900	-0.66775453
Cl	0.00000000	0.00000000	2.58388747

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$Cl^{-}\cdots C_6H_4(COCH_3)_2$

C	0.55233081	-0.06176317	-1.39756000
C	0.54041400	-1.27100945	-0.69297850
C	0.56422799	1.14549121	-0.69612400
C	0.55233081	-0.06176317	1.39756000
C	0.56422799	1.14549121	0.69612400
C	0.54041400	-1.27100945	0.69297850
H	0.57353709	2.09012334	-1.22454200
H	0.53129947	-2.19589754	-1.25465700
H	0.57353709	2.09012334	1.22454200
H	0.53129947	-2.19589754	1.25465700
C	0.55182444	-0.11314667	2.89832500
O	0.54127930	-1.18320472	3.47391700
C	0.55182444	-0.11314667	-2.89832500
O	0.54127930	-1.18320472	-3.47391700
C	0.56462123	1.18539527	-3.67119200
H	-0.31293983	1.78833726	-3.42615200
H	1.45389438	1.77092557	-3.42615200
H	0.56232489	0.95237659	-4.73347900
C	0.56462123	1.18539527	3.67119200
H	1.45389438	1.77092557	3.42615200
H	-0.31293983	1.78833726	3.42615200
H	0.56232489	0.95237659	4.73347900
Cl	-2.79751308	-0.02941536	0.00000000

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$Cl^{-}\cdots C_6H_4(COOCH_3)_2$

C	-0.44847038	0.24647586	-1.38733600
C	-0.44847038	0.24647586	1.38733600
C	-0.27874127	1.44635277	-0.69398200
C	-0.61831252	-0.95420009	-0.69502700
C	-0.61831252	-0.95420009	0.69502700
C	-0.27874127	1.44635277	0.69398200
H	-0.74876206	-1.87639539	-1.24420100
H	-0.14925059	2.36176955	-1.25636400
H	-0.74876206	-1.87639539	1.24420100
H	-0.14925059	2.36176955	1.25636400
C	-0.44065385	0.30173376	2.87785300
C	-0.44065385	0.30173376	-2.87785300
O	-0.29683310	1.31845503	3.51854700
O	-0.29683310	1.31845503	-3.51854700
O	-0.61102655	-0.90269285	3.44332400
O	-0.61102655	-0.90269285	-3.44332400
C	-0.61105932	-0.90292455	4.87894300
C	-0.61105932	-0.90292455	-4.87894300
H	-0.75765832	-1.93928629	5.16693500
H	-0.75765832	-1.93928629	-5.16693500
H	0.33996299	-0.52515403	5.24996700
H	-1.41999021	-0.27619909	-5.24996700
H	-1.41999021	-0.27619909	5.24996700
H	0.33996299	-0.52515403	-5.24996700
Cl	2.86847053	-0.22299514	0.00000000

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Cl⁻···C6H4(COOH)2

C	-0.55237862	-0.03855806	1.38503700
C	-0.55237862	-0.03855806	-1.38503700
C	-0.53346304	-1.25169260	0.69370300
C	-0.57130000	1.17494844	0.69506500
C	-0.57130000	1.17494844	-0.69506500
C	-0.53346304	-1.25169260	-0.69370300
H	-0.58582144	2.10626823	1.24400200
H	-0.51905508	-2.17573428	1.25637300
H	-0.58582144	2.10626823	-1.24400200
H	-0.51905508	-2.17573428	-1.25637300
C	-0.55157908	-0.08983582	-2.87245100
C	-0.55157908	-0.08983582	2.87245100
O	-0.53571680	-1.10714917	-3.52476600
O	-0.53571680	-1.10714917	3.52476600
O	-0.57061610	1.13108677	-3.44420800
O	-0.57061610	1.13108677	3.44420800
H	-0.56844033	0.99154573	-4.40491300
H	-0.56844033	0.99154573	4.40491300
Cl	2.79721229	0.01379385	0.00000000

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Cl⁻···C6H4F2

C	-1.36050000	0.00000000	-0.77066667
C	-0.69646100	1.21571600	-0.77066667
C	-0.69646100	-1.21571600	-0.77066667
C	1.36050000	0.00000000	-0.77066667
C	0.69646100	-1.21571600	-0.77066667
C	0.69646100	1.21571600	-0.77066667
F	-2.71324800	0.00000000	-0.77066667
F	2.71324800	0.00000000	-0.77066667
H	-1.26320000	2.13689900	-0.77066667
H	-1.26320000	-2.13689900	-0.77066667
H	1.26320000	-2.13689900	-0.77066667
H	1.26320000	2.13689900	-0.77066667
Cl	0.00000000	0.00000000	2.62933333

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Cl⁻···C6H4(NCH3_2)2

C	0.68757935	-1.19306886	-0.69535200
C	0.68757935	-1.19306886	0.69535200
C	0.71272603	-0.00126285	1.43630800
C	0.70028910	1.19081337	0.69527700
C	0.70028910	1.19081337	-0.69527700
C	0.71272603	-0.00126285	-1.43630800
H	0.66493267	-2.15106869	-1.19494900
H	0.66493267	-2.15106869	1.19494900
H	0.68822600	2.14897264	1.19495400
H	0.68822600	2.14897264	-1.19495400
N	0.75942214	-0.00123214	-2.83766800
N	0.75942214	-0.00123214	2.83766800
C	0.35589018	1.22317045	-3.50274800
H	0.40415153	1.06867336	-4.57947600
H	1.04207492	2.03505281	-3.26002400
H	-0.66445914	1.53496773	-3.23494100
C	0.35589018	1.22317045	3.50274800
H	1.04207492	2.03505281	3.26002400
H	0.40415153	1.06867336	4.57947600
H	-0.66445914	1.53496773	3.23494100
C	0.35243617	-1.22431819	-3.50285400
H	1.03534153	-2.03847863	-3.25841400
H	0.40303287	-1.07047872	-4.57956600
H	-0.66950716	-1.53239912	-3.23669500
C	0.35243617	-1.22431819	3.50285400
H	0.40303287	-1.07047872	4.57956600
H	1.03534153	-2.03847863	3.25841400
H	-0.66950716	-1.53239912	3.23669500
Cl	-2.94979684	0.00486825	0.00000000

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Cl⁻···C6H4(NH2)2

C	1.19711000	0.69536100	0.84692267
C	1.19711000	-0.69536100	0.84692267
C	-1.19711000	-0.69536100	0.84692267
C	-1.19711000	0.69536100	0.84692267
C	0.00000000	1.41573000	0.84277667
C	0.00000000	-1.41573000	0.84277667
H	2.14210500	1.22750900	0.85802867
H	2.14210500	-1.22750900	0.85802867
H	-2.14210500	-1.22750900	0.85802867
H	-2.14210500	1.22750900	0.85802867
H	0.82907400	-3.24493100	0.51079367
H	-0.82907400	-3.24493100	0.51079367
H	0.82907400	3.24493100	0.51079367
H	-0.82907400	3.24493100	0.51079367
N	0.00000000	-2.82161700	0.90078967
N	0.00000000	2.82161700	0.90078967
Cl	0.00000000	0.00000000	-2.85445933

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Cl⁻···C6H4(NHCH3)2

C	-0.72133510	0.27765854	1.42059600
C	-0.63016292	1.47550492	0.69123800
C	-0.80872406	-0.91286853	0.69957400
C	-0.63016292	1.47550492	-0.69123800
C	-0.80872406	-0.91286853	-0.69957400
C	-0.72133510	0.27765854	-1.42059600
H	-0.57337580	2.41844444	-1.22473100
H	-0.57337580	2.41844444	1.22473100

H	-0.87709512	-1.86181313	1.21439300
H	-0.87709512	-1.86181313	-1.21439300
N	-0.76265659	0.32317590	-2.82006400
H	-0.26775787	1.11660428	-3.19677400
N	-0.76265659	0.32317590	2.82006400
H	-0.26775787	1.11660428	3.19677400
C	-0.54753530	-0.89858549	-3.56851500
H	-0.49462685	-0.65238585	-4.62786600
H	-1.39168815	-1.57584521	-3.42760100
H	0.37165421	-1.42528472	-3.27858900
C	-0.54753530	-0.89858549	3.56851500
H	-1.39168815	-1.57584521	3.42760100
H	-0.49462685	-0.65238585	4.62786600
H	0.37165421	-1.42528472	3.27858900
Cl	2.91976823	0.00797556	0.00000000

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Cl⁻···C6H4(NHOH)2

C	-0.57761835	1.47278236	0.69282800
C	-0.79023752	-0.92415799	-0.69822700
C	-0.57761835	1.47278236	-0.69282800
C	-0.68328793	0.27047563	1.40062400
C	-0.79023752	-0.92415799	0.69822700
C	-0.68328793	0.27047563	-1.40062400
H	-0.51096722	2.41203582	-1.23117100
H	-0.51096722	2.41203582	1.23117100
H	-0.85392250	-1.85679566	1.24003900
H	-0.85392250	-1.85679566	-1.24003900
N	-0.74457854	0.33789583	-2.81979900
H	-0.01416716	0.94504692	-3.17391400
N	-0.74457854	0.33789583	2.81979900
H	-0.01416716	0.94504692	3.17391400
O	-0.50469410	-0.91801698	-3.41391300
H	-1.30988298	-1.09060623	-3.91745000
O	-0.50469410	-0.91801698	3.41391300
H	-1.30988298	-1.09060623	3.91745000
Cl	2.85240062	-0.04063715	0.00000000

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Cl⁻···C6H4(NO2)2

C	1.22142200	-0.52815534	-0.69475700
C	1.22142200	-0.52815534	0.69475700
C	-1.22142200	-0.52815534	0.69475700
C	-1.22142200	-0.52815534	-0.69475700
C	0.00000000	-0.52815534	-1.35543700
C	0.00000000	-0.52815534	1.35543700
H	2.14186600	-0.52815534	-1.25956200
H	2.14186600	-0.52815534	1.25956200
H	-2.14186600	-0.52815534	1.25956200
H	-2.14186600	-0.52815534	-1.25956200
O	1.07907900	-0.52815534	3.38817400
O	-1.07907900	-0.52815534	3.38817400
O	1.07907900	-0.52815534	-3.38817400
O	-1.07907900	-0.52815534	-3.38817400
N	0.00000000	-0.52815534	2.83087100
N	0.00000000	-0.52815534	-2.83087100
Cl	0.00000000	2.67184466	0.00000000

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Cl⁻···C6H4(NO)2

C	-0.61576437	-0.22344954	-1.36715600
C	-0.49373143	-1.43503235	-0.69622000
C	-0.73873834	0.99747600	-0.69129000
C	-0.61576437	-0.22344954	1.36715600
C	-0.73873834	0.99747600	0.69129000
C	-0.49373143	-1.43503235	0.69622000
H	-0.83084382	1.91192919	-1.26179100
H	-0.40183981	-2.34736228	-1.27173200
H	-0.83084382	1.91192919	1.26179100
H	-0.40183981	-2.34736228	1.27173200
N	-0.60532810	-0.32706428	2.81119700
O	-0.71123527	0.72441659	3.38558100
N	-0.60532810	-0.32706428	-2.81119700
O	-0.71123527	0.72441659	-3.38558100
Cl	2.61756086	0.10536302	0.00000000

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Cl⁻···C6H4(OCF3)2

C	-0.18887438	0.68420857	-1.37739900
C	0.20954389	1.82695364	-0.69268700
C	-0.58683933	-0.45723625	-0.69804200
C	-0.18887438	0.68420857	1.37739900
C	-0.58683933	-0.45723625	0.69804200
C	0.20954389	1.82695364	0.69268700
H	-0.89769900	-1.34884534	-1.22072200
H	0.51392133	2.69997034	-1.25378100
H	-0.89769900	-1.34884534	1.22072200
H	0.51392133	2.69997034	1.25378100
C	-0.50209255	-0.21416516	-3.56330900
C	-0.50209255	-0.21416516	3.56330900
O	-0.14540783	0.80887952	-2.76658500
O	-0.14540783	0.80887952	2.76658500
F	-1.77898672	-0.59285061	-3.37665100
F	0.26257777	-1.30464244	-3.37665100
F	-0.36421249	0.18130303	-4.82390900
F	0.26257777	-1.30464244	3.37665100
F	-1.77898672	-0.59285061	3.37665100
F	-0.36421249	0.18130303	4.82390900
Cl	2.92731852	-0.40176656	0.00000000

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Cl⁻···C6H4(OH)2

C	-0.80467636	0.00618668	-1.39434200
C	-0.80467636	0.00618668	1.39434200
C	-0.80295180	-1.19660908	-0.69798900
C	-0.80295180	-1.19660908	0.69798900
C	-0.80640531	1.21203944	0.69364700
C	-0.80640531	1.21203944	-0.69364700
H	-0.80159923	-2.13996511	-1.23383400
H	-0.80159923	-2.13996511	1.23383400
H	-0.80773551	2.13979049	1.25088900
H	-0.80773551	2.13979049	-1.25088900
O	-0.80477199	0.07288061	-2.76374400
O	-0.80477199	0.07288061	2.76374400
H	-0.80349596	-0.81708547	-3.13548600
H	-0.80349596	-0.81708547	3.13548600
Cl	2.74531853	0.01229564	0.00000000

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Cl⁻···C6H4(OMe)2

C	-0.64939578	0.27744559	-1.39967100
C	-0.76183918	-0.91778290	-0.70150500
C	-0.76183918	-0.91778290	0.70150500
C	-0.64939578	0.27744559	1.39967100
C	-0.53619699	1.48070362	0.69048800
C	-0.53619699	1.48070362	-0.69048800
H	-0.85080558	-1.86346028	-1.21718000
H	-0.85080558	-1.86346028	1.21718000
H	-0.44939243	2.40340146	1.24958100
H	-0.44939243	2.40340146	-1.24958100
O	-0.63920999	0.38571652	2.76183400
O	-0.63920999	0.38571652	-2.76183400
C	-0.75177206	-0.81077340	3.50781800
C	-0.75177206	-0.81077340	-3.50781800
H	-1.69713328	-1.31734665	3.29528200
H	-1.69713328	-1.31734665	-3.29528200
H	0.08252467	-1.48477136	3.29528200
H	0.08252467	-1.48477136	-3.29528200
H	-0.72404537	-0.51604975	4.55323800
H	-0.72404537	-0.51604975	-4.55323800
Cl	2.93503012	-0.05706624	0.00000000

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Cl⁻···C6H4(SCH3)2

C	-0.51035863	0.31931364	-1.40979300
C	-0.66877266	-0.86706579	-0.69886500
C	-0.66877266	-0.86706579	0.69886500
C	-0.51035863	0.31931364	1.40979300
C	-0.35083720	1.51398646	0.69166200
C	-0.35083720	1.51398646	-0.69166200
H	-0.79484593	-1.81124187	-1.21124200
H	-0.79484593	-1.81124187	1.21124200
H	-0.22600486	2.44886902	1.22611100
H	-0.22600486	2.44886902	-1.22611100
S	-0.49329467	0.44710742	3.17629700
S	-0.49329467	0.44710742	-3.17629700
C	-0.72265076	-1.27056458	3.69385800
C	-0.72265076	-1.27056458	-3.69385800
H	-1.67825497	-1.66536202	3.34963000
H	-1.67825497	-1.66536202	-3.34963000
H	0.09588882	-1.90225864	3.34963000
H	0.09588882	-1.90225864	-3.34963000
H	-0.72046125	-1.25416712	4.78284800
H	-0.72046125	-1.25416712	-4.78284800
Cl	2.90965981	-0.13453841	0.00000000

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Cl⁻···C6H4(SH)2

C	-0.64447854	-0.00604433	-1.40427000
C	-0.64447854	-0.00604433	1.40427000
C	-0.63570443	-1.20735829	-0.69576800
C	-0.63570443	-1.20735829	0.69576800
C	-0.65326681	1.19720958	0.69425900
C	-0.65326681	1.19720958	-0.69425900
H	-0.62878572	-2.15463902	-1.22180300
H	-0.62878572	-2.15463902	1.22180300
H	-0.66015667	2.14054042	1.22721600
H	-0.66015667	2.14054042	-1.22721600
S	-0.64506737	0.07457652	-3.17698300
S	-0.64506737	0.07457652	3.17698300
H	-0.63539104	-1.25026714	-3.38421000
H	-0.63539104	-1.25026714	3.38421000
Cl	2.80542472	0.01979995	0.00000000

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Cl⁻···C6H4(SiF3)2

C	0.39530906	-0.00013622	1.40247020
C	0.38774826	-1.20901951	0.69554840
C	0.38831685	1.20879266	0.69553320
C	0.39530906	-0.00013622	-1.40247020
C	0.38831685	1.20879266	-0.69553320
C	0.38774826	-1.20901951	-0.69554840
Si	0.41151006	0.00005093	3.23989000
F	1.88500065	0.00877281	3.85136460
F	-0.31272290	-1.30292406	3.80698190
F	-0.32792126	1.29432102	3.80733720
H	0.37169140	2.15281400	1.22754860
H	0.37082071	-2.15296407	1.22760460

Si	0.41151006	0.00005093	-3.23989000
F	1.88500065	0.00877281	-3.85136460
F	-0.32792126	1.29432102	-3.80733720
F	-0.31272290	-1.30292406	-3.80698190
H	0.37169140	2.15281400	-1.22754860
H	0.37082071	-2.15296407	-1.22760460
Cl	-2.90954194	0.00001030	0.00000000

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Cl^{-}···C6H4(SiH3)2

C	1.41691950	0.00000000	-0.65362403
C	0.69639075	-1.20091275	-0.65821103
C	0.69639075	1.20091275	-0.65821103
C	-1.41691950	0.00000000	-0.65362403
C	-0.69639075	1.20091275	-0.65821103
C	-0.69639075	-1.20091275	-0.65821103
H	1.22330000	-2.14946725	-0.66990128
H	-1.22330000	-2.14946725	-0.66990128
H	-1.22330000	2.14946725	-0.66990128
H	1.22330000	2.14946725	-0.66990128
Si	3.29416350	0.00000000	-0.62399703
Si	-3.29416350	0.00000000	-0.62399703
H	3.81061200	0.00000000	0.77281197
H	3.80275550	-1.21872075	-1.30998853
H	3.80275550	1.21872075	-1.30998853
H	-3.81061200	0.00000000	0.77281197
H	-3.80275550	-1.21872075	-1.30998853
H	-3.80275550	1.21872075	-1.30998853
Cl	0.00000000	0.00000000	2.79331797

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Cl⁻···C6H3(BF2)3

C	-0.00455139	1.38948822	-0.44199916
C	-1.22311812	0.70085205	-0.44199949
C	-1.20105640	-0.69868573	-0.44199916
C	0.00460338	-1.40967739	-0.44199949
C	1.20560780	-0.69080249	-0.44199916
C	1.21851474	0.70882534	-0.44199949
H	-0.00808890	2.47404401	-0.44199982
H	2.14662941	-1.23001681	-0.44199982
B	2.55825626	1.48817243	-0.44200049
H	-2.13854051	-1.24402719	-0.44199982
B	-2.56792326	1.47142870	-0.44200049
B	0.00966700	-2.95960113	-0.44200049
F	2.58371346	2.81759081	-0.44200149
F	3.72646778	0.85312610	-0.44199949
F	1.14824849	-3.64635690	-0.44200149
F	-1.12440502	-3.65377882	-0.44199949
F	-3.73196195	0.82876608	-0.44200149
F	-2.60206277	2.80065272	-0.44199949
Cl	0.00000000	0.00000000	2.80800051

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Cl⁻···C6H3(CCH)3

C	0.98825128	0.98825128	0.59052632
C	1.35097037	-0.36199142	0.59052632
C	0.36172507	-1.34997635	0.59052632
C	-0.98897895	-0.98897895	0.59052632
C	-1.34997635	0.36172507	0.59052632
C	-0.36199142	1.35097037	0.59052632
H	1.75283043	1.75283043	0.59052632
H	-2.39441090	0.64158047	0.59052632
H	0.64158047	-2.39441090	0.59052632
C	-0.73348541	2.73740481	0.59052632
C	-1.04588781	3.90330646	0.59052632
H	-1.32171395	4.93270363	0.59052632
C	2.73740481	-0.73348541	0.59052632
C	3.90330646	-1.04588781	0.59052632
H	4.93270363	-1.32171395	0.59052632
C	-2.00391940	-2.00391940	0.59052632
C	-2.85741864	-2.85741864	0.59052632
H	-3.61098967	-3.61098967	0.59052632
Cl	0.00000000	0.00000000	-2.70947368

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Cl⁻···C6H3(CF3)3

C	-1.12487391	0.82894635	-0.31478587
C	-1.26807203	-0.55433956	-0.31484487
C	-0.15545164	-1.38864256	-0.31478587
C	1.11410816	-0.82101281	-0.31484487
C	1.28032555	0.55969621	-0.31478587
C	0.15396387	1.37535237	-0.31484487
H	-1.99573694	1.47070624	-0.30043721
H	2.27153743	0.99300577	-0.30043721
H	-0.27580049	-2.46371201	-0.30043721
C	0.32115352	2.86885011	-0.35530221
C	2.32392031	-1.71255216	-0.35530221
C	-2.64507383	-1.15629794	-0.35530221
F	0.37184825	3.32170236	-1.62366454
F	1.45745856	3.25802385	0.24853546
F	-0.70097028	3.49964924	0.24853513
F	3.38127029	-1.14276655	0.24853513
F	2.69075450	-1.98288121	-1.62366454
F	2.09280215	-2.89120806	0.24853546
F	-3.06260275	-1.33882115	-1.62366454
F	-2.68030001	-2.35688269	0.24853513
F	-3.55026070	-0.36681579	0.24853546
Cl	0.00000000	0.00000000	2.88518479

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Cl⁻···C6H3(CH2OH)3

C	-0.78591301	-1.14931863	-0.56401869
C	0.61049624	-1.25416155	-0.56401869
C	1.38829563	-0.10596132	-0.56401869
C	0.78088764	1.15578603	-0.56401869
C	-0.60238262	1.25527995	-0.56401869
C	-1.39138388	0.09837552	-0.56401869
H	-1.40580653	-2.03771969	-0.56401869
H	-1.06181375	2.23632401	-0.56401869
H	2.46762028	-0.19860432	-0.56401869
C	-2.89201822	0.24848572	-0.56401869
C	1.66120405	2.38031839	-0.56401869
C	1.23081417	-2.62880410	-0.56401869
H	-3.19527692	0.81525084	0.32262331
H	-3.19527692	0.81525084	-1.45066069
H	0.89161052	-3.17481641	-1.45066069
H	0.89161052	-3.17481641	0.32262331
H	2.30366640	2.35956556	-1.45066069
H	2.30366640	2.35956556	0.32262331
O	0.85524251	3.55066440	-0.56401869
H	1.42766852	4.32542995	-0.56401869
O	-3.50258683	-1.03467046	-0.56401869
H	-4.45976648	-0.92631777	-0.56401869
O	2.64734431	-2.51599394	-0.56401869
H	3.03209796	-3.39911218	-0.56401869
Cl	0.00000000	0.00000000	2.98598131

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Cl⁻···C6H3(CH3)3

C	-1.27139255	0.74641163	-0.54271155
C	-0.15917229	0.75685774	-1.38571326
C	1.11431947	0.75078034	-0.81476951
C	1.28832068	0.72515641	0.56973875
C	0.15710306	0.71512684	1.38707577
C	-1.12911865	0.72072987	0.84541421
H	-2.26722786	0.76506083	-0.97533250
H	0.28014797	0.70927187	2.46597372
H	1.98711074	0.77285169	-1.46048210
C	-2.34173927	0.68312039	1.74242844
C	2.67189305	0.69230097	1.17069136
C	-0.33012578	0.75804747	-2.88480283
H	-3.19031677	1.18779666	1.27810202
H	-2.63963795	-0.34896600	1.94621143
H	-2.13782014	1.16474641	2.69994298
H	-1.25444040	1.25990323	-3.17491426
H	-0.37213729	-0.26450802	-3.26962650
H	0.50332009	1.26312123	-3.37536260
H	3.39231215	1.19985067	0.52744260
H	3.01175262	-0.33861693	1.30174658
H	2.68704828	1.17358142	2.14973189
Cl	-0.00003751	-2.81384018	-0.03750244

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Cl⁻···C6H3(CHO)3

C	-0.91277244	-1.05491449	-0.54702970
C	-1.36813397	0.26992310	-0.54702970
C	-0.45719653	1.31794137	-0.54702970
C	0.91782725	1.04987723	-0.54702970
C	1.36996897	-0.26302688	-0.54702970
C	0.45030673	-1.31980033	-0.54702970
H	-1.64185477	-1.85802643	-0.54702970
H	2.43002548	-0.49287473	-0.54702970
H	-0.78817070	2.35090116	-0.54702970
C	0.93386732	-2.72364251	-0.54702970
O	2.10526881	-3.02527224	-0.54702970
H	0.14752784	-3.49690948	-0.54702970
C	-2.82567727	0.55306844	-0.54702970
O	-3.67259702	-0.31058015	-0.54702970
H	-3.10217636	1.62069188	-0.54702970
C	1.89180995	2.17057408	-0.54702970
O	1.56732821	3.33585239	-0.54702970
H	2.95464852	1.87621760	-0.54702970
Cl	0.00000000	0.00000000	2.70297030

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Cl⁻···C6H3(CN)3

C	0.99055066	0.99055066	-0.56368421
C	1.34296369	-0.35984604	-0.56368421
C	0.36256671	-1.35311737	-0.56368421
C	-0.98311765	-0.98311765	-0.56368421
C	-1.35311737	0.36256671	-0.56368421
C	-0.35984604	1.34296369	-0.56368421
H	1.75533610	1.75533610	-0.56368421
H	-2.39783371	0.64249761	-0.56368421
H	0.64249761	-2.39783371	-0.56368421
C	-0.73230673	2.73300591	-0.56368421
N	-1.03127213	3.84876000	-0.56368421
C	2.73300591	-0.73230673	-0.56368421
N	3.84876000	-1.03127213	-0.56368421
C	-2.00069919	-2.00069919	-0.56368421
N	-2.81748786	-2.81748786	-0.56368421
Cl	0.00000000	0.00000000	2.58631579

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Cl⁻···C6H3(COCH3)3

C	-1.05602769	-0.90704276	-0.44200000
C	-1.31751278	0.46856028	-0.44200000
C	-0.25750823	1.36806818	-0.44200000
C	1.06454150	0.90671940	-0.44200000
C	1.31353591	-0.46102542	-0.44200000
C	0.25297129	-1.37527968	-0.44200000
H	-1.90403607	-1.57945119	-0.44200000
H	2.31986289	-0.85921801	-0.44200000
H	-0.41582683	2.43866920	-0.44200000
C	0.58407766	-2.83953973	-0.44200000
O	1.74532989	-3.19938929	-0.44200000
C	-2.75115237	0.91394378	-0.44200000
O	-3.64341735	0.08819462	-0.44200000
C	2.16707472	1.92559596	-0.44200000
O	1.89808746	3.11119467	-0.44200000
C	-0.54747061	-3.83775645	-0.44200000
H	-1.17783632	-3.70495386	0.44018800
H	-1.17783632	-3.70495386	-1.32418800
H	-0.12356934	-4.83902828	-0.44200000
C	-3.04985927	2.39300168	-0.44200000
H	-2.61966600	2.87251311	0.44018800
H	-2.61966600	2.87251311	-1.32418800
H	-4.12893675	2.52652833	-0.44200000
C	3.59732988	1.44475477	-0.44200000
H	3.79750232	0.83244075	0.44018800
H	3.79750232	0.83244075	-1.32418800
H	4.25250609	2.31249995	-0.44200000
Cl	0.00000000	0.00000000	2.80800000

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Cl⁻···C6H3(COOCH3)3

C	0.03092063	1.39600476	-0.37651007
C	1.22072569	0.66779279	-0.37651007
C	1.19351527	-0.72478043	-0.37651007
C	-0.03203732	-1.39107585	-0.37651007
C	-1.22443590	-0.67122433	-0.37651007
C	-1.18868836	0.72328306	-0.37651007
H	0.07107659	2.47638042	-0.37651007
H	-2.18014665	-1.17663607	-0.37651007
H	2.10907006	-1.29974435	-0.37651007
C	-2.49167447	1.44849486	-0.37651007
O	-3.57045771	0.89974109	-0.37651007
O	-2.34134175	2.77935421	-0.37651007
C	-0.00859611	-2.88210082	-0.37651007
O	1.00603022	-3.54197763	-0.37651007
O	-1.23632048	-3.41733854	-0.37651007
C	2.50027058	1.43360596	-0.37651007
O	2.56442750	2.64223654	-0.37651007
O	3.57766223	0.63798433	-0.37651007
C	-3.56539794	3.53061522	-0.37651007
H	-4.14598445	3.29201619	0.51224393
H	-3.26236499	4.57247386	-0.37651007
H	-4.14598445	3.29201619	-1.26526407
C	4.84030144	1.32241758	-0.37651007
H	4.92396187	1.94451977	0.51224393
H	5.59106102	0.53905403	-0.37651007
H	4.92396187	1.94451977	-1.26526407
C	-1.27490350	-4.85303280	-0.37651007
H	-2.32869603	-5.11152789	-0.37651007
H	-0.77797742	-5.23653595	-1.26526407
H	-0.77797742	-5.23653595	0.51224393
Cl	0.00000000	0.00000000	2.92348993

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Cl⁻···C6H3(COOH)3

C	-0.35849977	1.35026193	-0.44200000
C	0.98655884	0.97992809	-0.44200000
C	1.34861101	-0.36466105	-0.44200000
C	0.35536320	-1.34434906	-0.44200000
C	-0.99011124	-0.98560087	-0.44200000
C	-1.34192204	0.36442097	-0.44200000
H	-0.62070140	2.39942099	-0.44200000
H	-1.76760883	-1.73725368	-0.44200000
H	2.38831024	-0.66216731	-0.44200000
C	-2.79118900	0.70222669	-0.44200000
O	-3.68202890	-0.11384182	-0.44200000
O	-3.01953428	2.02908110	-0.44200000
H	-3.98256677	2.15347373	-0.44200000
C	0.78744834	-2.76835393	-0.44200000
O	1.93960436	-3.13180966	-0.44200000
O	-0.24746864	-3.62953394	-0.44200000
H	0.12632043	-4.52574086	-0.44200000
C	2.00374066	2.06612724	-0.44200000
O	1.74242455	3.24565148	-0.44200000
O	3.26700292	1.60045284	-0.44200000
H	3.85624634	2.37226713	-0.44200000
Cl	0.00000000	0.00000000	2.80800000

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Cl⁻···C6H3F3

C	-0.99700358	-0.99700358	0.68614458
C	0.35205860	-1.31390057	0.68614458
C	1.36193221	-0.36492864	0.68614458
C	0.96184198	0.96184198	0.68614458
C	-0.36492864	1.36193221	0.68614458
C	-1.31390057	0.35205860	0.68614458
H	-1.76071067	-1.76071067	0.68614458
H	-0.64446483	2.40517551	0.68614458
H	2.40517551	-0.64446483	0.68614458
F	-2.61376852	0.70035716	0.68614458
F	0.70035716	-2.61376852	0.68614458
F	1.91341136	1.91341136	0.68614458
Cl	0.00000000	0.00000000	-2.66385542

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Cl⁻···C6H3(NCH3_2)3

C	-1.28620898	-0.54734727	0.60693055
C	-0.16116635	-1.38705432	0.62499534
C	1.12556325	-0.82560078	0.60917480
C	1.29035337	0.56867363	0.60914425
C	0.16065945	1.40211359	0.59113047
C	-1.12917195	0.84782127	0.60689282
H	-2.27247292	-0.97462788	0.59534509
H	0.28384928	2.46967295	0.56742927
H	1.98863782	-1.46624470	0.59931064
N	-2.24765898	1.67809312	0.62448943
N	-0.32081166	-2.77050107	0.66052282
N	2.56848579	1.12243930	0.62897148
C	-3.53625533	1.09734915	0.30351907
H	-4.29114896	1.88061288	0.33402131
H	-3.81505858	0.34599769	1.04377933
H	-3.55266285	0.63049880	-0.69087413
C	0.82415467	-3.60000664	0.34155821
H	0.52351130	-4.64492584	0.38686990
H	1.61942208	-3.45685371	1.07456717
H	1.22966593	-3.39291662	-0.65829743
C	2.71211219	2.52477306	0.29192985
H	3.76764858	2.78732511	0.32664289
H	2.19565602	3.15081567	1.02103131

H	2.32299507	2.76027412	-0.70815326
C	-2.06756029	3.07621842	0.28748101
H	-1.63320368	3.21671197	-0.71183484
H	-1.42345373	3.56836281	1.01766291
H	-3.03564115	3.57224050	0.32031167
C	-1.62400040	-3.31755497	0.33927995
H	-1.96986389	-3.02377634	-0.66127534
H	-2.36712218	-2.99691453	1.07085719
H	-1.56928348	-4.40347350	0.38492200
C	3.69157182	0.26345304	0.31024617
H	3.60306572	-0.19507932	-0.68421464
H	3.79059583	-0.53148955	1.05085771
H	4.60493594	0.85424423	0.34230045
Cl	-0.00002864	-0.05751196	-3.09134355

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Cl⁻···C6H3(NH2)3

C	0.04070620	0.77634244	-1.39796769
C	-1.18747029	0.77648928	-0.73149017
C	-1.23192485	0.77264552	0.66517889
C	-0.04065167	0.77280496	1.39557461
C	1.19113112	0.77264586	0.73573488
C	1.22803521	0.77649158	-0.66113107
H	0.07224961	0.80352077	-2.48167619
H	2.11391694	0.79696117	1.30497475
H	-2.18625803	0.79695877	1.17978141
N	2.45593084	0.83311228	-1.32325606
H	2.44606858	0.48027128	-2.26748772
H	3.23902680	0.47761596	-0.79740591
N	-2.37492591	0.83310829	-1.46367164
H	-3.18715667	0.47771866	-0.98393477
H	-2.31050492	0.48015829	-2.40569703
N	-0.08110029	0.82573902	2.79017328
H	0.74104683	0.47046516	3.25279670
H	-0.92856311	0.47035486	3.20447572
Cl	0.00011101	-2.97542705	-0.00376133

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Cl⁻···C6H3(NHCH3)3

C	-1.28865838	-0.54315659	0.66990728
C	-0.15387604	-1.37967511	0.68468706
C	1.12362629	-0.82902206	0.67296383
C	1.28077741	0.57202367	0.66361650
C	0.16506438	1.40288934	0.64889656
C	-1.12686825	0.83854897	0.66076932
H	-2.27299715	-0.99186010	0.69170708
H	0.26846423	2.47992770	0.65422595
H	2.00456569	-1.45680897	0.69667437
N	-2.21905909	1.69676191	0.68865429
H	-2.01996419	2.61707482	0.33268143
N	-0.35071096	-2.75399047	0.73664620
H	-1.25055849	-3.04733183	0.39377864
N	2.56980388	1.08932742	0.69515240
H	3.27054411	0.45115717	0.35598740
C	-3.54824880	1.20583165	0.39556623
H	-4.23113744	2.05353217	0.35901276
H	-3.88828685	0.53984798	1.19108455
H	-3.60065524	0.66425333	-0.55797259
C	0.73627422	-3.66439506	0.44805647
H	0.34328842	-4.68005455	0.43160072
H	1.49046283	-3.61312165	1.23582531
H	1.22254653	-3.45450257	-0.51359414
C	2.81199838	2.48100695	0.38173734
H	3.88787106	2.64807714	0.35250727
H	2.39787356	3.12122602	1.16316709
H	2.37809964	2.78164737	-0.58088109
Cl	-0.00005228	-0.04953333	-3.08271638

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Cl⁻···C6H3(NHOH)3

C	-0.64062109	1.24888811	-0.62045507
C	-1.38318406	0.05890300	-0.61999307
C	-0.76125828	-1.17923819	-0.62045507
C	0.64058054	-1.22732403	-0.61999307
C	1.40187937	-0.06964992	-0.62045507
C	0.74260352	1.16842104	-0.61999307
H	-1.13182797	2.21154630	-0.61530674
H	2.48116926	-0.12558138	-0.61530674
H	-1.34934130	-2.08596492	-0.61530674
N	1.55479606	2.32407589	-0.68196140
H	2.34421824	2.24239605	-0.05197474
N	-2.79010679	0.18445494	-0.68196140
H	-3.11408106	0.90895452	-0.05197474
N	1.23531073	-2.50853083	-0.68196140
H	0.76986283	-3.15135057	-0.05197474
O	0.86677786	3.48924181	-0.29513474
H	0.91959406	4.05727686	-1.07394873
O	-3.45516098	-0.99396926	-0.29513474
H	-3.97350186	-1.23224661	-1.07394873
O	2.58838311	-2.49527255	-0.29513474
H	3.05390780	-2.82503025	-1.07394873
Cl	0.00000000	0.00000000	2.87977532

19

Cl⁻···C6H3(NO2)3

C	0.99514679	0.99514679	-0.42160000
C	-0.35319659	1.31814764	-0.42160000
C	-1.35939579	0.36424901	-0.42160000
C	-0.96495104	-0.96495104	-0.42160000
C	0.36424901	-1.35939579	-0.42160000
C	1.31814764	-0.35319659	-0.42160000
H	1.75904856	1.75904856	-0.42160000
H	0.64385646	-2.40290503	-0.42160000
H	-2.40290503	0.64385646	-0.42160000
N	-2.00806461	-2.00806461	-0.42160000
O	-3.16176896	-1.63369498	-0.42160000
O	-1.63369498	-3.16176896	-0.42160000
N	-0.73500266	2.74306726	-0.42160000
O	-1.92132475	2.99570584	-0.42160000
O	0.16606312	3.55501973	-0.42160000
N	2.74306726	-0.73500266	-0.42160000
O	3.55501973	0.16606312	-0.42160000
O	2.99570584	-1.92132475	-0.42160000
Cl	0.00000000	0.00000000	2.67840000

16

Cl⁻···C6H3(NO)3

C	0.17638629	1.39204420	-0.52178218
C	-1.10616063	0.82928577	-0.52178218
C	-1.29373879	-0.54326710	-0.52178218
C	-0.16510223	-1.37260609	-0.52178218
C	1.11735250	-0.84877711	-0.52178218
C	1.27126286	0.54332032	-0.52178218
H	0.31224288	2.46619660	-0.52178218
H	1.97966746	-1.50350856	-0.52178218
H	-2.29191034	-0.96268803	-0.52178218
N	-0.24743044	-2.81955904	-0.52178218
O	-1.36988614	-3.24699319	-0.52178218
N	2.56552498	1.19549848	-0.52178218
O	3.49692166	0.43714039	-0.52178218
N	-2.31809454	1.62406057	-0.52178218
O	-2.12703552	2.80985279	-0.52178218
Cl	0.00000000	0.00000000	2.57821782

25

Cl⁻···C6H3(OCF3)3

C	0.32874705	-1.36742944	-0.30391061
C	1.31493371	-0.38321655	-0.30391061
C	1.01985511	0.96841801	-0.30391061
C	-0.32559159	1.33037427	-0.30391061
C	-1.34860215	0.39901142	-0.30391061
C	-0.98934212	-0.94715772	-0.30391061
H	0.62461173	-2.40462178	-0.30391061
H	-2.39476941	0.66138126	-0.30391061
H	1.77015768	1.74324052	-0.30391061
O	-0.52120985	2.70404522	-0.30391061
O	2.60237678	-0.90064164	-0.30391061
O	-2.08116693	-1.80340358	-0.30391061
C	-1.76483715	3.23145337	-0.30391061
C	3.68093928	-0.08733288	-0.30391061
C	-1.91610214	-3.14412049	-0.30391061
F	3.72052330	0.70765185	-1.38496061
F	3.72052330	0.70765185	0.77713939
F	4.76360570	-0.85337877	-0.30391061
F	-1.24741717	-3.57589362	-1.38496061
F	-1.24741717	-3.57589362	0.77713939
F	-3.12085055	-3.69871417	-0.30391061
F	-1.64275516	4.55209294	-0.30391061
F	-2.47310613	2.86824177	0.77713939
F	-2.47310613	2.86824177	-1.38496061
Cl	0.00000000	0.00000000	2.89608939

16

Cl⁻···C6H3(OH)3

C	-0.82391826	1.13603651	-0.72710843
C	-1.37325608	-0.14571912	-0.72710843
C	-0.57187735	-1.28155240	-0.72710843
C	0.81282450	-1.11641510	-0.72710843
C	1.39579561	0.14551589	-0.72710843
C	0.56043159	1.26213421	-0.72710843
H	-1.48054653	1.99687609	-0.72710843
H	2.46961868	0.28375286	-0.72710843
H	-0.98907215	-2.28062895	-0.72710843
O	1.56298293	-2.25486601	-0.72710843
H	2.50083257	-2.02740434	-0.72710843
O	-2.73426272	-0.22614992	-0.72710843
H	-3.00619995	-1.15208236	-0.72710843
O	1.17127979	2.48101593	-0.72710843
H	0.50536738	3.17948670	-0.72710843
Cl	0.00000000	0.00000000	2.82289157

25

Cl⁻···C6H3(OMe)3

C	1.10308441	0.87111665	-0.55607477
C	-0.21085390	1.36819525	-0.55607477
C	-1.30595135	0.51974080	-0.55607477
C	-1.07946490	-0.86670246	-0.55607477
C	0.20286694	-1.39085744	-0.55607477
C	1.29031880	-0.50149279	-0.55607477
H	1.91558842	1.58148500	-0.55607477
H	0.41181197	-2.44969073	-0.55607477
H	-2.32740039	0.86820573	-0.55607477
O	-2.20754980	-1.62774254	-0.55607477
O	-0.30589149	2.72566548	-0.55607477
O	2.51344129	-1.09792294	-0.55607477
C	-2.04946588	-3.03614441	-0.55607477
H	-1.51586860	-3.36807778	-1.44991177
H	-1.51586860	-3.36807778	0.33776223
H	-3.05506571	-3.44788554	-0.55607477
C	-1.60464525	3.29296172	-0.55607477
H	-2.15890662	2.99681961	-1.44991177
H	-2.15890662	2.99681961	0.33776223
H	-1.45842361	4.36970729	-0.55607477
C	3.65411113	-0.25681731	-0.55607477
H	3.67477522	0.37125817	-1.44991177
H	3.67477522	0.37125817	0.33776223
H	4.51348933	-0.92182175	-0.55607477
Cl	0.00000000	0.00000000	2.94392523

25

Cl⁻···C6H3(SCH3)3

C	-0.64758857	1.24010962	-0.44122137
C	-1.39308933	0.04895243	-0.44122137
C	-0.75017215	-1.18088297	-0.44122137
C	0.65415062	-1.23092697	-0.44122137

C	1.39776072	-0.05922665	-0.44122137
C	0.73893871	1.18197454	-0.44122137
H	-1.17340927	2.18488911	-0.44122137
H	2.47887411	-0.07624232	-0.44122137
H	-1.30546484	-2.10864679	-0.44122137
C	3.13635473	-2.52037836	-0.44122137
H	3.43796365	-1.97642873	-1.33571137
H	3.43796365	-1.97642873	0.45326863
H	3.62101558	-3.49545571	-0.44122137
C	-3.75088906	-1.45597369	-0.44122137
H	-3.43061931	-1.98914949	-1.33571137
H	-3.43061931	-1.98914949	0.45326863
H	-4.83766124	-1.38816363	-0.44122137
C	0.61453433	3.97635205	-0.44122137
H	-0.00734433	3.96557822	-1.33571137
H	-0.00734433	3.96557822	0.45326863
H	1.21664565	4.88361934	-0.44122137
S	1.35934423	-2.85558440	-0.44122137
S	-3.15268074	0.25056556	-0.44122137
S	1.79333652	2.60501883	-0.44122137
Cl	0.00000000	0.00000000	2.95877863

16
Cl⁻···C6H3(SH)3

C	0.98773758	-0.98974713	-0.53224299
C	1.34338932	0.36075556	-0.53224299
C	0.36327737	1.35027940	-0.53224299
C	-0.98411814	0.98303150	-0.53224299
C	-1.35101494	-0.36053227	-0.53224299
C	-0.35927119	-1.34378706	-0.53224299
H	1.75947439	-1.75029892	-0.53224299
H	-2.39554053	-0.64860006	-0.53224299
H	0.63606614	2.39889898	-0.53224299
S	-2.17718576	2.29429544	-0.53224299
S	3.07551101	0.73835045	-0.53224299
S	-0.89832526	-3.03264590	-0.53224299
H	-3.26257309	1.50653973	-0.53224299
H	0.32658487	-3.57874104	-0.53224299
H	2.93598822	2.07220132	-0.53224299
Cl	0.00000000	0.00000000	2.81775701

22
Cl⁻···C6H3(SiF3)3

C	1.28132352	-0.54081176	0.29950265
C	0.17322731	-1.39544912	0.30377452
C	-1.11009084	-0.83743910	0.29971295
C	-1.29618343	0.54952168	0.30225721
C	-0.17127065	1.38189946	0.29800238
C	1.12291642	0.84958323	0.30204430
H	2.28046858	-0.96348549	0.27698989
H	-0.30481208	2.45849449	0.27431915
H	-1.97569445	-1.49141385	0.27736360
Si	-2.98998891	1.26603466	0.30546128
Si	2.59033597	1.95820982	0.30497141
Si	0.39961464	-3.22057990	0.30896241
F	3.08106419	2.33009854	1.77479859
F	2.24588446	3.32782408	-0.43246437
F	3.81424994	1.25187308	-0.43084426
F	1.75846427	-3.60793340	-0.42709763
F	0.47531175	-3.82981044	1.77954630
F	-0.82354518	-3.92820180	-0.42687151
F	-4.00436917	0.28206343	-0.43015682
F	-3.55645078	1.50679121	1.77538202
F	-2.99072521	2.67828282	-0.43200406
Cl	0.00012245	-0.01162431	-2.89909189

22
Cl⁻···C6H3(SiH3)3

C	1.27244234	0.55662190	-0.55851350
C	0.16200669	1.40884697	-0.54867872
C	-1.11339897	0.83202509	-0.55700324
C	-1.29626555	-0.55578042	-0.55979895
C	-0.15898746	-1.37184248	-0.56942893
C	1.13431532	-0.83634753	-0.56133708
H	2.26945616	0.98846626	-0.57185733
H	-0.28357683	-2.45105638	-0.59132496
H	-1.98582192	1.47966189	-0.56916410
H	3.77736438	-1.27687750	-1.21110621
H	3.05178638	-2.26769382	0.86549019
H	2.32476355	-3.23386606	-1.22218275
H	1.64631040	3.64401954	-1.18336216
H	0.43581518	3.77294384	0.89954699
H	-0.77481863	3.92349595	-1.18182977
H	-3.97098194	-0.38247044	-1.20620156
H	-3.48762672	-1.51283511	0.86963002
H	-3.00245413	-2.61893450	-1.21881047
Si	-3.01912972	-1.30206936	-0.52748978
Si	2.64188310	-1.95553204	-0.53107266
Si	0.37730012	3.27370185	-0.50158994
Cl	-0.00009642	-0.02890595	2.84069812

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Cl^-···C6H2(CCH)4

C	-0.70609071	-1.21629871	-0.51635514
C	-1.39027996	0.00000000	-0.51635514
C	-0.70609071	1.21629871	-0.51635514
C	0.70609071	1.21629871	-0.51635514
C	1.39027996	0.00000000	-0.51635514
C	0.70609071	-1.21629871	-0.51635514
H	-2.47163542	0.00000000	-0.51635514
H	2.47163542	0.00000000	-0.51635514
C	1.44175986	-2.44371057	-0.51635514
C	2.07690346	-3.46994141	-0.51635514
H	2.62896654	-4.38152017	-0.51635514
C	-1.44175986	-2.44371057	-0.51635514
C	-2.07690346	-3.46994141	-0.51635514
H	-2.62896654	-4.38152017	-0.51635514
C	1.44175986	2.44371057	-0.51635514
C	2.07690346	3.46994141	-0.51635514
H	2.62896654	4.38152017	-0.51635514
C	-1.44175986	2.44371057	-0.51635514
C	-2.07690346	3.46994141	-0.51635514
H	-2.62896654	4.38152017	-0.51635514
Cl	0.00000000	0.00000000	2.73364486

25

Cl^-···C6H2(CH3)4

C	1.40984785	-0.00000478	-0.66318689
C	0.68192085	-1.18994578	-0.66332089
C	-0.71275015	-1.21640678	-0.66304989
C	-1.40984415	-0.00000478	-0.66318689
C	-0.68193715	1.18993622	-0.66305289
C	0.71274385	1.21641622	-0.66332389
H	1.22200785	-2.13236378	-0.66352989
H	-1.22201215	2.13236122	-0.66284489
C	1.45403685	2.52919422	-0.66332789
H	0.75663285	3.36779022	-0.66399389
H	2.09598385	2.62436422	0.21701411
H	2.09696285	2.62380222	-1.54301689
C	2.91727085	-0.02409378	-0.66332789
H	3.32383285	0.48161222	-1.54373989
H	3.32401485	0.48284322	0.21629111
H	3.28823685	-1.04976378	-0.66263889
C	-2.91726615	0.02410822	-0.66304489
H	-3.32384515	-0.48157378	0.21736811
H	-3.28822115	1.04978122	-0.66374589
H	-3.32402915	-0.48282578	-1.54265289
C	-1.45402115	-2.52919778	-0.66304589
H	-2.09695215	-2.62382478	0.21663311
H	-2.09595815	-2.62439378	-1.54338789
H	-0.75660915	-3.36778578	-0.66237089
Cl	-0.00000315	-0.00000178	2.88681311

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Cl^-···C6H2(CN)4

C	-0.70307290	-1.20599043	-0.48457944
C	-1.40074847	0.00000000	-0.48457944
C	-0.70307290	1.20599043	-0.48457944
C	0.70307290	1.20599043	-0.48457944
C	1.40074847	0.00000000	-0.48457944
C	0.70307290	-1.20599043	-0.48457944
H	-2.48191068	0.00000000	-0.48457944
H	2.48191068	0.00000000	-0.48457944
C	1.43287331	-2.44377297	-0.48457944
N	2.03575562	-3.42872310	-0.48457944
C	-1.43287331	-2.44377297	-0.48457944
N	-2.03575562	-3.42872310	-0.48457944
C	-1.43287331	2.44377297	-0.48457944
N	-2.03575562	3.42872310	-0.48457944
C	1.43287331	2.44377297	-0.48457944
N	2.03575562	3.42872310	-0.48457944
Cl	0.00000000	0.00000000	2.56542056

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Cl^-···C6H2F4

C	1.18973430	0.69385715	-0.60714286
C	0.00000000	1.40279465	-0.60714286
C	-1.18973430	0.69385715	-0.60714286
C	-1.18973430	-0.69385715	-0.60714286
C	0.00000000	-1.40279465	-0.60714286
C	1.18973430	-0.69385715	-0.60714286
H	0.00000000	2.48393286	-0.60714286
H	0.00000000	-2.48393286	-0.60714286
F	2.35996263	-1.34715714	-0.60714286
F	2.35996263	1.34715714	-0.60714286
F	-2.35996263	-1.34715714	-0.60714286
F	-2.35996263	1.34715714	-0.60714286
Cl	0.00000000	0.00000000	2.64285714

21

Cl^-···C6H2(NH2)4

C	-0.66231966	-0.00184628	1.38683332
C	-0.66781217	1.21298237	0.70468389
C	-0.68550078	1.21300132	-0.69574206
C	-0.68335771	-0.00224098	-1.37732059
C	-0.67831599	-1.21707603	-0.69501373
C	-0.66235691	-1.21709042	0.70535238
H	-0.63611503	-0.00150689	2.47257329
H	-0.70809368	-0.00280376	-2.46307271
N	-0.64152409	-2.46612709	-1.35484751
H	-1.31494999	-3.11578090	-0.96369810

H	-0.78289311	-2.38490923	-2.35182606
N	-0.68953697	-2.46673349	1.36532680
H	-0.00882789	-3.10962004	0.97543556
H	-0.54905972	-2.38366234	2.36231768
N	-0.69817837	2.46306062	1.36448062
H	-0.57794545	2.37848865	2.36396558
H	-0.00551469	3.10153461	0.98857383
N	-0.65624504	2.46132687	-1.35604810
H	-0.81095374	2.38112627	-2.35106302
H	-1.32148653	3.11267347	-0.95411944
Cl	2.92660061	0.00925835	-0.02260168

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Cl^{-}···C6(CCH)6

C	-0.99574297	-0.99574297	-0.40877863
C	-1.36021020	0.36446722	-0.40877863
C	-0.36446722	1.36021020	-0.40877863
C	0.99574297	0.99574297	-0.40877863
C	1.36021020	-0.36446722	-0.40877863
C	0.36446722	-1.36021020	-0.40877863
C	-0.73400063	2.73932766	-0.40877863
C	-1.04619836	3.90446544	-0.40877863
H	-1.32200375	4.93378517	-0.40877863
C	-2.73932766	0.73400063	-0.40877863
C	-3.90446544	1.04619836	-0.40877863
H	-4.93378517	1.32200375	-0.40877863
C	-2.00532703	-2.00532703	-0.40877863
C	-2.85826708	-2.85826708	-0.40877863
H	-3.61178142	-3.61178142	-0.40877863
C	0.73400063	-2.73932766	-0.40877863
C	1.04619836	-3.90446544	-0.40877863
H	1.32200375	-4.93378517	-0.40877863
C	2.73932766	-0.73400063	-0.40877863
C	3.90446544	-1.04619836	-0.40877863
H	4.93378517	-1.32200375	-0.40877863
C	2.00532703	2.00532703	-0.40877863
C	2.85826708	2.85826708	-0.40877863
H	3.61178142	3.61178142	-0.40877863
Cl	0.00000000	0.00000000	2.74122137

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Cl^{-}···C6(CH3)6

C	-0.82830551	1.15514358	-0.50625848
C	0.56613274	1.30724101	-0.52613794
C	1.39444117	0.17509744	-0.53820134
C	0.82831133	-1.10671493	-0.60483614
C	-0.56612692	-1.25881236	-0.58495667
C	-1.39443535	-0.12666879	-0.57289328
C	1.72148246	-2.32404883	-0.72407247
H	1.23090773	-3.11797220	-1.28611262
H	1.99598132	-2.73130865	0.25545392
H	2.64367081	-2.08471308	-1.25242191
C	2.89807348	0.33564225	-0.45340810
H	3.36019702	0.41811183	-1.44351970
H	3.35583517	-0.51213730	0.05511001
H	3.16691257	1.22733118	0.11181911
C	1.17659548	2.69289170	-0.56051408
H	0.52325191	3.39762767	-1.07369748
H	2.12493759	2.69141822	-1.09671388
H	1.36420834	3.08562285	0.44509227
C	-1.72147663	2.37247748	-0.38702215
H	-1.99597550	2.77973729	-1.36654854
H	-1.23090191	3.16640085	0.17501800
H	-2.64366499	2.13314172	0.14132729
C	-2.89806766	-0.28721360	-0.65768651
H	-3.35582935	0.56056595	-1.16620463
H	-3.36019120	-0.36968318	0.33242508
H	-3.16690675	-1.17890254	-1.22291373
C	-1.17658966	-2.64446305	-0.55058054
H	-1.36420252	-3.03719420	-1.55618689
H	-2.12493177	-2.64298957	-0.01438074
H	-0.52324609	-3.34919902	-0.03739714
Cl	-0.00001541	-0.12819348	2.94113281

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Cl^{-}···C6(CN)6

C	-1.40195600	0.00000000	-0.38282443
C	-0.70097800	1.21413000	-0.38282443
C	0.70097800	1.21413000	-0.38282443
C	1.40195600	0.00000000	-0.38282443
C	0.70097800	-1.21413000	-0.38282443
C	-0.70097800	-1.21413000	-0.38282443
C	1.41830700	2.45658000	-0.38282443
N	1.99557800	3.45644200	-0.38282443
C	2.83661500	0.00000000	-0.38282443
N	3.99115500	0.00000000	-0.38282443
C	1.41830700	-2.45658000	-0.38282443
N	1.99557800	-3.45644200	-0.38282443
C	-1.41830700	-2.45658000	-0.38282443
N	-1.99557800	-3.45644200	-0.38282443
C	-2.83661500	0.00000000	-0.38282443
N	-3.99115500	0.00000000	-0.38282443
C	-1.41830700	2.45658000	-0.38282443
N	-1.99557800	3.45644200	-0.38282443
Cl	0.00000000	0.00000000	2.56717557

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Cl^{-}···C6F6

C	-1.38796700	0.00000000	-0.50046729
C	-0.69398300	1.20201400	-0.50046729
C	0.69398300	1.20201400	-0.50046729
C	1.38796700	0.00000000	-0.50046729
C	0.69398300	-1.20201400	-0.50046729
C	-0.69398300	-1.20201400	-0.50046729
F	1.35959500	2.35488800	-0.50046729
F	2.71919100	0.00000000	-0.50046729
F	1.35959500	-2.35488800	-0.50046729
F	-1.35959500	-2.35488800	-0.50046729
F	-2.71919100	0.00000000	-0.50046729
F	-1.35959500	2.35488800	-0.50046729
Cl	0.00000000	0.00000000	2.64953271

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Cl^{-}···C6(NH2)6

C	−0.65935772	−1.34888475	0.00000000
C	−0.56976385	−0.65567633	−1.20760400
C	−0.53923780	0.73929393	−1.20760400
C	−0.44964394	1.43250235	0.00000000
C	−0.53923780	0.73929393	1.20760400
C	−0.56976385	−0.65567633	1.20760400
N	−0.58068283	−1.36720331	2.43905600
H	−0.13367225	−2.27053689	2.33349600
H	−0.05294611	−0.86718072	3.14506350
N	−0.77092952	−2.76677641	0.00000000
H	−1.28816708	−3.08426474	0.81156700
H	−1.28816708	−3.08426474	−0.81156700
N	−0.52831883	1.45082092	−2.43905600
H	−1.05605555	0.95079833	−3.14506350
H	−0.97532941	2.35415450	−2.33349600
N	−0.33807213	2.85039402	0.00000000
H	0.17916542	3.16788235	0.81156700
H	0.17916542	3.16788235	−0.81156700
N	−0.52831883	1.45082092	2.43905600
H	−0.97532941	2.35415450	2.33349600
H	−1.05605555	0.95079833	3.14506350
N	−0.58068283	−1.36720331	−2.43905600
H	−0.05294611	−0.86718072	−3.14506350
H	−0.13367225	−2.27053689	−2.33349600
Cl	2.93559263	−0.22134072	0.00000000