Supporting Information for:

The Hydrogen Bond Basicity of the Chlorogroup;

Hexachlorocyclohexanes as Strong Hydrogen Bond Bases

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Energies and optimised coordinates are supplied in the XYZ format recognised by the Babel file conversion program.

TABLE OF CONTENTS

α-HCH

```
18
Energy = -2992.727534276
C     1.5733755    0.1021989   -0.7628245
C     0.3030509   -0.4802759   -1.4009472
C    -0.9812379    0.0867799   -0.7689189
C    -0.9812132   -0.0867961    0.7689022
C     0.3030763    0.4802907    1.4009338
C     1.5734126   -0.1020818    0.7627524
Cl    1.7429692    1.8858738   -1.0962813
Cl    0.3281856   -0.2391502   -3.1859885
Cl   -2.4235991   -0.7435996   -1.4685267
Cl   -2.4235013    0.7435554    1.4687094
Cl    0.3282669    0.2390132    3.1859623
Cl    1.7432198   -1.8857377    1.0961572
H     2.4681112   -0.3706043   -1.2103578
H     2.4681283    0.3707870    1.2102575
H     0.3325256    1.5773686    1.2402863
H    -1.0794565   -1.1606631    1.0246069
H    -1.0795974    1.1606613   -1.0245221
H     0.3325047   -1.5773421   -1.2401920
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β-HCH

```
18
Energy = -2992.721691648
C    -1.4236535    0.3680091    0.2295405
C    -1.0309240   -1.0490103   -0.2288665
C     0.3932903   -1.4170634    0.2288944
C     1.4237537   -0.3677043   -0.2295815
C     1.0303169    1.0486457    0.2302914
C    -0.3929526    1.4164414   -0.2303349
Cl   -3.0526151    0.7887536   -0.4245274
Cl   -2.2093269   -2.2488196    0.4269517
Cl    0.8429015   -3.0372735   -0.4270136
Cl    3.0524342   -0.7892794    0.4245249
Cl    2.2099838    2.2490488   -0.4220153
Cl   -0.8433006    3.0378702    0.4221002
H    -1.5137682    0.3922105    1.3352462
H    -0.4171897    1.5052832   -1.3362638
H     1.0947219    1.1146037    1.3362270
H     1.5142728   -0.3903297   -1.3352784
H     0.4188553   -1.5080474    1.3346067
H    -1.0975821   -1.1161524   -1.3345862
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γ-HCH

```
18
Energy = -2992.722935990
C    -0.4595856   -1.2557083    0.4380977
C     1.0561587   -1.3009479    0.1679916
C     1.7512935    0.0048085    0.6040901
C     1.0482015    1.3074145    0.1710735
C    -0.4676758    1.2522335    0.4391843
C    -1.1372915   -0.0036578   -0.1540769
Cl   -1.2396652   -2.7815177   -0.1151625
Cl    1.4296476   -1.6548486   -1.5702567
Cl    1.8310116    0.0025900    2.4395182
Cl    1.4220861    1.6678272   -1.5658782
Cl   -1.2567839    2.7735508   -0.1134054
Cl   -2.8932810   -0.0092377    0.2594048
H    -0.5933902   -1.2375038    1.5399428
H    -1.0624914   -0.0030483   -1.2597809
H    -0.6020752    1.2324849    1.5409602
H     1.4810990    2.1534347    0.7385865
H     2.8053031    0.0085703    0.2682070
H     1.4950235   -2.1457624    0.7326952
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δ-HCH

```
18
Energy = -2992.723510786
C    -1.2513368   -0.7865855    0.6729063
C    -0.0025428   -1.6064546    0.3058223
C     1.2566931   -0.7985409    0.6639394
C     1.2952421    0.5489307   -0.0777074
C     0.0019500    1.3581924    0.1735552
C    -1.2884550    0.5485366   -0.0887874
Cl   -2.7464948   -1.7549213    0.4020221
Cl   -0.0120149   -2.0635800   -1.4482907
Cl    2.7435191   -1.7682125    0.3600580
Cl    2.7200885    1.5136012    0.4649553
Cl    0.0088816    2.8398037   -0.8576493
Cl   -2.7188136    1.5200558    0.4268174
H    -1.2215665   -0.5825275    1.7644206
H    -1.4054154    0.3538445   -1.1728609
H    -0.0037103    1.7143560    1.2246831
H     1.4250664    0.3686004   -1.1629573
H     1.2424662   -0.6092790    1.7585047
H    -0.0044562   -2.5612793    0.8654023
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ε-HCH

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18
Energy = -2992.725516511
C    -1.2682556   -0.5072893    0.5771190
C     0.0000870   -1.3850705    0.5279810
C     1.2684799   -0.5073943    0.5770333
C     1.2683568    0.5074704   -0.5766889
C    -0.0000173    1.3852936   -0.5271816
C    -1.2682130    0.5072046   -0.5768650
Cl   -2.7486496   -1.5292718    0.5901638
Cl   -0.0000633   -2.4370115   -0.9552586
Cl    2.7488359   -1.5294118    0.5894461
Cl    2.7488093    1.5291837   -0.5895345
Cl   -0.0002976    2.4377294    0.9549695
Cl   -2.7488143    1.5287325   -0.5902662
H    -1.2702803    0.0465109    1.5390494
H    -1.2695484   -0.0464652   -1.5388603
H     0.0000565    2.0827023   -1.3872433
H     1.2700995   -0.0459689   -1.5388003
H     1.2706604    0.0461628    1.5391010
H     0.0001114   -2.0837582    1.3869764
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η-HCH

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18
Energy = -2992.723024075
C    -0.9472916   -0.7905766    0.6368618
C     0.5725164   -1.0653654    0.7390174
C     1.3315917    0.2704767    0.8681339
C     0.9989702    1.3339075   -0.1920034
C    -0.5280985    1.5108340   -0.3281812
C    -1.2554487    0.1682163   -0.5236290
Cl   -1.8661167   -2.3325512    0.5221102
Cl    1.1593466   -2.0831344   -0.6341227
Cl    3.1043406    0.0283359    1.0442390
Cl    1.6865278    0.9940475   -1.8343173
Cl   -1.1303869    2.3833511    1.1617811
Cl   -3.0205567    0.4427350   -0.7383448
H    -1.2770865   -0.3154721    1.5840522
H    -0.8876580   -0.2767384   -1.4714729
H    -0.7522412    2.1872751   -1.1739283
H     1.4499174    2.2968236    0.1149280
H     1.0020527    0.7162539    1.8318280
H     0.7637084   -1.6678879    1.6483573
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θ-HCH

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18
Energy = -2992.716997827
C    -0.7207593   -1.2536820    0.6035033
C     0.8180298   -1.3064815    0.4741189
C     1.4135682   -0.0063728    1.0489445
C     0.8263228    1.3000173    0.4794894
C    -0.7134529    1.2561294    0.6039737
C    -1.3331027    0.0030527   -0.0477472
Cl   -1.4585748   -2.7728166   -0.0195810
Cl    1.3393916   -1.6524369   -1.2160040
Cl    3.2119507   -0.0122153    1.0086619
Cl    1.3551689    1.6520025   -1.2071894
Cl   -1.4401855    2.7795321   -0.0210317
Cl   -3.1196520    0.0088073    0.1982786
H    -0.9658011   -1.2361995    1.6876524
H    -1.1504828    0.0022335   -1.1407401
H    -0.9618401    1.2400564    1.6874012
H     1.2029008    2.1478613    1.0849216
H     1.1561909   -0.0080505    2.1318983
H     1.1919815   -2.1595252    1.0738637
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ζ-HCH

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18
Energy = -2992.708766009
C     0.7783993   -1.2181170    0.9811073
C     1.5111796    0.0680088    0.5415011
C     0.6658629    1.2832269    0.9809363
C    -0.8143943    1.2745847    0.5411492
C    -1.4442059   -0.0648564    0.9809742
C    -0.6967370   -1.3424987    0.5413894
Cl    1.7233105   -2.6974182    0.5922413
Cl    1.9598777    0.0880585   -1.1980940
Cl    1.4741548    2.8413992    0.5921665
Cl   -1.0559531    1.6522292   -1.1986954
Cl   -3.1979538   -0.1435552    0.5922738
Cl   -0.9034761   -1.7408532   -1.1982934
H     0.7584194   -1.1866081    2.0936695
H    -1.1414662   -2.1994476    1.0853088
H    -1.4067970   -0.0630626    2.0934311
H    -1.3342810    2.0882678    1.0847834
H     0.6486956    1.2502089    2.0935688
H     2.4755907    0.1114032    1.0853990
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