

## Supporting Information Material

Simultaneous interaction of tetrafluoroethene with anions and hydrogen bond donors.

A cooperative study.

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Optimized geometries of the complexes at the MP2/6-311++G(d,p) computational level.

C<sub>2</sub>F<sub>4</sub>:Cl-

C,0.,0.5918579043,-0.7334617374  
C,0.,-0.7201698585,-0.9081030748  
F,-1.1024158087,1.3105557702,-0.663344204  
F,1.1024158087,1.3105557702,-0.663344204  
F,-1.1031369705,-1.4463427505,-0.9760943843  
F,1.1031369705,-1.4463427505,-0.9760943843  
Cl,0.,-0.0501140845,2.3182119884

C<sub>2</sub>F<sub>4</sub>:Br-

C,0.,0.6218176966,-0.8152210882  
C,0.,-0.7005307877,-0.8844813184  
F,-1.1026215303,1.3459501003,-0.7772157443  
F,1.1026215303,1.3459501003,-0.7772157443  
F,-1.1026407999,-1.4246901755,-0.9219487885  
F,1.1026407999,-1.4246901755,-0.9219487885  
Br,0.,-0.2138067579,2.4958014719

C<sub>2</sub>F<sub>4</sub>:CN-

C,0.7115102807,0.3244950551,0.  
C,-0.5857892949,0.0572056495,0.  
F,1.4362449386,0.4308637236,1.1039469469  
F,1.4362449386,0.4308637236,-1.1039469469  
F,-1.2975558624,-0.0407426119,1.1021410576  
F,-1.2975558624,-0.0407426119,-1.1021410576  
C,-0.2080414528,-2.9295546936,0.  
N,0.004873298,-4.1044764821,0.

C<sub>2</sub>F<sub>4</sub>:NC-

C,0.6908626853,0.0745777974,0.  
C,-0.6329481794,0.0401989507,0.  
F,1.4178448797,0.0709368438,1.1033054656  
F,1.4178448797,0.0709368438,-1.1033054656  
F,-1.354934127,0.0424670993,1.1028068228  
F,-1.354934127,0.0424670993,-1.1028068228  
N,-0.5133889681,-2.8079880059,0.  
C,0.5295525447,-3.3924038296,0.

C<sub>2</sub>F<sub>4</sub>:NNN-

C,0.,0.6652067898,-0.3449384329  
C,0.,-0.6652067898,-0.3449384329  
F,-1.1063925996,1.3863014128,-0.4109809076  
F,1.1063925996,1.3863014128,-0.4109809076  
F,-1.1063925996,-1.3863014128,-0.4109809076  
F,1.1063925996,-1.3863014128,-0.4109809076  
N,0.,0.,2.4882232442  
N,0.,1.2111606875,2.4497231223  
N,0.,-1.2111606875,2.4497231223

C<sub>2</sub>F<sub>4</sub>:NO<sub>2</sub>-

C,-0.0184784255,0.6625776409,0.4531714852  
C,-0.0184784255,-0.6625776409,0.4531714852  
F,1.0880014517,1.3857574266,0.4592431298  
F,-1.1197427099,1.38796144,0.4945384766  
F,1.0880014517,-1.3857574266,0.4592431298  
F,-1.1197427099,-1.38796144,0.4945384766  
N,0.3470664087,0.,-2.8230951036  
O,-0.0649173738,1.0717594912,-2.29019365  
O,-0.0649173738,-1.0717594912,-2.29019365

C<sub>2</sub>F<sub>4</sub>:HCO<sub>2</sub>-

C,0.,0.6622456282,-0.3832313923  
C,0.,-0.6622456282,-0.3832313923  
F,-1.1044921637,1.3866357934,-0.4087623026  
F,1.1044921637,1.3866357934,-0.4087623026  
F,-1.1044921637,-1.3866357934,-0.4087623026  
F,1.1044921637,-1.3866357934,-0.4087623026  
C,0.,0.,2.8928857363  
O,0.,1.1384741357,2.3544532609  
O,0.,-1.1384741357,2.3544532609  
H,0.,0.,4.0212700358

C<sub>2</sub>F<sub>4</sub>:CCH-

C,0.,0.7229045488,-0.2686524666  
C,0.,-0.6008429448,-0.2377092656  
F,-1.1026935996,1.4443781254,-0.3169709175  
F,1.1026935996,1.4443781254,-0.3169709175  
F,-1.1033109504,-1.3275802663,-0.1947512653  
F,1.1033109504,-1.3275802663,-0.1947512653  
C,0.,-0.7389044945,3.1376613476  
C,0.,0.4446661148,2.7059400534  
H,0.,-1.7404011037,3.5215584023

C<sub>2</sub>F<sub>4</sub>:OCN-

C,0.,0.582094235,-0.0185504864  
C,0.,-0.7396390301,-0.1418484847  
F,-1.1044916803,1.3056177558,0.0187745543  
F,1.1044916803,1.3056177558,0.0187745543  
F,-1.1045338763,-1.4533685775,-0.248139059  
F,1.1045338763,-1.4533685775,-0.248139059

O,0.,0.8147945665,2.8466650049  
C,0.,-0.4173531573,2.8341362506  
N,0.,-1.6233089678,2.773544723

C<sub>2</sub>F<sub>4</sub>:NCO-

C,0.,0.6803153654,-0.2077342726  
C,0.,-0.6068784232,-0.5205206918  
F,-1.1019862567,1.3888764209,-0.087573163  
F,1.1019862567,1.3888764209,-0.087573163  
F,-1.1042600822,-1.328234796,-0.6465009234  
F,1.1042600822,-1.328234796,-0.6465009234  
N,0.,0.2608543794,2.5115362094  
C,0.,-0.6202762476,3.338395833  
O,0.,-1.5142154334,4.1816981478

FH:C<sub>2</sub>F<sub>4</sub>:Cl-

C,0.,0.7894801372,-0.4805506045  
C,0.,-0.5075032495,-0.1559144197  
F,-1.1057511512,1.5202038208,-0.4981501635  
F,1.1057511512,1.5202038208,-0.4981501635  
F,-1.0994986858,-1.220758571,-0.1261801718  
F,1.0994986858,-1.220758571,-0.1261801718  
Cl,0.,-0.1914748077,2.6358840055  
H,0.,-0.0144456151,-2.4317791296  
F,0.,-0.1549469641,-3.3527391812

FH:C<sub>2</sub>F<sub>4</sub>:Br-

C,0.,0.729688529,-0.3634747136  
C,0.,-0.5997109472,-0.3167518128  
F,-1.1024920478,1.4477868426,-0.3756048634  
F,1.1024920478,1.4477868426,-0.3756048634  
F,-1.1025040101,-1.3169521109,-0.2769056878  
F,1.1025040101,-1.3169521109,-0.2769056878  
Br,0.,0.189709344,2.8737462244  
H,0.,-0.0116065431,-2.4975517131  
F,0.,-0.0497498464,-3.4247068823

FH:C<sub>2</sub>F<sub>4</sub>:NC-

C,0.,0.6935647879,-0.1789591203  
C,0.,-0.6340083323,-0.2695769076  
F,-1.1017832407,1.4089282335,-0.155587207  
F,1.1017832407,1.4089282335,-0.155587207  
F,-1.1037366977,-1.3537015516,-0.2611545661  
F,1.1037366977,-1.3537015516,-0.2611545661  
C,0.,-0.6585939288,3.0774750811  
N,0.,0.4094751949,2.5401051796  
H,0.,0.0812214305,-2.3701777691  
F,0.,0.1165065264,-3.2980852248

FH:C<sub>2</sub>F<sub>4</sub>:NNN-

C,0.,0.668914172,-0.3175178259  
C,0.,-0.668914172,-0.3175178259

F,-1.1072314745,1.3835609867,-0.3848066607  
F,1.1072314745,1.3835609867,-0.3848066607  
F,-1.1072314745,-1.3835609867,-0.3848066607  
F,1.1072314745,-1.3835609867,-0.3848066607  
N,0.,0.,2.4395108607  
N,0.,1.2110769861,2.3941881379  
N,0.,-1.2110769861,2.3941881379  
H,0.,0.,-2.4685481404  
F,0.,0.,-3.3956640112

FH:C<sub>2</sub>F<sub>4</sub>:NO<sub>2</sub>-

C,-0.019735528,0.6659282557,0.4288312622  
C,-0.019735528,-0.6659282557,0.4288312622  
F,1.0871191531,1.38152094,0.4242635056  
F,-1.1213062699,1.3848774295,0.4683259566  
F,1.0871191531,-1.38152094,0.4242635056  
F,-1.1213062699,-1.3848774295,0.4683259566  
N,0.3287067392,0.,-2.7823639912  
O,-0.0520345782,1.0709680102,-2.2250268396  
O,-0.0520345782,-1.0709680102,-2.2250268396  
H,0.0141687509,0.,2.5530402728  
F,0.0376133103,0.,3.4822493807

FH:C<sub>2</sub>F<sub>4</sub>:HCO<sub>2</sub>-

C,0.,0.6658389217,-0.384822102  
C,0.,-0.6658389217,-0.384822102  
F,-1.1052264147,1.3821224988,-0.405331086  
F,1.1052264147,1.3821224988,-0.405331086  
F,-1.1052264147,-1.3821224988,-0.405331086  
F,1.1052264147,-1.3821224988,-0.405331086  
C,0.,0.,2.8008497111  
O,0.,1.1370895468,2.2586934893  
O,0.,-1.1370895468,2.2586934893  
H,0.,0.,3.9267333265  
H,0.,0.,-2.501207183  
F,0.,0.,-3.4315962553

FH:C<sub>2</sub>F<sub>4</sub>:OCN-

C,0.,0.5474585168,-0.0644906641  
C,0.,-0.784422367,-0.1491890588  
F,-1.105053123,1.2646849201,-0.0355378077  
F,1.105053123,1.2646849201,-0.0355378077  
F,-1.1047659276,-1.4938689797,-0.2343544306  
F,1.1047659276,-1.4938689797,-0.2343544306  
O,0.,0.850685736,2.7198125284  
C,0.,-0.3811135042,2.731439714  
N,0.,-1.5873265092,2.6783976685  
H,0.,0.0392328016,-2.257727378  
F,0.,0.0949394483,-3.1832403354

FH:C<sub>2</sub>F<sub>4</sub>:NCO-

C,0.,0.57889727,-0.1916852144

C,0.,-0.7212567265,-0.4862470798  
F,-1.1002002819,1.2875883814,-0.1224391824  
F,1.1002002819,1.2875883814,-0.1224391824  
F,-1.1055419515,-1.447743989,-0.5297303361  
F,1.1055419515,-1.447743989,-0.5297303361  
N,0.,0.2915896318,2.3877902041  
C,0.,-0.5487665088,3.2566066716  
O,0.,-1.396574504,4.1424160663  
H,0.,0.1517182139,-2.4749804862  
F,0.,0.2857838388,-3.3943331248

ClH:C<sub>2</sub>F<sub>4</sub>:Br-

C,0.,0.66415685,-0.50439637  
C,0.,-0.66415685,-0.50439637  
F,-1.102459,1.38360526,-0.49729028  
F,1.102459,1.38360526,-0.49729028  
F,-1.102459,-1.38360526,-0.49729028  
F,1.102459,-1.38360526,-0.49729028  
Br,0.,0.,2.73345261  
H,0.,0.,-2.76177024  
Cl,0.,0.,-4.04955132

ClH:C<sub>2</sub>F<sub>4</sub>:Cl-

C,0.,0.7977498193,-0.4213406897  
C,0.,-0.4986102882,-0.1019620801  
F,-1.105220942,1.5276169433,-0.4584621815  
F,1.105220942,1.5276169433,-0.4584621815  
F,-1.0998009631,-1.2129113753,-0.0741979458  
F,1.0998009631,-1.2129113753,-0.0741979458  
Cl,0.,-0.2079372401,2.7138109452  
H,0.,-0.0061958816,-2.4391110906  
Cl,0.,-0.1944175447,-3.7198368304

ClH:C<sub>2</sub>F<sub>4</sub>:HCO<sub>2</sub>-

C,0.,0.6653805773,-0.3777413627  
C,0.,-0.6653805773,-0.3777413627  
F,-1.1049018006,1.3820386419,-0.4052230018  
F,1.1049018006,1.3820386419,-0.4052230018  
F,-1.1049018006,-1.3820386419,-0.4052230018  
F,1.1049018006,-1.3820386419,-0.4052230018  
C,0.,0.,2.8098490161  
O,0.,1.1372121575,2.267877023  
O,0.,-1.1372121575,2.267877023  
H,0.,0.,3.9359853618  
H,0.,0.,-2.5453498636  
Cl,0.,0.,-3.838670606

ClH:C<sub>2</sub>F<sub>4</sub>:NC-

C,0.,0.6684432025,-0.2019702816  
C,0.,-0.6607192114,-0.1800876513  
F,-1.103577265,1.3888588463,-0.1646402431  
F,1.103577265,1.3888588463,-0.1646402431

F,-1.1017265535,-1.3770472849,-0.2027121854  
F,1.1017265535,-1.3770472849,-0.2027121854  
N,0.,-0.5711144757,2.5597430492  
C,0.,0.458986511,3.1667469571  
H,0.,0.0890883663,-2.4270388023  
Cl,0.,0.1101197555,-3.7157627475

OH<sub>2</sub>:C<sub>2</sub>F<sub>4</sub>:Br-

C,-0.8122322517,-0.2938689907,0.  
C,0.5086427068,-0.4178212996,0.  
F,-1.5293586885,-0.207567222,1.1024175298  
F,-1.5293586885,-0.207567222,-1.1024175298  
F,1.2272241471,-0.5016961673,1.1020762448  
F,1.2272241471,-0.5016961673,-1.1020762448  
Br,0.3796604412,2.8788290866,0.  
H,-0.0703042141,-2.8111949424,0.  
O,0.2000369262,-3.7364210631,0.  
H,1.1578685355,-3.6670694012,0.

OH<sub>2</sub>:C<sub>2</sub>F<sub>4</sub>:Cl-

C,-1.0117821989,-0.2169536695,0.  
C,0.3014679577,-0.406468429,0.  
F,-1.7207572133,-0.0414644121,1.1038481159  
F,-1.7207572133,-0.0414644121,-1.1038481159  
F,0.9988451799,-0.5938152118,1.1010227959  
F,0.9988451799,-0.5938152118,-1.1010227959  
Cl,0.9757199512,2.4662536259,0.  
H,-0.0979525059,-3.1311589417,0.  
O,0.6395665841,-3.7481915483,0.  
H,1.3973964756,-3.1571405601,0.

OH<sub>2</sub>:C<sub>2</sub>F<sub>4</sub>:HCO<sub>2</sub>-

C,0.,0.1746157658,-0.5055048391  
C,0.,-1.1233409563,-0.2323523662  
F,-1.1040228707,0.8765311496,-0.6898511236  
F,1.1040228707,0.8765311496,-0.6898511236  
F,-1.1047201264,-1.8321578171,-0.101951362  
F,1.1047201264,-1.8321578171,-0.101951362  
C,0.,0.2494818889,2.7712626189  
O,0.,1.2345829611,1.9856442185  
O,0.,-0.9811179211,2.5038844464  
H,0.,0.506614324,3.8685698067  
H,0.,1.1468010728,-3.30953804  
H,0.,-0.333316969,-3.1091057033  
O,0.,0.3263200414,-3.8097952535

OH<sub>2</sub>:C<sub>2</sub>F<sub>4</sub>:NC-

C,0.,0.3448939112,-0.3624761809  
C,0.,-0.9507618794,-0.0822491342  
F,-1.1025708773,1.0616739876,-0.4907657739  
F,1.1025708773,1.0616739876,-0.4907657739  
F,-1.101996026,-1.6576764553,0.0540608532

F,1.101996026,-1.6576764553,0.0540608532  
N,0.,-0.2065825939,2.6336445897  
C,0.,0.9485145541,2.9428523227  
H,0.,0.0021652727,-3.0590296977  
O,0.,0.7377649212,-3.6785567058  
H,0.,1.498230217,-3.0912635681