Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPLEMENTARY MATERIAL

Reduced nucleophilicity: An intrinsic property of the Lewis base atom interacting with H in hydrogen-bonds with Lewis acids HX (X = F, Cl, Br, I, CN, CCH, CP)

Ibon Alkorta[a] and Anthony Legon[b]

[a]*Instituto de Química Médica (IQM-CSIC), Juan de la Cierva, 3, E-28006 Madrid, Spain,*

E-mail: ibon@iqm.csic.es; Tel: +34 915622900

[b]*School of Chemistry, University of Bristol, Cantock's Close, Bristol BS8 1TS, U. K.*

E-mail: a.c.legon@bristol.ac.uk; Tel: +44 (0)117 331 7708

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Table S1. Optimised geometries (Å) and counterpoise corrected energies (au) of complexes B□HX (X = F, Cl, Br, I, CN, CCH, CP), all calculated at the CCSD(T)(F12c)/cc-pVDZ-F12 level.

OC□HX

OC□HF

F	0.0000000000	0.0000000000	-2.1601895773
H	0.0000000000	0.0000000000	-1.2369758735
C	0.0000000000	0.0000000000	0.8658219416
O	0.0000000000	0.0000000000	1.9930714075

E(OC□HF) = -213.56590658 au

OC□HCl

Cl	0.0000000000	0.0000000000	-1.8949134033
H	0.0000000000	0.0000000000	-0.6166943494
C	0.0000000000	0.0000000000	1.7759346824
O	0.0000000000	0.0000000000	2.9045890224

E(OC□HCl) = -573.54637931 au

OC□HBr

Br	0.0000000000	0.0000000000	-1.1841361949
H	0.0000000000	0.0000000000	0.2358073361
C	0.0000000000	0.0000000000	2.7245777905
O	0.0000000000	0.0000000000	3.8535591978

E(OC□HBr) = -529.49888890 au

OC□HI

I	0.0000000000	0.0000000000	-0.9017883128
H	0.0000000000	0.0000000000	0.7129295000
C	0.0000000000	0.0000000000	3.3975886289
O	0.0000000000	0.0000000000	4.5271169056

E(OC□HI) = -408.62269541 au

OC□HCN

N	0.0000000000	0.0000000000	-1.4053632397
C	0.0000000000	0.0000000000	-0.2500152102
H	0.0000000000	0.0000000000	0.8191371857
C	0.0000000000	0.0000000000	3.3755177122
O	0.0000000000	0.0000000000	4.5041381708

E(OC□HCN) = -206.48967900 au

OC□HCCH

H	0.0000000000	0.0000000000	-4.1314927618
C	0.0000000000	0.0000000000	-3.0684392910
C	0.0000000000	0.0000000000	-1.8626815198
H	0.0000000000	0.0000000000	-0.7980917383
C	0.0000000000	0.0000000000	1.8972585391
O	0.0000000000	0.0000000000	3.0268152830

E(OC□HCCH) = -190.39583915 au

OC□HCP

P	0.0000000000	0.0000000000	-4.2954597411
C	0.0000000000	0.0000000000	-2.7519071413
H	0.0000000000	0.0000000000	-1.6790304204
C	0.0000000000	0.0000000000	1.0449134214
O	0.0000000000	0.0000000000	2.1745235915

E(OC□HCP)) = -492.69176728 au

SC□HX

SC□HF

F	0.0000000000	0.0000000000	-2.7637157120
H	0.0000000000	0.0000000000	-1.8322082973
C	0.0000000000	0.0000000000	0.1229244962
S	0.0000000000	0.0000000000	1.6503433348

E(SC□HF) = -536.10005174 au

SC□HCl

Cl	0.0000000000	0.0000000000	-2.6623801949
H	0.0000000000	0.0000000000	-1.3751317886
C	0.0000000000	0.0000000000	0.7991176060
S	0.0000000000	0.0000000000	2.3301966294

E(SC□HCl) = -896.07863341au

SC□HBr

Br	0.0000000000	0.0000000000	5.2090568439
H	0.0000000000	0.0000000000	3.7803192497
C	0.0000000000	0.0000000000	1.5494905709
S	0.0000000000	0.0000000000	0.0175333355

E(SC□HBr) = -852.03068408 au

SC□HI

I	0.0000000000	0.0000000000	-3.1077378642
H	0.0000000000	0.0000000000	-1.4869759202
C	0.0000000000	0.0000000000	0.9084854007
S	0.0000000000	0.0000000000	2.4422306356

E(SC□HI) = -731.15357784 au

SC□HCN

N	0.0000000000	0.0000000000	-1.3403672811
C	0.0000000000	0.0000000000	-0.1846415417
H	0.0000000000	0.0000000000	0.8889303946
C	0.0000000000	0.0000000000	3.2732638905
S	0.0000000000	0.0000000000	4.8049716086

E(SC□HCN) = -529.02187141 au

SC□HCCH

H	0.0000000000	0.0000000000	-2.5005415406
C	0.0000000000	0.0000000000	-1.4375787629
C	0.0000000000	0.0000000000	-0.2312343282
H	0.0000000000	0.0000000000	0.8358979846
C	0.0000000000	0.0000000000	3.3854382272
S	0.0000000000	0.0000000000	4.9201754908

E(SC□HCCH) = -512.92608957 au

SC□HCP

P	0.0000000000	0.0000000000	-1.7833727227
C	0.0000000000	0.0000000000	-0.2389712479
H	0.0000000000	0.0000000000	0.8361863437
C	0.0000000000	0.0000000000	3.3934125473
S	0.0000000000	0.0000000000	4.9282224541

E(SC□HCP)= -815.22204259 au

SeC□HX

SeC□HF

F	0.0000000000	0.0000000000	-3.5637765662
H	0.0000000000	0.0000000000	-2.6317393738
C	0.0000000000	0.0000000000	-0.6784128926
Se	0.0000000000	0.0000000000	0.9913592672

E(SeC□HF)= -510.38634126 au

SeC□HCl

Cl	0.0000000000	0.0000000000	-4.0089523826
H	0.0000000000	0.0000000000	-2.7205444974
C	0.0000000000	0.0000000000	-0.5635259784
Se	0.0000000000	0.0000000000	1.1104532931

E(SeC□HCl)= -870.36502067 au

SeC□HBr

Br	0.0000000000	0.0000000000	-4.1887831075
H	0.0000000000	0.0000000000	-2.7585055681
C	0.0000000000	0.0000000000	-0.5551122754
Se	0.0000000000	0.0000000000	1.1198313857

E(SeC□HBr)= -826.31710046 au

SeC□HI

I	0.0000000000	0.0000000000	-4.4598104691
H	0.0000000000	0.0000000000	-2.8376714697
C	0.0000000000	0.0000000000	-0.4810149965
Se	0.0000000000	0.0000000000	1.1959273700

E(SeC□HI)= -789.50830083 au

SeC□HCN

N	0.0000000000	0.0000000000	-4.9827247034
C	0.0000000000	0.0000000000	-3.8269757047
H	0.0000000000	0.0000000000	-2.7530387578
C	0.0000000000	0.0000000000	-0.3792731850
Se	0.0000000000	0.0000000000	1.2955349787

E(SeC□HCN)= -503.30820866 au

SeC□HCCH

H	0.0000000000	0.0000000000	-6.1327620186
C	0.0000000000	0.0000000000	-5.0697728543
C	0.0000000000	0.0000000000	-3.8633926736
H	0.0000000000	0.0000000000	-2.7960585948
C	0.0000000000	0.0000000000	-0.2564055541
Se	0.0000000000	0.0000000000	1.4219143232

E(SeC□HCN)= -487.21230353 au

SeC□HCP

P	0.0000000000	0.0000000000	-5.4229866603
C	0.0000000000	0.0000000000	-3.8785657184
H	0.0000000000	0.0000000000	-2.8031343016
C	0.0000000000	0.0000000000	-0.2601406790
Se	0.0000000000	0.0000000000	1.4183499872

E(SeC□HCP)= -789.50828329 au

$H_3CNC\square HX$

$H_3CNC\square HF$

C	-0.0000000000	0.0000000000	-0.0074634094
N	-0.0000000000	0.0000000000	1.1579956789
C	0.0000000000	0.0000000000	2.5838810107
H	1.0266242557	0.0000000000	2.9407684827
H	-0.5133121279	0.8890826856	2.9407684827
H	-0.5133121279	-0.8890826856	2.9407684827
H	-0.0000000000	0.0000000000	-1.9141938391
F	0.0000000000	0.0000000000	-2.8490822044

E($H_3CNC\cdots HF$)= -232.91269137 au

$H_3CNC\square HCl$

C	-0.0000000000	0.0000000000	0.8512480515
N	-0.0000000000	0.0000000000	2.0186059302
C	0.0000000000	0.0000000000	3.4441965725
H	1.0263468190	0.0000000000	3.8024202379
H	-0.5131734095	0.8888424183	3.8024202379
H	-0.5131734095	-0.8888424183	3.8024202379
H	-0.0000000000	0.0000000000	-1.2496344222
Cl	0.0000000000	0.0000000000	-2.5415302205

E($H_3CNC\cdots HCl$)= -592.89027711 au

$H_3CNC\square HBr$

C	-0.0000000000	0.0000000000	1.8999562972
N	-0.0000000000	0.0000000000	3.0677164025
C	-0.0000000000	0.0000000000	4.4933213568
H	1.0262664454	0.0000000000	4.8517396422
H	-0.5131332227	0.8887728128	4.8517396422
H	-0.5131332227	-0.8887728128	4.8517396422
H	-0.0000000000	0.0000000000	-0.2455677527
Br	0.0000000000	0.0000000000	-1.6792840289

E($H_3CNC\cdots HBr$)= -548.84204881 au

$H_3CNC\square HI$

C	-0.0000000000	0.0000000000	2.6250994828
N	-0.0000000000	0.0000000000	3.7938465978
C	-0.0000000000	0.0000000000	5.2192252943
H	1.0260713261	0.0000000000	5.5785110540
H	-0.5130356630	0.8886038345	5.5785110540
H	-0.5130356630	-0.8886038345	5.5785110540
H	-0.0000000000	0.0000000000	0.3279121597
I	0.0000000000	0.0000000000	-1.2966854454

E($H_3CNC\cdots HI$)= -427.96439054 au

$H_3CNC\square HCN$

C	-0.0000000000	0.0000000000	0.7382580586
N	-0.0000000000	0.0000000000	1.9063146866
C	0.0000000000	0.0000000000	3.3321385961
H	1.0262258276	0.0000000000	3.6906299077
H	-0.5131129138	0.8887376367	3.6906299077
H	-0.5131129138	-0.8887376367	3.6906299077
H	-0.0000000000	0.0000000000	-1.5752324479
C	0.0000000000	0.0000000000	-2.6509949347
N	0.0000000000	0.0000000000	-3.8068690494

E($H_3CNC\cdots HCN$)= -225.83372685 au

$H_3CNC\square HCCH$

C	-0.0000000000	0.0000000000	0.7706856853
N	-0.0000000000	0.0000000000	1.9402890367
C	0.0000000000	0.0000000000	3.3652995711
H	1.0257984588	0.0000000000	3.7255175794
H	-0.5128992294	0.8883675245	3.7255175794
H	-0.5128992294	-0.8883675245	3.7255175794
H	-0.0000000000	0.0000000000	-1.7125078706
C	0.0000000000	0.0000000000	-2.7811669426
C	0.0000000000	0.0000000000	-3.9878540706
H	0.0000000000	0.0000000000	-5.0507404794

E($H_3CNC\cdots HCCH$)= -209.73660446 au

$H_3CNC\square HCP$

C	-0.0000000000	0.0000000000	1.7288543109
N	-0.0000000000	0.0000000000	2.8984695987
C	-0.0000000000	0.0000000000	4.3235696566
H	1.0258188412	0.0000000000	4.6837393160
H	-0.5129094206	0.8883851762	4.6837393160
H	-0.5129094206	-0.8883851762	4.6837393160
H	-0.0000000000	0.0000000000	-0.7576287071
C	0.0000000000	0.0000000000	-1.8341289052
P	0.0000000000	0.0000000000	-3.3790885078

E($H_3CNC\cdots HCP$)= -512.03256991 au

HNC□HX

HNC□HF

H	0.0000000000	0.0000000000	0.9375481277
N	0.0000000000	0.0000000000	-0.0598122320
C	0.0000000000	0.0000000000	-1.2248614503
H	0.0000000000	0.0000000000	-3.1679686679
F	0.0000000000	0.0000000000	-4.0996997507

E(HNC□HF) = -193.66203371 au

HNC□HCl

H	0.0000000000	0.0000000000	0.9101756808
N	0.0000000000	0.0000000000	-0.0870671589
C	0.0000000000	0.0000000000	-1.2541585102
H	0.0000000000	0.0000000000	-3.4181834588

Cl	0.0000000000	0.0000000000	-4.7055605261

E(HNC□HCl) = -553.64017031 au

HNC□HBr

H	0.0000000000	0.0000000000	0.9030664902
N	0.0000000000	0.0000000000	-0.0941438094
C	0.0000000000	0.0000000000	-1.2617309724
H	0.0000000000	0.0000000000	-3.4866485185
Br	0.0000000000	0.0000000000	-4.9153371631

E(HNC□HBr) = -509.59206813 au

HNC□HI

H	0.0000000000	0.0000000000	0.9120155037
N	0.0000000000	0.0000000000	-0.0850518160
C	0.0000000000	0.0000000000	-1.2536299453
H	0.0000000000	0.0000000000	-3.6437633862
I	0.0000000000	0.0000000000	-5.2643643294

E(HNC□HI) = -388.71479243 au

HNC□HCN

H	0.0000000000	0.0000000000	1.0936623126
N	0.0000000000	0.0000000000	0.0963513079
C	0.0000000000	0.0000000000	-1.0712269059
H	0.0000000000	0.0000000000	-3.4324148947
C	0.0000000000	0.0000000000	-4.5062672367
N	0.0000000000	0.0000000000	-5.6620128749

E(HNC□HCN) = -186.58369257 au

HNC□HCCH

H	0.0000000000	0.0000000000	1.2110255039
N	0.0000000000	0.0000000000	0.2142277774
C	0.0000000000	0.0000000000	-0.9549414562
H	0.0000000000	0.0000000000	-3.4818664123
C	0.0000000000	0.0000000000	-4.5493760242
C	0.0000000000	0.0000000000	-5.7558333714
H	0.0000000000	0.0000000000	-6.8187443088

E(HNC□HCCH) = -170.48736156 au

HNC□HCP

H	0.0000000000	0.0000000000	1.1759404679
N	0.0000000000	0.0000000000	0.1790938716
C	0.0000000000	0.0000000000	-0.9901070650
H	0.0000000000	0.0000000000	-3.5246815434
C	0.0000000000	0.0000000000	-4.6000778053
P	0.0000000000	0.0000000000	-6.1446762174

E(HNC□HCP) = -472.78329734 au

FNC□HX

FNC□HF

F	0.0000000000	0.0000000000	1.1883479181
N	0.0000000000	0.0000000000	-0.1088055850
C	0.0000000000	0.0000000000	-1.2798653071
H	0.0000000000	0.0000000000	-3.2750337908

F	0.0000000000	0.0000000000	-4.2029583067

E(FNC□HF) = -292.70570193 au

FNC□HCl

F	0.0000000000	0.0000000000	1.2692907511
N	0.0000000000	0.0000000000	-0.0308316611
C	0.0000000000	0.0000000000	-1.2048248812
H	0.0000000000	0.0000000000	-3.4385294361
Cl	0.0000000000	0.0000000000	-4.7217198441

E(HNC□HCl) = -652.68486001 au

FNC□HBr

F	0.0000000000	0.0000000000	1.2810533339
N	0.0000000000	0.0000000000	-0.0198960231
C	0.0000000000	0.0000000000	-1.1945943070
H	0.0000000000	0.0000000000	-3.4983474822
Br	0.0000000000	0.0000000000	-4.9229722865

E(FNC□HBr) = -608.63701862 au

FNC□HI

F	0.0000000000	0.0000000000	1.2526748439
N	0.0000000000	0.0000000000	-0.0497460074
C	0.0000000000	0.0000000000	-1.2257281103
H	0.0000000000	0.0000000000	-3.6971121295
I	0.0000000000	0.0000000000	-5.3148480737

E(FNC□HI) = -487.76021762 au

FNC□HCN

F	0.0000000000	0.0000000000	1.3890777908
N	0.0000000000	0.0000000000	0.0890417963
C	0.0000000000	0.0000000000	-1.0853235221
H	0.0000000000	0.0000000000	-3.4951787163
C	0.0000000000	0.0000000000	-4.5670698542
N	0.0000000000	0.0000000000	-5.7226680988

E(FNC□HCN) = -285.62841191 au

FNC□HCCH

F	0.0000000000	0.0000000000	1.5163513989
N	0.0000000000	0.0000000000	0.2134793674
C	0.0000000000	0.0000000000	-0.9629399735
H	0.0000000000	0.0000000000	-3.5320348143
C	0.0000000000	0.0000000000	-4.5982647625
C	0.0000000000	0.0000000000	-5.8044273723
H	0.0000000000	0.0000000000	-6.8673976391

E(FNC□HCCh) = -269.53303776

FNC□HCP

F	0.0000000000	0.0000000000	1.4823166313
N	0.0000000000	0.0000000000	0.1793756776
C	0.0000000000	0.0000000000	-0.9971300599
H	0.0000000000	0.0000000000	-3.5753311933
C	0.0000000000	0.0000000000	-4.6496553041
P	0.0000000000	0.0000000000	-6.1938245111

E(FNC□HCP) = -571.82897815 au

$H_3CCN\square HX$

$H_3CCN\square HF$

H	-0.0000000000	0.0000000000	1.8189975659
F	-0.0000000000	0.0000000000	2.7510792054
N	0.0000000000	0.0000000000	0.0044495452
C	0.0000000000	0.0000000000	-1.1496241290
C	0.0000000000	0.0000000000	-2.6105156211
H	1.0247765586	0.0000000000	-2.9753063122
H	-0.5123882793	-0.8874825329	-2.9753063122
H	-0.5123882793	0.8874825329	-2.9753063122

E($CH_3CN\square HF$) = -232.95097095 au

$H_3CCN\square HCl$

H	0.0000000000	0.0000000000	1.1794122276
Cl	-0.0000000000	0.0000000000	2.4674898305
N	0.0000000000	0.0000000000	-0.8363422990
C	0.0000000000	0.0000000000	-1.9917578342
C	-0.0000000000	0.0000000000	-3.4532859955
H	1.0244556152	0.0000000000	-3.8191458872
H	-0.5122278076	-0.8872045879	-3.8191458872
H	-0.5122278076	0.8872045879	-3.8191458872

E($CH_3CN\square HCl$) = -592.92863788 au

$H_3CCN\square HBr$

H	0.0000000000	0.0000000000	0.2086173073
Br	0.0000000000	0.0000000000	1.6374908350
N	0.0000000000	0.0000000000	-1.8686229026
C	0.0000000000	0.0000000000	-3.0243282656
C	0.0000000000	0.0000000000	-4.4860395431
H	1.0244097082	0.0000000000	-4.8521648922
H	-0.5122048541	-0.8871648312	-4.8521648922
H	-0.5122048541	0.8871648312	-4.8521648922

E($CH_3CN\square HBr$) = -548.88034569 au

$H_3CCN\square HI$

H	0.0000000000	0.0000000000	-0.3549407972
I	0.0000000000	0.0000000000	1.2658727751
N	0.0000000000	0.0000000000	-2.5802506989
C	0.0000000000	0.0000000000	-3.7365053520
C	0.0000000000	0.0000000000	-5.1985601357
H	1.0242257090	0.0000000000	-5.5652991260
H	-0.5121128545	-0.8870054832	-5.5652991260
H	-0.5121128545	0.8870054832	-5.5652991260

E($CH_3CN\square HI$) = -428.00285321 au

$H_3CCN\square HCN$

N	-0.0000000000	0.0000000000	3.5530096569
C	-0.0000000000	0.0000000000	2.3971446485
H	0.0000000000	0.0000000000	1.3221749205
N	0.0000000000	0.0000000000	-0.8401824017

C	0.0000000000	0.0000000000	-1.9960740155
C	-0.0000000000	0.0000000000	-3.4577392765
H	1.0243981893	0.0000000000	-3.8238076491
H	-0.5121990946	-0.8871548555	-3.8238076491
H	-0.5121990946	0.8871548555	-3.8238076491

E($CH_3CN\cdots HCN$) = -225.87272827 au

$H_3CCN\cdots HCCH$

H	0.0000000000	0.0000000000	4.7394045816
C	0.0000000000	0.0000000000	3.6765527207
C	-0.0000000000	0.0000000000	2.4698392614
H	-0.0000000000	0.0000000000	1.4014924307
N	-0.0000000000	0.0000000000	-0.9222763387
C	-0.0000000000	0.0000000000	-2.0787257188
C	0.0000000000	0.0000000000	-3.5408735635
H	1.0240151301	0.0000000000	-3.9081675962
H	-0.5120075650	-0.8868231166	-3.9081675962
H	-0.5120075650	0.8868231166	-3.9081675962

E($CH_3CN\cdots HCCH$) = -209.77545252 au

$H_3CCN\cdots HCP$

P	0.0000000000	0.0000000000	4.0625446102
C	-0.0000000000	0.0000000000	2.5175496415
H	-0.0000000000	0.0000000000	1.4414489354
N	-0.0000000000	0.0000000000	-0.8903990812
C	-0.0000000000	0.0000000000	-2.0469125066
C	0.0000000000	0.0000000000	-3.5090438124
H	1.0240103610	0.0000000000	-3.8763590673
H	-0.5120051804	-0.8868189863	-3.8763590673
H	-0.5120051804	0.8868189863	-3.8763590673

E($CH_3CN\cdots HCP$) = -512.07139725 au

HCN···HX

HCN···HF

F	0.0000000000	0.0000000000	-1.9635857216
H	0.0000000000	0.0000000000	-1.0347148699
N	0.0000000000	0.0000000000	0.8242638477
C	0.0000000000	0.0000000000	1.9760332815
H	0.0000000000	0.0000000000	3.0432928311

E(HCN···HF) = -193.68517740au

HCN···HCl

Cl	0.0000000000	0.0000000000	-1.7097811080
H	0.0000000000	0.0000000000	-0.4257769854
N	0.0000000000	0.0000000000	1.6641462633
C	0.0000000000	0.0000000000	2.8173576452
H	0.0000000000	0.0000000000	3.8845935508

E(HCN···HCl) = -553.66353812 au

HCN···HBr

Br	0.0000000000	0.0000000000	-1.0602471671

H	0.0000000000	0.0000000000	0.3647246916
N	0.0000000000	0.0000000000	2.5256410440
C	0.0000000000	0.0000000000	3.6791627217
H	0.0000000000	0.0000000000	4.7463630487

E(HCN□HBr) = -509.61542595 au

HCN□HI

I	0.0000000000	0.0000000000	-0.8011417304
H	0.0000000000	0.0000000000	0.8169692118
N	0.0000000000	0.0000000000	3.1357423687
C	0.0000000000	0.0000000000	4.2898091308
H	0.0000000000	0.0000000000	5.3569217389

E(HCN□HI) = -388.73831553 au

HCN□HCN

N	0.0000000000	0.0000000000	-3.6841007575
C	0.0000000000	0.0000000000	-2.5284058081
H	0.0000000000	0.0000000000	-1.4555059138
N	0.0000000000	0.0000000000	0.7625672393
C	0.0000000000	0.0000000000	1.9160545306
H	0.0000000000	0.0000000000	2.9833567472

E(HCN□HCN) = -186.60757895 au

HCN□HCCH

H	0.0000000000	0.0000000000	-4.0302052661
C	0.0000000000	0.0000000000	-2.9673069916
C	0.0000000000	0.0000000000	-1.7608886068
H	0.0000000000	0.0000000000	-0.6938001963
N	0.0000000000	0.0000000000	1.6813499701
C	0.0000000000	0.0000000000	2.8355593437
H	0.0000000000	0.0000000000	3.9025380766

E(HCN□HCCH) = -170.51121892 au

HCN□HCP

P	0.0000000000	0.0000000000	-4.1467634618
C	0.0000000000	0.0000000000	-2.6022035951
H	0.0000000000	0.0000000000	-1.5272852262
N	0.0000000000	0.0000000000	0.8598714976
C	0.0000000000	0.0000000000	2.0141419716
H	0.0000000000	0.0000000000	3.0811361228

E(HCN□HCP) = -472.80713698 au

FCN□HX

FCN□HF

N	0.0000000000	0.0000000000	-0.0700935424
C	0.0000000000	0.0000000000	1.0843655073
F	0.0000000000	0.0000000000	2.3440437505
H	0.0000000000	0.0000000000	-1.9472150604
F	0.0000000000	0.0000000000	-2.8746322131

E(FCN···HF) = -292.82075963 au

FCN□HCl

N	0.0000000000	0.0000000000	0.7669179873
C	0.0000000000	0.0000000000	1.9231221206
F	0.0000000000	0.0000000000	3.1849569204
H	0.0000000000	0.0000000000	-1.3405361236
Cl	0.0000000000	0.0000000000	-2.6231741083

E(FCN···HCl) = -652.79955326 au

FCN□HBr

Proton tranfers

FCN□HI

Proton tranfers

FCN□HCN

N	0.0000000000	0.0000000000	0.6173526329
C	0.0000000000	0.0000000000	1.7739442083
F	0.0000000000	0.0000000000	3.0354983852
H	0.0000000000	0.0000000000	-1.6117949444
C	0.0000000000	0.0000000000	-2.6839617072
N	0.0000000000	0.0000000000	-3.8396042703

E(FCN···HCN) = -285.74356858 au

FCN□HCCH

N	0.0000000000	0.0000000000	0.6408803231
C	0.0000000000	0.0000000000	1.7981864945
F	0.0000000000	0.0000000000	3.0621233900
H	0.0000000000	0.0000000000	-1.7422898353
C	0.0000000000	0.0000000000	-2.8088663479
C	0.0000000000	0.0000000000	-4.0151728036
H	0.0000000000	0.0000000000	-5.0780817068

E(FCN···HCCH) = -269.64760049 au

FCN□HCP

N	0.0000000000	0.0000000000	1.5696148454
C	0.0000000000	0.0000000000	2.7270108406
F	0.0000000000	0.0000000000	3.9909680161
H	0.0000000000	0.0000000000	-0.8305401070
C	0.0000000000	0.0000000000	-1.9050710729
P	0.0000000000	0.0000000000	-3.4494717023

E(FCN···HCP) = -571.94351738 au

N_2□HX

N_2□HF

F	0.0000000000	0.0000000000	-2.1005650526
H	0.0000000000	0.0000000000	-1.1803137730
N	0.0000000000	0.0000000000	0.9179185013
N	0.0000000000	0.0000000000	2.0160743965

E(N_2□HF) = -209.78158728 au

N_2□HCl

Cl	0.0000000000	0.0000000000	-1.8549706581
H	0.0000000000	0.0000000000	-0.5789133926

N	0.0000000000	0.0000000000	1.8193710831
N	0.0000000000	0.0000000000	2.9180376946

E(N_2□HCl) = -569.76293294 au

N_2□HBr

Br	0.0000000000	0.0000000000	-1.1629249982
H	0.0000000000	0.0000000000	0.2552232652
N	0.0000000000	0.0000000000	2.7585128364
N	0.0000000000	0.0000000000	3.8572574247

E(N_2□HBr) = -525.71563388 au

N_2□HI

I	0.0000000000	0.0000000000	-0.8855240524
H	0.0000000000	0.0000000000	0.7282246751
N	0.0000000000	0.0000000000	3.4165153286
N	0.0000000000	0.0000000000	4.5154323304

E(N_2□HI) = -404.83974022 au

N_2□HCN

N	0.0000000000	0.0000000000	-1.3722450524
C	0.0000000000	0.0000000000	-0.2169612492
H	0.0000000000	0.0000000000	0.8511397654
N	0.0000000000	0.0000000000	3.3414037302
N	0.0000000000	0.0000000000	4.4400774247

E(N_2□HCN) = -202.70652732 au

N_2□HCCH

H	0.0000000000	0.0000000000	-4.1001357383
C	0.0000000000	0.0000000000	-3.0370556549
C	0.0000000000	0.0000000000	-1.8314597384
H	0.0000000000	0.0000000000	-0.7675774582
N	0.0000000000	0.0000000000	1.8503734208
N	0.0000000000	0.0000000000	2.9492236801

E(N_2□HCCH) = -186.61297970 au

N_2□HCP

P	0.0000000000	0.0000000000	-4.2524717379
C	0.0000000000	0.0000000000	-2.7091182432
H	0.0000000000	0.0000000000	-1.6368264192
N	0.0000000000	0.0000000000	0.9962814555
N	0.0000000000	0.0000000000	2.0951746548

E(N_2□HCP) = -488.90892677

PN□HX

PN□HF

F	0.0000000000	0.0000000000	-1.4160585635
H	0.0000000000	0.0000000000	-0.4834849492
N	0.0000000000	0.0000000000	1.3390678417
P	0.0000000000	0.0000000000	2.8257604504

E(PN□HF) = -495.96002431 au

PN□HCl

Cl	0.0000000000	0.0000000000	-2.7418581565
H	0.0000000000	0.0000000000	-1.4531192391
N	0.0000000000	0.0000000000	0.5655962399
P	0.0000000000	0.0000000000	2.0546659350

E(PN□HCl) = -855.93799719 au

PN□HBr

Br	0.0000000000	0.0000000000	-2.3501742930
H	0.0000000000	0.0000000000	-0.9202416150
N	0.0000000000	0.0000000000	1.1530188006
P	0.0000000000	0.0000000000	2.6426818868

E(PN□HBr) = -811.88982365 au

PN□HI

I	0.0000000000	0.0000000000	-2.5627807765
H	0.0000000000	0.0000000000	-0.9410651943
N	0.0000000000	0.0000000000	1.2792138602
P	0.0000000000	0.0000000000	2.7699168900

E(PN□HI) = -691.01242324 au

PN□HCN

N	0.0000000000	0.0000000000	-1.2524906379
C	0.0000000000	0.0000000000	-0.0966248576
H	0.0000000000	0.0000000000	0.9783783456
N	0.0000000000	0.0000000000	3.1593785691
P	0.0000000000	0.0000000000	4.6490990532

E(PN□HCN) = -488.88169132au

PN□HCCH

H	0.0000000000	0.0000000000	-4.0202130294
C	0.0000000000	0.0000000000	-2.9573008465
C	0.0000000000	0.0000000000	-1.7506728193
H	0.0000000000	0.0000000000	-0.6825090632
N	0.0000000000	0.0000000000	1.6608111049
P	0.0000000000	0.0000000000	3.1519514751

E(PN□HCCH) = -472.78490997 au

PN□HCP

P	0.0000000000	0.0000000000	-3.3032263478
C	0.0000000000	0.0000000000	-1.7583637220
H	0.0000000000	0.0000000000	-0.6823348598
N	0.0000000000	0.0000000000	1.6690848286
P	0.0000000000	0.0000000000	3.1603207985

E(PN□HCP) = -775.08086196

OCO□HX

OCO□HF

F	0.0000000000	0.0000000000	-2.1005809452
H	0.0000000000	0.0000000000	-1.1802895155
O	0.0000000000	0.0000000000	0.8025477134
C	0.0000000000	0.0000000000	1.9661400735

O	0.0000000000	0.0000000000	3.1239105721

E(OCO□HF) = -288.76134746 au

OCO□HCl

Cl	0.0000000000	0.0000000000	-2.7147884738
H	0.0000000000	0.0000000000	-1.4384339318
O	0.0000000000	0.0000000000	0.7847950750
C	0.0000000000	0.0000000000	1.9480992437
O	0.0000000000	0.0000000000	3.1073264458

E(OCO□HCl) = -648.74256446 au

OCO□HBr

Br	0.0000000000	0.0000000000	-2.9506279974
H	0.0000000000	0.0000000000	-1.5321522723
O	0.0000000000	0.0000000000	0.7818619650
C	0.0000000000	0.0000000000	1.9449958667
O	0.0000000000	0.0000000000	3.1047092707

E(OCO□HBr) = -604.69518604 au

OCO□HI

I	0.0000000000	0.0000000000	-3.2809884449
H	0.0000000000	0.0000000000	-1.6671156244
O	0.0000000000	0.0000000000	0.7866996261
C	0.0000000000	0.0000000000	1.9495844625
O	0.0000000000	0.0000000000	3.1098870832

E(OCO□HI) = - -483.81916127 au

OCO□HCN

N	0.0000000000	0.0000000000	-3.7858006664
C	0.0000000000	0.0000000000	-2.6304607765
H	0.0000000000	0.0000000000	-1.5620014526
O	0.0000000000	0.0000000000	0.7078105727
C	0.0000000000	0.0000000000	1.8717241532
O	0.0000000000	0.0000000000	3.0304265285

E(OCO□HCN) = -281.68647853 au

OCO□HCCH

H	0.0000000000	0.0000000000	-4.9607442480
C	0.0000000000	0.0000000000	-3.8976983535
C	0.0000000000	0.0000000000	-2.6919738022
H	0.0000000000	0.0000000000	-1.6277593772
O	0.0000000000	0.0000000000	0.7761330810
C	0.0000000000	0.0000000000	1.9388576718
O	0.0000000000	0.0000000000	3.0991611652

E(OCO□HCCH) = -265.59240156 au

OCO□HCP

P	0.0000000000	0.0000000000	-4.2494771117
C	0.0000000000	0.0000000000	-2.7058942686
H	0.0000000000	0.0000000000	-1.6333426269
O	0.0000000000	0.0000000000	0.7899373635
C	0.0000000000	0.0000000000	1.9527151499

O	0.0000000000	0.0000000000	3.1130605192

E(OCO□HCP) = -567.88834926 au

SCO□HX

SCO□HF

F	0.0000000000	0.0000000000	-2.9036463599
H	0.0000000000	0.0000000000	-1.9829541535
O	0.0000000000	0.0000000000	-0.0112674477
C	0.0000000000	0.0000000000	1.1501098219
S	0.0000000000	0.0000000000	2.7071981391

E(SCO□HF) = -611.34363959 au

SCO□HCl

Cl	0.0000000000	0.0000000000	-3.4853323128
H	0.0000000000	0.0000000000	-2.2086873647
O	0.0000000000	0.0000000000	0.0020080877
C	0.0000000000	0.0000000000	1.1624167190
S	0.0000000000	0.0000000000	2.7220348709

E(SCO□HCl) = -971.32478720 au

SCO□HBr

Br	0.0000000000	0.0000000000	-3.7243917554
H	0.0000000000	0.0000000000	-2.3056646325
O	0.0000000000	0.0000000000	-0.0044755745
C	0.0000000000	0.0000000000	1.1555993857
S	0.0000000000	0.0000000000	2.7160048895

E(SCO□HBr) = -927.27740161 au

SCO□HI

I	0.0000000000	0.0000000000	-4.0551378154
H	0.0000000000	0.0000000000	-2.4410915777
O	0.0000000000	0.0000000000	-0.0022096011
C	0.0000000000	0.0000000000	1.1573574707
S	0.0000000000	0.0000000000	2.7188455916

E(SCO□HI) = -806.40136189

SCO□HCN

N	0.0000000000	0.0000000000	-4.4956032679
C	0.0000000000	0.0000000000	-3.3402328721
H	0.0000000000	0.0000000000	-2.2715300071
O	0.0000000000	0.0000000000	-0.0122131353
C	0.0000000000	0.0000000000	1.1489782685
S	0.0000000000	0.0000000000	2.7077010139

E(SCO□HCN) = -604.26878026 au

SCO□HCCH

H	0.0000000000	0.0000000000	-5.0151384308
C	0.0000000000	0.0000000000	-3.9521101617
C	0.0000000000	0.0000000000	-2.7463522474
H	0.0000000000	0.0000000000	-1.6820348030
O	0.0000000000	0.0000000000	0.7170929005
C	0.0000000000	0.0000000000	1.8764777740

S	0.0000000000	0.0000000000	3.4380411055

E(SCO□HCCH) = -588.17453882 au

SCO□HCP

P	0.0000000000	0.0000000000	-5.0433396370
C	0.0000000000	0.0000000000	-3.4997006984
H	0.0000000000	0.0000000000	-2.4270596393
O	0.0000000000	0.0000000000	-0.0098620407
C	0.0000000000	0.0000000000	1.1495784945
S	0.0000000000	0.0000000000	2.7112596681

E(SCO□HCP) = -890.47051893 au

HB□HX

HB□HF

F	0.0000000000	0.0000000000	-2.3568625499
H	0.0000000000	0.0000000000	-1.4201237381
B	0.0000000000	0.0000000000	0.6362002508
H	0.0000000000	0.0000000000	1.8537166365

E(HB□HF) = -125.61980187 au

HB□HCl

Cl	0.0000000000	0.0000000000	-1.9728969272
H	0.0000000000	0.0000000000	-0.6779899909
B	0.0000000000	0.0000000000	1.5715067465
H	0.0000000000	0.0000000000	2.7936732651

E(HB□HCl) = -485.59782029 au

HB□HBr

Br	0.0000000000	0.0000000000	-3.0760381092
H	0.0000000000	0.0000000000	-1.6368848855
B	0.0000000000	0.0000000000	0.6279907637
H	0.0000000000	0.0000000000	1.8512686605

E(HB□HBr) = - -441.54991866 au

HB□HI

I	0.0000000000	0.0000000000	-3.4002869071
H	0.0000000000	0.0000000000	-1.7710805256
B	0.0000000000	0.0000000000	0.6557469451
H	0.0000000000	0.0000000000	1.8815180968

E(HB□HI) = - -320.67240670 au

HB□HCN

N	0.0000000000	0.0000000000	-4.0740519667
C	0.0000000000	0.0000000000	-2.9181884654
H	0.0000000000	0.0000000000	-1.8430702749
B	0.0000000000	0.0000000000	0.7198849949
H	0.0000000000	0.0000000000	1.9434754661

E(HB□HCN) = -118.54023338 au

HB□HCCH

H	0.0000000000	0.0000000000	-5.3553391268
C	0.0000000000	0.0000000000	-4.2923743037
C	0.0000000000	0.0000000000	-3.0858915319

H	0.0000000000	0.0000000000	-2.0179386208
B	0.0000000000	0.0000000000	0.7260543070
H	0.0000000000	0.0000000000	1.9542754554

E(HB□HCCH) = -102.44425577 au

HB□HCP

P	0.0000000000	0.0000000000	-4.5442489655
C	0.0000000000	0.0000000000	-2.9995678981
H	0.0000000000	0.0000000000	-1.9235451863
B	0.0000000000	0.0000000000	0.8217156745
H	0.0000000000	0.0000000000	2.0500011142

E(HB□HCP) = -404.74021411 au

FB□HX

FB□HF

F	0.0000000000	0.0000000000	-2.3419078412
H	0.0000000000	0.0000000000	-1.4137635638
B	0.0000000000	0.0000000000	0.7386020043
F	0.0000000000	0.0000000000	1.9966525679

E(FB□HF) = -224.91931989 au

FB□HCl

Cl	0.0000000000	0.0000000000	-2.0325327054
H	0.0000000000	0.0000000000	-0.7486571194
B	0.0000000000	0.0000000000	1.6389829182
F	0.0000000000	0.0000000000	2.9000636589

E(FB□HCl) = -584.89892220 au

FB□HBr

Br	0.0000000000	0.0000000000	-3.1552283884
H	0.0000000000	0.0000000000	-1.7293745211
B	0.0000000000	0.0000000000	0.7167393390
F	0.0000000000	0.0000000000	1.9784990017

E(FB□HBr) = - -540.85126520 au

FB□HI

I	0.0000000000	0.0000000000	-3.4874568267
H	0.0000000000	0.0000000000	-1.8685716875
B	0.0000000000	0.0000000000	0.7522261234
F	0.0000000000	0.0000000000	2.0154378221

E(FB□HI) = - -419.97457059 au

FB□HCN

N	0.0000000000	0.0000000000	-4.0987700695
C	0.0000000000	0.0000000000	-2.9431869928
H	0.0000000000	0.0000000000	-1.8716763296
B	0.0000000000	0.0000000000	0.7620831460
F	0.0000000000	0.0000000000	2.0234425040

E(HB□HCN) = -217.84204527 au

FB□HCCH

H	0.0000000000	0.0000000000	-5.3725963617
C	0.0000000000	0.0000000000	-4.3095855543
C	0.0000000000	0.0000000000	-3.1035453488
H	0.0000000000	0.0000000000	-2.0376481290
B	0.0000000000	0.0000000000	0.7642615729
F	0.0000000000	0.0000000000	2.0284060788

E(FB□HCCH) = -102.44425577 au

FB□HCP

P	0.0000000000	0.0000000000	-4.5663794175
C	0.0000000000	0.0000000000	-3.0224862528
H	0.0000000000	0.0000000000	-1.9483544177
B	0.0000000000	0.0000000000	0.8589748268
F	0.0000000000	0.0000000000	2.1231375192

E(FB□HCP) = -504.04316286 au

H_3CB□HX

H_3CB□HF

C	0.0000000000	0.0000000000	-2.1277187379
H	0.5142564297	-0.8907182644	-2.5031520460
H	-1.0285128595	0.0000000000	-2.5031520460
H	0.5142564297	0.8907182644	-2.5031520460
B	0.0000000000	0.0000000000	-0.5990038590
H	-0.0000000000	0.0000000000	1.4244044731
F	-0.0000000000	0.0000000000	2.3655997374

E(H_3CB□HF) = -164.90618891 au

H_3CB□HCl

C	-0.0000561882	0.0000000000	-1.9877346482
H	0.5142854898	-0.8908084615	-2.3632081957
H	-1.0286744329	0.0000000000	-2.3633311150
H	0.5142854898	0.8908084615	-2.3632081957
B	-0.0000439439	0.0000000000	-0.4557146592
H	0.0002388253	0.0000000000	1.7201639491
Cl	-0.0000352401	0.0000000000	3.0235583404

E(H_3CB□HCl) = -524.88370145 au

H_3CB□HBr

C	-0.0000000001	0.0000000000	-1.8964752276
H	0.5143740300	-0.8909219540	-2.2717491065
H	-1.0287480600	0.0000000000	-2.2717491066
H	0.5143740300	0.8909219540	-2.2717491065
B	0.0000000000	0.0000000000	-0.3645341400
H	0.0000000000	0.0000000000	1.7910011160
Br	0.0000000000	0.0000000000	3.2431810469

E(H_3CB□HBr) = -480.83163401 au

H_3CB□HI

C	0.0000000000	0.0000000000	-1.9697264893
H	0.5143995647	-0.8909661815	-2.3453774175
H	-1.0287991295	0.0000000000	-2.3453774174
H	0.5143995647	0.8909661815	-2.3453774175

B	0.0000000001	0.0000000000	-0.4352665569
H	0.0000000001	0.0000000000	1.8495089219
I	-0.0000000001	0.0000000000	3.4910418524

E($H_3CB\square HI$) = -359.95346460 au

$H_3CB\square HCN$

B	0.0082025774	0.0000000000	0.0021406062
C	1.5420933140	0.0000000000	0.0002281945
H	1.9197570345	0.0000000000	1.0281742804
H	1.9178388080	-0.8906026434	-0.5144221203
H	1.9178388080	0.8906026434	-0.5144221203
H	-2.5105171147	0.0000000000	-0.0020071487
C	-3.5881764073	0.0000000000	-0.0006005021
N	-4.7442630200	0.0000000000	0.0009088104

E($H_3CB\square HCN$) = -157.82582407au

$H_3CB\square HCCH$

C	0.0000000000	0.0000000000	-2.0878671089
H	0.5142431289	-0.8906952266	-2.4640345220
H	-1.0284862578	0.0000000000	-2.4640345219
H	0.5142431289	0.8906952266	-2.4640345220
B	0.0000000001	0.0000000000	-0.5490004453
H	0.0000000000	0.0000000000	2.1591300595
C	-0.0000000001	0.0000000000	3.2285275980
C	0.0000000000	0.0000000000	4.4353305856
H	0.0000000001	0.0000000000	5.4982386277

E($H_3CB\square HCCH$) = -141.72883466 au

$H_3CB\square HCP$

B	0.0155766041	0.0000000000	-0.0003094171
C	1.5542194629	0.0000000000	-0.0004274631
H	1.9305126584	0.0000000000	1.0280671431
H	1.9303954792	-0.8906965200	-0.5146917998
H	1.9303954792	0.8906965200	-0.5146917998
H	-2.6869005508	0.0000000000	0.0047253318
C	-3.7643501110	0.0000000000	0.0011953767
P	-5.3095520220	0.0000000000	-0.0038673719

E($H_3CB\square HCP$) = -444.02484476 au

Oxirene□HX

Oxirene□HF

O	0.0000000000	-0.0455850982	0.0586572810
C	0.6341857444	1.3126835802	-0.0368627688
C	-0.6341857444	1.3126835802	-0.0368627688
H	1.6566627257	1.6248774549	-0.0634088556
H	-1.6566627257	1.6248774549	-0.0634088556
H	0.0000000000	-0.7004575036	-1.4403875455
F	0.0000000000	-0.9466794683	-2.3517264868

E(oxirene□HF) = -252.66790085 au

Oxirene□HCl

O	0.0000000000	-0.0605010955	0.0550279629
C	0.6342572804	1.2963999206	-0.0491315015
C	-0.6342572804	1.2963999206	-0.0491315015
H	1.6560979385	1.6107845043	-0.0792459814
H	-1.6560979385	1.6107845043	-0.0792459814
H	0.0000000000	-0.6739436908	-1.5443425853
Cl	0.0000000000	-0.8975240635	-2.8362039250

E(oxirene□HCl) = -612.64576208 au

Oxirene□HBr

O	0.0000000000	-0.0995626710	0.0284140696
C	0.6361838756	1.2654460237	-0.0887266942
C	-0.6361838756	1.2654460237	-0.0887266942
H	1.6586483949	1.5765248238	-0.1229653731
H	-1.6586483949	1.5765248238	-0.1229653731
H	0.0000000000	-0.6067443938	-1.4573083381
Br	0.0000000000	-0.7952346301	-2.9299951101

E(oxirene□HBr) = -568.58598638au

Oxirene□HI

O	0.0000000000	-0.0540432971	0.0812103231
C	0.6344518819	1.2986810312	-0.0477666955
C	-0.6344518819	1.2986810312	-0.0477666955
H	1.6556483468	1.6150181191	-0.0810692426
H	-1.6556483468	1.6150181191	-0.0810692426
H	0.0000000000	-0.7092125593	-1.5480585313
I	0.0000000000	-0.9865078140	-3.1777583187

E(oxirene□HI) = -447.70807635 au

Oxirene□HCN

O	0.0000000000	-0.1326992225	0.0720255439
C	0.6345236957	1.2050640629	-0.1710832241
C	-0.6345236957	1.2050640629	-0.1710832241
H	1.6543769226	1.5245798285	-0.2154446540
H	-1.6543769226	1.5245798285	-0.2154446540
H	0.0000000000	-1.0325241165	-1.6557901190
C	0.0000000000	-1.3019369161	-2.7037267705
N	0.0000000000	-1.5719085027	-3.8280148489

E(oxirene□HCN) = -245.58738797 au

Oxirene□HCCH

O	0.0000000000	-0.0939174903	0.2181179880
C	0.6345849717	1.2011100004	-0.1881672104
C	-0.6345849717	1.2011100004	-0.1881672104
H	1.6534137714	1.5100586835	-0.2873005565
H	-1.6534137714	1.5100586835	-0.2873005565
H	0.0000000000	-1.1226477713	-1.6159227369
C	0.0000000000	-1.3247384669	-2.6688926063
C	0.0000000000	-1.5468235887	-3.8553441027
H	0.0000000000	-1.7462910257	-4.8995849591

E(oxirene□HCCH) = -229.49056285 au

Oxirene□HCP

O	0.0000000000	-0.0887916484	0.2359763993
C	0.6346043971	1.1923481463	-0.2115021470
C	-0.6346043971	1.1923481463	-0.2115021470
H	1.6534261033	1.4988398010	-0.3193336345
H	-1.6534261033	1.4988398010	-0.3193336345
H	0.0000000000	-1.1726030262	-1.5800521340
C	0.0000000000	-1.3841428408	-2.6386194432
P	0.0000000000	-1.6750653610	-4.1563531895

E(oxirene□HCP) = -531.78639217 au

$(CH_3)_2O$□HX

$(CH_3)_2O$□HF

O	0.0000000000	0.0831917191	0.0622398212
C	1.1751910228	-0.0051675218	-0.7272609077
C	-1.1751910228	-0.0051675218	-0.7272609077
H	2.0239751335	0.0567031883	-0.0513606963
H	-2.0239751335	0.0567031883	-0.0513606963
H	1.2071784119	-0.9542893963	-1.2701021376
H	1.2135882624	0.8207277395	-1.4422658837
H	-1.2135882624	0.8207277395	-1.4422658837
H	-1.2071784119	-0.9542893963	-1.2701021376
H	0.0000000000	-0.8864679121	1.3954539481
F	0.0000000000	-1.4794277591	2.1251381504

E[$(CH_3)_2O\cdots HF$] = -255.21202946 au

$(CH_3)_2O$□HCl

O	0.0000000000	0.2096202745	0.0495077200
C	1.1723705824	0.0244516484	-0.7256937352
C	-1.1723705824	0.0244516484	-0.7256937352
H	2.0235540526	0.1662401374	-0.0645403082
H	-2.0235540526	0.1662401374	-0.0645403082
H	1.2033935123	-0.9842289954	-1.1491414991
H	-1.2033935123	-0.9842289954	-1.1491414991
H	1.2128392763	0.7562687850	-1.5371419107
H	-1.2128392763	0.7562687850	-1.5371419107
H	0.0000000000	-0.8996246925	1.4169563244
Cl	0.0000000000	-1.8251787328	2.3339508621

E[$(CH_3)_2O\cdots HCl$] = -615.18959577 au

$(CH_3)_2O$□HBr

O	0.0000000000	0.3158007004	0.0427870720
C	1.1713001479	0.0500479247	-0.7114061828
C	-1.1713001479	0.0500479247	-0.7114061828
H	2.0235794514	0.2818739321	-0.0776148659
H	-2.0235794514	0.2818739321	-0.0776148659
H	1.2127684731	-1.0031632087	-1.0070251446
H	1.1985524583	0.6769094978	-1.6070144247
H	-1.1985524583	0.6769094978	-1.6070144247
H	-1.2127684731	-1.0031632087	-1.0070251446
H	0.0000000000	-0.8816430393	1.3628455706
Br	0.0000000000	-2.0308997296	2.2422021260

$E[(CH_3)_2O\cdots HBr]$ = -571.14148978 au

$(CH_3)_2O$□HI

O	0.0000000000	0.3482730805	0.0100469742
C	1.1692431969	0.0710657606	-0.7394041514
C	-1.1692431969	0.0710657606	-0.7394041514
H	2.0229485306	0.3041507219	-0.1076868706
H	-2.0229485306	0.3041507219	-0.1076868706
H	1.2067668401	-0.9850102308	-1.0274900982
H	1.2026519022	0.6888527940	-1.6417080466
H	-1.2026519022	0.6888527940	-1.6417080466
H	-1.2067668401	-0.9850102308	-1.0274900982
H	0.0000000000	-0.9027241315	1.4264367399
I	0.0000000000	-2.1890728170	2.4378081521

$E[(CH_3)_2O\cdots HI]$ = -450.26337414 au

$(CH_3)_2O$□HCN

O	0.0000000000	-0.3341828217	-0.1766083946
C	1.1693866318	-0.0104170036	-0.9026036058
C	-1.1693866318	-0.0104170036	-0.9026036058
H	2.0237211538	-0.2846671816	-0.2879169536
H	-2.0237211538	-0.2846671816	-0.2879169536
H	1.2081436056	-0.5652971249	-1.8453365771
H	1.2082511330	1.0617580538	-1.1195502188
H	-1.2082511330	1.0617580538	-1.1195502188
H	-1.2081436056	-0.5652971249	-1.8453365771
H	0.0000000000	-1.1390480566	1.6240176029
C	0.0000000000	-1.5827411377	2.6063253534
N	0.0000000000	-2.0586706743	3.6598463834

$E[(CH_3)_2O\cdots HCN]$ = -248.13210504 au

$(CH_3)_2O$□HCCH

O	0.9568799660	-0.1578871176	0.0000000000
C	2.1270626783	-0.9461886407	0.0000000000
C	1.2618857632	1.2206467549	0.0000000000
H	1.8194782994	-1.9892249086	0.0000000000
H	0.3193376077	1.7640985044	0.0000000000
H	2.7337418464	-0.7475684149	-0.8902890149
H	2.7337418464	-0.7475684149	0.8902890149
H	1.8377793345	1.4945839231	0.8906221928
H	1.8377793345	1.4945839231	-0.8906221928
H	-1.1488828077	-0.3966939719	0.0000000000
C	-2.2051013122	-0.2280100716	0.0000000000
C	-3.3955382452	-0.0295795211	0.0000000000
H	-4.4445846715	0.1424700657	0.0000000000

$E[(CH_3)_2O\cdots HCCH]$ = -232.03543192 au

$(CH_3)_2O$□HCP

O	0.0000000000	-0.3061010328	-0.2416547330
C	1.1665202957	0.0183382076	-0.9668809976
C	-1.1665202957	0.0183382076	-0.9668809976
H	2.0208807179	-0.2565896924	-0.3524768656
H	-2.0208807179	-0.2565896924	-0.3524768656

H	1.2073963473	-0.5343985481	-1.9117702341
H	1.2074549336	1.0911799934	-1.1844550921
H	-1.2074549336	1.0911799934	-1.1844550921
H	-1.2073963473	-0.5343985481	-1.9117702341
H	0.0000000000	-1.1763491814	1.6996840239
C	0.0000000000	-1.6171819029	2.6829764282
P	0.0000000000	-2.2493083677	4.0929076170

E[$(CH_3)_2O\cdots HCP$] = -534.33087630 au

$H_2C{=}O\square HX$

$H_2C{=}O\square HF$

C	-1.3971771989	0.4984670407	0.0000000000
H	-0.8380055961	1.4440692824	0.0000000000
H	-2.4934274320	0.5514281849	0.0000000000
O	-0.8263140077	-0.5705997461	0.0000000000
H	0.8822651672	-0.3109822909	0.0000000000
F	1.7364740043	0.0674914382	0.0000000000

E($H_2C{=}O\square HF$) = -214.75382343au

$H_2C{=}O\square HCl$

C	-1.9909703705	0.5383507931	0.0000000000
H	-1.3071858428	1.4001316120	0.0000000000
H	-3.0697793893	0.7460635559	0.0000000000
O	-1.5721730192	-0.5973665256	0.0000000000
H	0.3206570130	-0.4584615197	0.0000000000
Cl	1.5096117178	0.0459525410	0.0000000000

E($H_2C{=}O\square HCl$) = -574.73215810 au

$H_2C{=}O\square HBr$

C	-2.0007444160	0.5398377997	0.0000000000
H	-1.3155667010	1.4012203254	0.0000000000
H	-3.0792263480	0.7511161638	0.0000000000
O	-1.5844200844	-0.5962147258	0.0000000000
H	0.3450863271	-0.4652674544	0.0000000000
Br	1.6854196136	0.0439783480	0.0000000000

E($H_2C{=}O\square HBr$) = -530.68416521 au

$H_2C{=}O\square HI$

C	-1.9772219557	0.5298909844	0.0000000000
H	-1.2536315241	1.3604497606	0.0000000000
H	-3.0449077472	0.7934054762	0.0000000000
O	-1.6139030756	-0.6231117619	0.0000000000
H	0.4559676232	-0.5247807010	0.0000000000
I	1.9395254571	0.1388166984	0.0000000000

E($H_2C{=}O\square HI$) = -409.80682763 au

$H_2C{=}O\square HCN$

C	0.0000000000	-0.3151375263	-2.4458996512
H	0.0000000000	-1.4034843948	-2.2836015769
H	0.0000000000	0.0345040280	-3.4884672306
O	0.0000000000	0.4642106406	-1.5220604116

H	0.0000000000	0.2162841268	0.5494620183
C	0.0000000000	0.0060660417	1.6026926399
N	0.0000000000	-0.2325792028	2.7335410621

E($H_2C{=}O\cdots HCN$) = -207.67490184 au

$H_2C{=}O\cdots HCCH$

C	0.0000000000	-0.2827152801	-2.1062882961
H	0.0000000000	-1.0775972563	-1.3435463642
H	0.0000000000	-0.6007323287	-3.1600669274
O	0.0000000000	0.8858690397	-1.8008869365
H	0.0000000000	0.7200871667	0.4180272296
C	0.0000000000	0.0815244326	1.2745158685
C	0.0000000000	-0.6573154878	2.2283654107
H	0.0000000000	-1.2992565728	3.0755468653

E($H_2C{=}O\cdots HCCH$) = -191.58083148 au

$H_2C{=}O\cdots HCP$

C	0.0000000000	-0.2648111581	-2.1417680718
H	0.0000000000	-1.0720949032	-1.3919023000
H	0.0000000000	-0.5656589433	-3.2006268692
O	0.0000000000	0.8986233451	-1.8168137700
H	0.0000000000	0.7052868412	0.4455775726
C	0.0000000000	0.0281344142	1.2818818872
P	0.0000000000	-0.9596158828	2.4693184011

E($H_2C{=}O\cdots HCP$) = -493.87527645 au

$H_2C{=}C{=}O\cdots HX$

$H_2C{=}C{=}O\cdots HF$

C	-0.0156656717	-0.0767269891	0.0000000000
O	1.1502108165	-0.1458003261	0.0000000000
C	-1.3223993182	0.0117082668	0.0000000000
H	-1.8441860752	0.0416850341	0.9423467170
H	-1.8441860752	0.0416850341	-0.9423467170
H	2.2105245351	-1.7025646867	0.0000000000
F	2.6612564243	-2.5092038533	0.0000000000

E($H_2C{=}C{=}O\cdots HF$) = -252.78142966 au

$H_2C{=}C{=}O\cdots HCl$

C	-0.0652285190	0.0401713719	0.0000000000
O	1.1008621693	0.0511458359	0.0000000000
C	-1.3768470267	0.0325076688	0.0000000000
H	-1.8993453714	0.0251354373	0.9421777542
H	-1.8993453714	0.0251354373	-0.9421777542
H	2.2879078305	-1.6806956643	0.0000000000
Cl	2.8471758768	-2.8317294575	0.0000000000

E($H_2C{=}C{=}O\cdots HCl$) = -612.76176345 au

$H_2C{=}C{=}O\cdots HBr$

C	-0.0699407322	0.0959439758	0.0000000000

O	1.0945496751	0.1618033704	0.0000000000
C	-1.3809392268	0.0239250466	0.0000000000
H	-1.9025620543	-0.0097038560	0.9425474338
H	-1.9025620543	-0.0097038560	-0.9425474338
H	2.3080384378	-1.6434757355	0.0000000000
Br	2.8487948574	-2.9586050407	0.0000000000

E($H_2C{=}C{=}O\cdots HBr$) = -568.71421086 au

$H_2C{=}C{=}O\square HI$

C	-0.0690983275	0.1518021207	0.0000000000
O	1.0892787008	0.2737804405	0.0000000000
C	-1.3748396730	0.0138018755	0.0000000000
H	-1.8941053467	-0.0455049187	0.9420307295
H	-1.8941053467	-0.0455049187	-0.9420307295
H	2.3210417802	-1.6872555543	0.0000000000
I	2.8872071157	-3.2009351403	0.0000000000

E($H_2C{=}C{=}O\cdots HI$) = -447.83786564 au

$H_2C{=}C{=}O\square HCN$

C	-0.3301740110	-0.1029623378	0.0000000000
O	0.7724214888	-0.4810102630	0.0000000000
C	-1.5702516892	0.3250687690	0.0000000000
H	-2.0644663675	0.4957206940	0.9420366412
H	-2.0644663675	0.4957206940	-0.9420366412
H	2.3199227083	-2.0577978592	0.0000000000
C	3.0658653924	-2.8246599974	0.0000000000
N	3.8696735848	-3.6548694813	0.0000000000

E($H_2C{=}C{=}O\cdots HCN$) = -245.70564860 au

$H_2C{=}C{=}O\square HCCH$

C	0.0000000000	0.0000000000	-1.9629564149
O	0.0000000000	0.0000000000	-0.7994517800
C	0.0000000000	0.0000000000	-3.2765736319
H	0.0000000000	0.9420801329	-3.7989134854
H	0.0000000000	-0.9420801329	-3.7989134854
H	0.0000000000	0.0000000000	1.5587600867
C	0.0000000000	0.0000000000	2.6235238870
C	0.0000000000	0.0000000000	3.8294179224
H	0.0000000000	0.0000000000	4.8923927614

E($H_2C{=}C{=}O\cdots HCCH$) = -229.61084736 au

$H_2C{=}C{=}O\square HCP$

C	0.0000000000	0.0000000000	-2.7644529825
O	0.0000000000	0.0000000000	-1.6008863518
C	0.0000000000	0.0000000000	-4.0780735718
H	0.0000000000	0.9420042350	-4.6005850909
H	0.0000000000	-0.9420042350	-4.6005850909
H	0.0000000000	0.0000000000	0.7727965352
C	0.0000000000	0.0000000000	1.8457785608
P	0.0000000000	0.0000000000	3.3896197118

E($H_2C{=}C{=}O\cdots HCP$) = -531.90681301 au

$H_2O\cdots HX$

$H_2O\cdots HF$

H	0.0000000000	0.0407699617	0.3709228947
F	0.0000000000	-0.0067456336	1.3030326093
O	0.0000000000	0.0523281989	-1.3496858648
H	0.7631047937	-0.3676027283	-1.7511262755
H	-0.7631047937	-0.3676027283	-1.7511262755

$E(H_2O\cdots HF)$ = -176.74686032 au

$H_2O\cdots HCl$

H	0.0000000000	0.0420145505	-0.1895332751
Cl	0.0000000000	-0.0033682021	1.0984813580
O	0.0000000000	0.0472535451	-2.1019860286
H	0.7615813642	-0.3370279948	-2.5401910108
H	-0.7615813642	-0.3370279948	-2.5401910108

$E(H_2O\cdots HCl)$ = -536.72441599 au

$H_2O\cdots HBr$

H	0.0000000000	0.0491812422	-0.7869899812
Br	0.0000000000	-0.0014584193	0.6419813900
O	0.0000000000	0.0476639987	-2.7556805117
H	0.7611242987	-0.3448188521	-3.1875975299
H	-0.7611242987	-0.3448188521	-3.1875975299

$E(H_2O\cdots HBr)$ = -492.67614448au

$H_2O\cdots HI$

H	0.0000000000	0.0376880244	-1.1418426539
I	0.0000000000	-0.0007823121	0.4790473015
O	0.0000000000	0.0426964115	-3.2583747229
H	0.7601061163	-0.3084631048	-3.7257872467
H	-0.7601061163	-0.3084631048	-3.7257872467

$E(H_2O\cdots HI)$ = -371.79866491 au

$H_2O\cdots HCN$

N	0.0000000000	0.0593680336	1.1546691136
C	0.0000000000	-0.0053534964	0.0007467906
H	0.0000000000	-0.0651614667	-1.0719959108
O	0.0000000000	-0.1677950296	-3.1245573680
H	0.7604499900	-0.1976439196	-3.7068559209
H	-0.7604499900	-0.1976439196	-3.7068559209

$E(H_2O\cdots HCN)$ = -169.66800457 au

$H_2O\cdots HCCH$

H	0.0000000000	0.1169579480	2.3157978973
C	0.0000000000	0.0623900842	1.2542441023
C	0.0000000000	-0.0020545882	0.0494063768
H	0.0000000000	-0.0579863605	-1.0170990623
O	0.0000000000	-0.1725279659	-3.2133971328
H	0.7595615643	-0.2035044580	-3.7969006988
H	-0.7595615643	-0.2035044580	-3.7969006988

$E(H_2O\cdots HCCH)$ = -153.57154086 au

H_2O□HCP

P	0.0000000000	0.0547876112	1.7830442347
C	0.0000000000	-0.0131912975	0.2398400601
H	0.0000000000	-0.0622438235	-0.8347543193
O	0.0000000000	-0.1641404460	-3.0463481932
H	0.7593875560	-0.1947209213	-3.6302349337
H	-0.7593875560	-0.1947209213	-3.6302349337

E(H_2O□HCP) = -455.86737442 au

H_2S□HX

H_2S□HF

H	0.0000000000	0.0499940268	1.1165547949
F	0.0000000000	-0.0068387636	2.0430272851
S	0.0000000000	0.0565055049	-1.1673964877
H	0.9665407245	-0.8606818436	-1.2849704274
H	-0.9665407245	-0.8606818436	-1.2849704274

E(H_2S□HF) = -499.33178799 au

H_2S□HCl

H	0.0000000000	0.0705336149	0.5562188546
Cl	0.0000000000	-0.0026304987	1.8391613302
S	0.0000000000	0.0550529082	-1.9240131887
H	0.9657405173	-0.8645508751	-2.0242073148
H	-0.9657405173	-0.8645508751	-2.0242073148

E(H_2S□HCl) = -859.31181138 au

H_2S□HBr

H	0.0000000000	0.0454134223	-0.2404282764
Br	0.0000000000	-0.0010738344	1.1861990014
S	0.0000000000	0.0553959963	-2.7667700747
H	0.9652490923	-0.8611454943	-2.8955389900
H	-0.9652490923	-0.8611454943	-2.8955389900

E(H_2S□HBr) = -815.26426121 au

H_2S□HI

H	0.0000000000	0.0440309020	-0.7062623213
I	0.0000000000	-0.0005443137	0.9137681769
S	0.0000000000	0.0551419496	-3.3761294380
H	0.9651474451	-0.8647117228	-3.4781515645
H	-0.9651474451	-0.8647117228	-3.4781515645

E(H_2S□HI) = -694.38763731 au

H_2S□HCN

No convergence

H_2S□HCCH

H	0.0000000000	-0.0440538750	2.7458008245
C	0.0000000000	0.0283400488	1.6851014525
C	0.0000000000	0.1105006243	0.4817389224
H	0.0000000000	0.1825132319	-0.5820801771

S	0.0000000000	0.0090518883	-3.4431502842
H	0.9646732253	-0.9145734131	-3.4985092712
H	-0.9646732253	-0.9145734131	-3.4985092712

E(H_2S□HCCH) = -476.16013995 au

H_2S□HCP

P	0.0000000000	0.0452430699	1.9531502342
C	0.0000000000	0.1034398719	0.4102514178
H	0.0000000000	0.1428735827	-0.6633866383
S	0.0000000000	0.0008847225	-3.5293709848
H	0.9648907882	-0.9176180775	-3.6401259166
H	-0.9648907882	-0.9176180775	-3.6401259166

E(H_2S□HCP) = -778.45610783 au

$(CH_3)_2S$□HX

$(H_3C)_2S$□HF

S	0.0000000000	-0.1056033893	-0.0040382526
C	1.3693346285	-0.0681858977	-1.1757665604
C	-1.3693346285	-0.0681858977	-1.1757665604
H	2.2922035180	-0.1028151803	-0.6002309487
H	-2.2922035180	-0.1028151803	-0.6002309487
H	1.3276915102	-0.9318509040	-1.8380794600
H	1.3440005705	0.8524890974	-1.7567143874
H	-1.3440005705	0.8524890974	-1.7567143874
H	-1.3276915102	-0.9318509040	-1.8380794600
H	0.0000000000	-2.2556577922	0.0683170357
F	0.0000000000	-3.1658421037	-0.1551614103

E[$(H_3C)_2S\cdots HF$] = -577.83023138 au

$(H_3C)_2S$□HCl

S	0.0000000000	0.0124465562	0.0141328733
C	1.3668878495	-0.0578581454	-1.1578713729
C	-1.3668878495	-0.0578581454	-1.1578713729
H	2.2912888714	-0.0293883791	-0.5843758284
H	-2.2912888714	-0.0293883791	-0.5843758284
H	1.3294787525	-0.9839245250	-1.7313029632
H	1.3355523070	0.7993497880	-1.8287272897
H	-1.3355523070	0.7993497880	-1.8287272897
H	-1.3294787525	-0.9839245250	-1.7313029632
H	0.0000000000	-2.2195620155	0.0690727507
Cl	0.0000000000	-3.4644283553	-0.3138462981

E[$(H_3C)_2S\cdots HCl$] = -937.81022652 au

$(H_3C)_2S$□HBr

S	0.0000000000	0.0269381923	0.0118962322
C	1.3666947167	-0.0508223090	-1.1587418437
C	-1.3666947167	-0.0508223090	-1.1587418437
H	2.2910077152	-0.0224581392	-0.5850098175
H	-2.2910077152	-0.0224581392	-0.5850098175
H	1.3269234785	-0.9799850692	-1.7274924291
H	1.3376285543	0.8038424904	-1.8328892495

H	-1.3376285543	0.8038424904	-1.8328892495
H	-1.3269234785	-0.9799850692	-1.7274924291
H	0.0000000000	-2.1732245204	0.0798067046
Br	0.0000000000	-3.5700539558	-0.3186318400

$E[(H_3C)_2S\cdots HBr]$ = -893.76305908 au

$(H_3C)_2S\cdots HI$

S	0.0000000000	0.0675020740	0.0089628531
C	1.3661068818	-0.0292363031	-1.1607516799
C	-1.3661068818	-0.0292363031	-1.1607516799
H	2.2911525800	0.0070675136	-0.5885632353
H	-2.2911525800	0.0070675136	-0.5885632353
H	1.3256791465	-0.9669015470	-1.7159727220
H	1.3368387749	0.8145598791	-1.8485999653
H	-1.3368387749	0.8145598791	-1.8485999653
H	-1.3256791465	-0.9669015470	-1.7159727220
H	0.0000000000	-2.1669271476	0.0941940361
I	0.0000000000	-3.7667403495	-0.3105772671

$E[(H_3C)_2S\cdots HI]$ = -772.88592837 au

$(H_3C)_2S\cdots HCN$

S	0.0000000000	0.1657742260	0.0060484894
C	1.3652821744	-0.0267476760	-1.1540307425
C	-1.3652821744	-0.0267476760	-1.1540307425
H	2.2914963933	0.0703699448	-0.5908531791
H	-2.2914963933	0.0703699448	-0.5908531791
H	1.3378192865	-1.0076501605	-1.6301258130
H	1.3295251286	0.7503748868	-1.9162663860
H	-1.3295251286	0.7503748868	-1.9162663860
H	-1.3378192865	-1.0076501605	-1.6301258130
H	0.0000000000	-2.3259027016	0.2275344474
C	0.0000000000	-3.3187170331	-0.1918128412
N	0.0000000000	-4.3713761010	-0.6698028780

$E[(H_3C)_2S\cdots HCN]$ = -570.75161545 au

$(H_3C)_2S\cdots HCCH$

S	-0.5549217315	1.3461189748	0.0000000000
C	0.5679671056	0.9920891394	1.3632768361
C	0.5679671056	0.9920891394	-1.3632768361
H	0.0223701762	1.1596095782	2.2902085718
H	0.0223701762	1.1596095782	-2.2902085718
H	0.9019679358	-0.0452804942	1.3280544118
H	1.4295144664	1.6584114114	1.3331421726
H	1.4295144664	1.6584114114	-1.3331421726
H	0.9019679358	-0.0452804942	-1.3280544118
H	-0.9496576424	-1.2957821002	0.0000000000
C	-0.4500560745	-2.2409991176	0.0000000000
C	0.1337731180	-3.2969450363	0.0000000000
H	0.6402069624	-4.2318378900	0.0000000000

$E[(H_3C)_2S\cdots HCCH]$ = -554.65688148 au

$(H_3C)_2S\cdots HCP$

S	0.0000000000	0.3343851242	-0.0180387798

C	1.3630820868	-0.0043772973	-1.1457939790
C	-1.3630820868	-0.0043772973	-1.1457939790
H	2.2902111772	0.1565434958	-0.5985376842
H	-2.2902111772	0.1565434958	-0.5985376842
H	1.3283984258	-1.0374140044	-1.4932136409
H	1.3323490894	0.6728719234	-1.9988300920
H	-1.3323490894	0.6728719234	-1.9988300920
H	-1.3283984258	-1.0374140044	-1.4932136409
H	0.0000000000	-2.3206492863	0.3528794728
C	0.0000000000	-3.2680656510	-0.1596284256
P	0.0000000000	-4.6155428318	-0.9147664586

E[$(H_3C)_2S\cdots HCP$] = -856.95285543 au

$H_2C{=}S\square HX$

$H_2C{=}S\square HF$

H	-0.8116507796	0.0000000000	-0.5787570615
H	1.0324952179	0.0000000000	-0.3964232499
C	0.0543664398	0.0000000000	0.0756790561
S	-0.1073033848	0.0000000000	1.6808759062
H	2.1002314066	0.0000000000	1.8068507697
F	2.9928611002	0.0000000000	1.5359717692

E($H_2C{=}S\square HF$) = -537.34223785 au

$H_2C{=}S\square HCl$

H	-0.8806183751	0.0000000000	-0.5993494637
H	0.9668494996	0.0000000000	-0.4678034825
C	0.0019065435	0.0000000000	0.0330939883
S	-0.1144275551	0.0000000000	1.6412653013
H	2.2266200561	0.0000000000	1.6341644169
Cl	3.4386698311	0.0000000000	1.1828264297

E($H_2C{=}S\square HCl$) = -897.32233758 au

$H_2C{=}S\square HBr$

H	-0.8355888892	0.0000000000	-0.5604009295
H	1.0150597271	0.0000000000	-0.4788839505
C	0.0636690750	0.0000000000	0.0480681809
S	-0.0086387707	0.0000000000	1.6583642182
H	2.3320955849	0.0000000000	1.5899023415
Br	3.6724032731	0.0000000000	1.0671473293

E($H_2C{=}S\square HBr$) = -853.27496961au

$H_2C{=}S\square HI$

H	-0.8300676940	0.0000000000	-0.5730687070
H	1.0182689270	0.0000000000	-0.4658537836
C	0.0598468400	0.0000000000	0.0492200139
S	-0.0350971661	0.0000000000	1.6578407962
H	2.3949013265	0.0000000000	1.5904519363
I	3.9111477667	0.0000000000	0.9856069341

E($H_2C{=}S\square HI$) = -732.39815654 au

$H_2C{=}S{\square}HCN$

H	-0.8073720138	0.0000000000	-0.6570488424
H	1.0221708689	0.0000000000	-0.4082040308
C	0.0289112507	0.0000000000	0.0356762018
S	-0.1977776728	0.0000000000	1.6317594344
H	2.3941188481	0.0000000000	1.7528449374
C	3.3235788326	0.0000000000	1.2134782191
N	4.3041005731	0.0000000000	0.6013912703

E($H_2C{=}S{\square}HCN$) = -530.26446902 au

$H_2C{=}S{\square}HCCH$

H	-0.6943874938	0.0000000000	-0.7549106129
H	1.0907661048	0.0000000000	-0.2695221517
C	0.0477367572	0.0000000000	0.0383682036
S	-0.3786683838	0.0000000000	1.5927658147
H	2.3714617016	0.0000000000	1.8918125883
C	3.2740407621	0.0000000000	1.3214474908
C	4.2816745457	0.0000000000	0.6581810986
H	5.1751066929	0.0000000000	0.0817547586

E($H_2C{=}S{\square}HCCH$) = -514.17019887 au

$H_2C{=}S{\square}HCP$

H	-0.7536831364	0.0000000000	-0.6907924073
H	1.0610303896	0.0000000000	-0.3330644595
C	0.0424919633	0.0000000000	0.0483094783
S	-0.2721207652	0.0000000000	1.6289506915
H	2.4908875420	0.0000000000	1.7432084319
C	3.3770363049	0.0000000000	1.1329632594
P	4.6373134964	0.0000000000	0.2403221957

E($H_2C{=}S{\square}HCP$) = -816.46607508 au

Thiirene□HX

Thiirene□HF

S	0.0000000000	-0.7757711018	-1.1168378034
C	0.6401064057	0.8895816326	-1.5812532177
C	-0.6401064057	0.8895816326	-1.5812532177
H	1.5922263473	1.3672819760	-1.7060690835
H	-1.5922263473	1.3672819760	-1.7060690835
H	0.0000000000	-0.3483177041	1.0024845878
F	0.0000000000	0.0170131507	1.8651633767

E(thiirene□HF) = -575.31862909 au

Thiirene□HCl

S	0.0000000000	-0.8368668868	-1.2593142942
C	0.6401916863	0.8676000012	-1.5453306180
C	-0.6401916863	0.8676000012	-1.5453306180
H	1.5915558183	1.3573134728	-1.6189993918
H	-1.5915558183	1.3573134728	-1.6189993918

H	0.0000000000	-0.4061411054	0.9363089163
Cl	0.0000000000	0.1998326063	2.0891022979

E(thiirene□HCl) = -935.29841196 au

Thiirene□HBr

S	0.0000000000	-0.8364754666	-1.2487563892
C	0.6402984810	0.8656880042	-1.5382484968
C	-0.6402984810	0.8656880042	-1.5382484968
H	1.5917953970	1.3551596670	-1.6126819711
H	-1.5917953970	1.3551596670	-1.6126819711
H	0.0000000000	-0.4024118222	0.9146774229
Br	0.0000000000	0.3040435085	2.1842745046

E(thiirene□HBr) = -891.25116724 au

Thiirene□HI

S	0.0000000000	-0.8327435285	-1.1753802537
C	0.6404741071	0.8670699241	-1.4721953969
C	-0.6404741071	0.8670699241	-1.4721953969
H	1.5911278787	1.3579395017	-1.5490305450
H	-1.5911278787	1.3579395017	-1.5490305450
H	0.0000000000	-0.3344429810	1.0133459723
I	0.0000000000	0.5238192201	2.4216141494

E(thiirene□HI) = -770.37400669 au

Thiirene□HCN

S	0.0000000000	-0.8666061223	-1.3862546087
C	0.6405113586	0.8615925142	-1.4675703499
C	-0.6405113586	0.8615925142	-1.4675703499
H	1.5890282992	1.3619576693	-1.4970203702
H	-1.5890282992	1.3619576693	-1.4970203702
H	0.0000000000	-0.4673434092	1.0734231744
C	0.0000000000	0.1548946671	1.9536001349
N	0.0000000000	0.8386060594	2.8858496399

E(thiirene□HCN) = -568.24055657 au

Thiirene□HCCH

S	0.0000000000	-0.8831244125	-1.5160699690
C	0.6405189112	0.8458908131	-1.5031469571
C	-0.6405189112	0.8458908131	-1.5031469571
H	1.5878624529	1.3485903873	-1.4917335395
H	-1.5878624529	1.3485903873	-1.4917335395
H	0.0000000000	-0.4689417982	1.1004546694
C	0.0000000000	0.1734472289	1.9553255159
C	0.0000000000	0.9031624333	2.9164942729
H	0.0000000000	1.5421457099	3.7659934043

E(thiirene□HCCH) = -552.14481947au

Thiirene□HCP

S	0.0000000000	-0.8774904429	-1.4673364751
C	0.6405257130	0.8514766588	-1.4664271412
C	-0.6405257130	0.8514766588	-1.4664271412
H	1.5878596541	1.3543940002	-1.4594011515

H	-1.5878596541	1.3543940002	-1.4594011515
H	0.0000000000	-0.4413433984	1.1469140723
C	0.0000000000	0.2252610223	1.9933919198
P	0.0000000000	1.1892520514	3.2009356491

E(thiirene□HCP) = -854.44083359 au

S_2□HX

S_2□HF

S	0.0000000000	-0.1086675994	0.0942640641
S	0.0000000000	-0.2419116581	1.9942079077
H	0.0000000000	2.1716209513	-0.0749357760
F	0.0000000000	3.0989583061	-0.1045361957

E(S_2□HF) = -895.83267815 au

S_2□HCl

Cl	0.0000000000	-0.3172478163	-2.4373966680
H	0.0000000000	0.2498499819	-1.2840485913
S	0.0000000000	1.0127519832	1.0377476762
S	0.0000000000	-0.7834812485	1.6700309489

E(S_2□HCl) = -1255.81362317 au

S_2□HBr

Br	0.0000000000	-0.0489963915	-1.7881095860
H	0.0000000000	0.3248218679	-0.4099445540
S	0.0000000000	0.9741039857	1.9819087327
S	0.0000000000	-0.8622010938	2.4875331848

E(S_2□HBr) = -1211.76631589 au

S_2□HI

I	0.0000000000	-0.0180703332	-1.4279577451
H	0.0000000000	0.3595600511	0.1476096595
S	0.0000000000	0.9713372221	2.6783840899
S	0.0000000000	-0.9111123967	2.9693628578

E(S_2□HI) = -1090.89008501 au

S_2□HCN

S	0.0000000000	0.9651358546	-1.2313374711
S	0.0000000000	-0.9403439341	-1.2375181951
H	0.0000000000	-0.4999625258	1.3678465180
C	0.0000000000	-0.1878631018	2.3927558474
N	0.0000000000	0.1403276269	3.5007114421

E(S_2□HCN) = -888.75693991 au

S_2□HCCH

S	0.0000000000	0.8258627900	-1.3574652526
S	0.0000000000	-1.0770029290	-1.2651471961
H	0.0000000000	-0.4738801281	1.4631230251
C	0.0000000000	-0.1335480089	2.4731193785
C	0.0000000000	0.2468196284	3.6174940910

H	0.0000000000	0.5840650015	4.6255878353

E(S_2□HCCH) = -872.66240622 au

S_2□HCP

S	0.0000000000	0.9770103640	-1.9183684192
S	0.0000000000	-0.9265336887	-1.9952782272
H	0.0000000000	-0.5091864521	0.7685889421
C	0.0000000000	-0.2700352633	1.8156396197
P	0.0000000000	0.0690371699	3.3218173213

E(S_2□HCP) = -1174.95849367 au

$(CH_3)_3N$□HX

(CH_3)N□HF

N	-0.0000000000	0.0000000000	-0.3629305312
C	1.3860784376	0.0000000000	-0.8263266282
C	-0.6930392188	-1.2003791386	-0.8263266282
C	-0.6930392188	1.2003791386	-0.8263266282
H	1.4432713342	0.0000000000	-1.9233599508
H	-0.7216356671	-1.2499096400	-1.9233599508
H	-0.7216356671	1.2499096400	-1.9233599508
H	1.8950268910	-0.8849921824	-0.4462059992
H	1.8950268910	0.8849921824	-0.4462059992
H	-1.7139391576	-1.1986453373	-0.4462059992
H	-0.1810877334	-2.0836375197	-0.4462059992
H	-0.1810877334	2.0836375197	-0.4462059992
H	-1.7139391576	1.1986453373	-0.4462059992
H	-0.0000000000	0.0000000000	1.2509461171
F	-0.0000000000	0.0000000000	2.2166071207

E[(CH_3)N···HF] = -274.60638179 au

(CH_3)N□HCl

Proton tranfer

(CH_3)N□HBr

Proton tranfer

(CH_3)N□HI

Proton tranfer

(CH_3)N□HCN

N	-0.0000000000	0.0000000000	-0.8902851499
C	1.3812125679	0.0000000000	-1.3554900451
C	-0.6906062839	-1.1961651718	-1.3554900451
C	-0.6906062839	1.1961651718	-1.3554900451
H	1.4444629411	0.0000000000	-2.4544125307
H	-0.7222314705	-1.2509416018	-2.4544125307
H	-0.7222314705	1.2509416018	-2.4544125307
H	1.8948363668	-0.8854698384	-0.9800666470
H	1.8948363668	0.8854698384	-0.9800666470

H	-1.7142575577	-1.1982415105	-0.9800666470
H	-0.1805788091	-2.0837113489	-0.9800666470
H	-0.1805788091	2.0837113489	-0.9800666470
H	-1.7142575577	1.1982415105	-0.9800666470
H	-0.0000000000	0.0000000000	1.1129965903
C	-0.0000000000	0.0000000000	2.2037319880
N	-0.0000000000	0.0000000000	3.3605533830

E[(CH_3)N···HCN] = -267.52197046 au

(CH_3)N□HCCH

N	-0.0000000000	0.0000000000	-0.9221009098
C	1.3792906640	0.0000000000	-1.3849383805
C	-0.6896453320	-1.1945007542	-1.3849383805
C	-0.6896453320	1.1945007542	-1.3849383805
H	1.4470379437	0.0000000000	-2.4851034269
H	-0.7235189719	-1.2531716195	-2.4851034269
H	-0.7235189719	1.2531716195	-2.4851034269
H	1.8927434775	-0.8850750086	-1.0081227510
H	1.8927434775	0.8850750086	-1.0081227510
H	-1.7128691805	-1.1966264300	-1.0081227510
H	-0.1798742970	-2.0817014387	-1.0081227510
H	-0.1798742970	2.0817014387	-1.0081227510
H	-1.7128691805	1.1966264300	-1.0081227510
H	-0.0000000000	0.0000000000	1.2559517413
C	-0.0000000000	0.0000000000	2.3320199560
C	-0.0000000000	0.0000000000	3.5396832913
H	-0.0000000000	0.0000000000	4.6028460968

E[(CH_3)N···HCCH] = -251.42446667 au

(CH_3)N□HCP

N	-0.0000000000	0.0000000000	-1.6340152459
C	1.3793416060	0.0000000000	-2.0966569856
C	-0.6896708030	-1.1945448713	-2.0966569856
C	-0.6896708030	1.1945448713	-2.0966569856
H	1.4473191948	0.0000000000	-3.1967593236
H	-0.7236595974	-1.2534151901	-3.1967593236
H	-0.7236595974	1.2534151901	-3.1967593236
H	1.8927557203	-0.8850990359	-1.7198318960
H	1.8927557203	0.8850990359	-1.7198318960
H	-1.7128961101	-1.1966250190	-1.7198318960
H	-0.1798596102	-2.0817240549	-1.7198318960
H	-0.1798596102	2.0817240549	-1.7198318960
H	-1.7128961101	1.1966250190	-1.7198318960
H	-0.0000000000	0.0000000000	0.5459727095
C	-0.0000000000	0.0000000000	1.6298956052
P	0.0000000000	0.0000000000	3.1761196446

E[(CH_3)N···HCP] = -553.72037504 au

Aza-tetrahedrane□HX

Azatetrahedrane□HF

N	-0.0000000000	0.0000000000	0.0683615403

C	0.8356939033	0.0000000000	1.2930551772
C	-0.4178469517	-0.7237321501	1.2930551772
C	-0.4178469517	0.7237321501	1.2930551772
H	1.8921492950	0.0000000000	1.4567247616
H	-0.9460746475	-1.6386493572	1.4567247616
H	-0.9460746475	1.6386493572	1.4567247616
H	0.0000000000	0.0000000000	-1.7090224306
F	0.0000000000	0.0000000000	-2.6440358269

E(Azatetrahedrane···HF) = -270.82516549 au

Azatetrahedrane□HCl

N	-0.0000000000	0.0000000000	0.7565956071
C	0.8352725389	0.0000000000	1.9853159296
C	-0.4176362695	-0.7233672378	1.9853159296
C	-0.4176362695	0.7233672378	1.9853159296
H	1.8914482008	0.0000000000	2.1507913801
H	-0.9457241004	-1.6380421919	2.1507913801
H	-0.9457241004	1.6380421919	2.1507913801
H	0.0000000000	0.0000000000	-1.1734916887
Cl	0.0000000000	0.0000000000	-2.4667896471

E(Azatetrahedrane···HCl) = -630.80304413 au

Azatetrahedrane□HBr

N	-0.0000000000	0.0000000000	1.6792348388
C	0.8352603338	0.0000000000	2.9086952852
C	-0.4176301669	-0.7233566678	2.9086952852
C	-0.4176301669	0.7233566678	2.9086952852
H	1.8914518695	0.0000000000	3.0740855035
H	-0.9457259348	-1.6380453690	3.0740855035
H	-0.9457259348	1.6380453690	3.0740855035
H	0.0000000000	0.0000000000	-0.2834818051
Br	0.0000000000	0.0000000000	-1.7188038697

E(Azatetrahedrane···HBr) = -586.75486057 au

Azatetrahedrane□HI

N	-0.0000000000	0.0000000000	2.3445047288
C	0.8349931504	0.0000000000	3.5759205404
C	-0.4174965752	-0.7231252803	3.5759205404
C	-0.4174965752	0.7231252803	3.5759205404
H	1.8909036354	0.0000000000	3.7428965846
H	-0.9454518177	-1.6375705844	3.7428965846
H	-0.9454518177	1.6375705844	3.7428965846
H	-0.0000000000	0.0000000000	0.2612198558
I	0.0000000000	0.0000000000	-1.3653560740

E(Azatetrahedrane···HI) = -465.87697759 au

Azatetrahedrane□HCN

N	-0.0000000000	0.0000000000	0.6545612818
C	0.8347484940	0.0000000000	1.8864707490
C	-0.4173742470	-0.7229134016	1.8864707490
C	-0.4173742470	0.7229134016	1.8864707490
H	1.8905436157	0.0000000000	2.0545205625
H	-0.9452718078	-1.6372587981	2.0545205625

H	-0.9452718078	1.6372587981	2.0545205625
H	-0.0000000000	0.0000000000	-1.4484370728
C	0.0000000000	0.0000000000	-2.5253827311
N	0.0000000000	0.0000000000	-3.6813549749

E(Azatetrahedrane···HCN) = -263.74642556 au

Azatetrahedrane□HCCH

N	-0.0000000000	0.0000000000	0.6791776776
C	0.8347349419	0.0000000000	1.9116888614
C	-0.4173674709	-0.7229016651	1.9116888614
C	-0.4173674709	0.7229016651	1.9116888614
H	1.8904258744	0.0000000000	2.0792711568
H	-0.9452129372	-1.6371568312	2.0792711568
H	-0.9452129372	1.6371568312	2.0792711568
H	0.0000000000	0.0000000000	-1.5797865936
C	0.0000000000	0.0000000000	-2.6491793084
C	0.0000000000	0.0000000000	-3.8560171359
H	0.0000000000	0.0000000000	-4.9189632697

E(Azatetrahedrane···HCCH) = -247.64929357 au

Azatetrahedrane□HCP

N	-0.0000000000	0.0000000000	1.4944146178
C	0.8347081109	0.0000000000	2.7272247642
C	-0.4173540554	-0.7228784288	2.7272247642
C	-0.4173540554	0.7228784288	2.7272247642
H	1.8903615895	0.0000000000	2.8951376180
H	-0.9451807948	-1.6371011589	2.8951376180
H	-0.9451807948	1.6371011589	2.8951376180
H	0.0000000000	0.0000000000	-0.7681500407
C	0.0000000000	0.0000000000	-1.8453438497
P	0.0000000000	0.0000000000	-3.3905346996

E(Azatetrahedrane···HCP) = -549.94524573 au

H_3N□HX

H_3N□HF

F	-0.0000000000	0.0000000000	-1.2755099300
H	-0.0000000000	0.0000000000	-0.3268906373
N	0.0000000000	0.0000000000	1.3758104940
H	0.9404250901	0.0000000000	1.7499629552
H	-0.4702125451	0.8144320184	1.7499629552
H	-0.4702125451	-0.8144320184	1.7499629552

E(H_3N···HF) = -156.88546362 au

H_3N□HCl

Cl	-0.0000000000	0.0000000000	-1.0439618345
H	-0.0000000000	0.0000000000	0.2699577364
N	0.0000000000	0.0000000000	2.0908955228
H	0.9407284038	0.0000000000	2.4647404270
H	-0.4703642019	0.8146946957	2.4647404270
H	-0.4703642019	-0.8146946957	2.4647404270

E($H_3N\cdots HCl$) = -516.86143489 au

$H_3N\square HBr$

Br	-0.0000000000	0.0000000000	-0.5940083940
H	-0.0000000000	0.0000000000	0.8709023696
N	0.0000000000	0.0000000000	2.6695900883
H	0.9419630530	0.0000000000	3.0404196978
H	-0.4709815265	0.8157639333	3.0404196978
H	-0.4709815265	-0.8157639333	3.0404196978

E($H_3N\cdots HBr$) = -472.81309990 au

$H_3N\square HI$

Proton tranfer

$H_3N\square HCN$

C	-0.0000000000	0.0000000000	-0.9209155486
H	-0.0000000000	0.0000000000	0.1607289486
N	0.0000000000	0.0000000000	2.2798593116
H	0.9365080982	0.0000000000	2.6654912619
H	-0.4682540491	0.8110398039	2.6654912619
H	-0.4682540491	-0.8110398039	2.6654912619
N	0.0000000000	0.0000000000	-2.0771601941

E($H_3N\cdots HCN$) = -149.80274841 au

$H_3N\square HCCH$

C	-0.0000000000	0.0000000000	-0.9907347424
H	-0.0000000000	0.0000000000	0.0811340771
N	0.0000000000	0.0000000000	2.3689334568
H	0.9369848738	0.0000000000	2.7524841518
H	-0.4684924369	0.8114527037	2.7524841518
H	-0.4684924369	-0.8114527037	2.7524841518
C	0.0000000000	0.0000000000	-2.1979218978
H	0.0000000000	0.0000000000	-3.2608887965

E($H_3N\cdots HCCH$) = -133.70539742 au

$H_3N\square HCP$

C	-0.0000000000	0.0000000000	-0.1945114490
H	-0.0000000000	0.0000000000	0.8850080699
N	0.0000000000	0.0000000000	3.1813286670
H	0.9369419905	0.0000000000	3.5651243113
H	-0.4684709952	0.8114155656	3.5651243113
H	-0.4684709952	-0.8114155656	3.5651243113
P	0.0000000000	0.0000000000	-1.7400524978

E($H_3N\cdots HCP$) = -436.00122192 au

$\underline{Cl_3N\square HX}$

$Cl_3N\square HF$

N	-0.0000000000	0.0000000000	0.0707348031
Cl	1.6349541772	0.0000000000	-0.5417920114
Cl	-0.8174770886	-1.4159118514	-0.5417920114

Cl	-0.8174770886	1.4159118514	-0.5417920114
H	-0.0000000000	0.0000000000	1.9490297880
F	-0.0000000000	0.0000000000	2.8775676721

$E(Cl_3N\cdots HF)$ = -1534.19488501 au

Cl_3N□HCl

N	-0.0000000000	0.0000000000	-0.3492960626
Cl	1.6350976242	0.0000000000	-0.9665536877
Cl	-0.8175488121	-1.4160360802	-0.9665536877
Cl	-0.8175488121	1.4160360802	-0.9665536877
H	-0.0000000000	0.0000000000	1.7045570391
Cl	-0.0000000000	0.0000000000	2.9891991540

$E(Cl_3N\cdots HCl)$ = -1894.17544743 au

Cl_3N□HBr

N	-0.0000000000	0.0000000000	-1.0803823668
Cl	1.6352149510	0.0000000000	-1.6986580923
Cl	-0.8176074755	-1.4161376882	-1.6986580923
Cl	-0.8176074755	1.4161376882	-1.6986580923
H	-0.0000000000	0.0000000000	1.0108954850
Br	-0.0000000000	0.0000000000	2.4376908007

$E(Cl_3N\cdots HBr)$ = -1850.12807591 au

Cl_3N□HI

N	-0.0000000000	0.0000000000	-1.6996560604
Cl	1.6350010768	0.0000000000	-2.3215401455
Cl	-0.8175005384	-1.4159524677	-2.3215401455
Cl	-0.8175005384	1.4159524677	-2.3215401455
H	-0.0000000000	0.0000000000	0.5094168534
I	-0.0000000000	0.0000000000	2.1292222337

$E(Cl_3N\cdots HI)$ = -1729.25168030 au

Cl_3N□HCN

N	-0.0000000000	0.0000000000	-0.2611451898
Cl	1.6348986707	0.0000000000	-0.8830854495
Cl	-0.8174493353	-1.4158637814	-0.8830854495
Cl	-0.8174493353	1.4158637814	-0.8830854495
H	-0.0000000000	0.0000000000	1.9797250766
C	-0.0000000000	0.0000000000	3.0517977752
N	-0.0000000000	0.0000000000	4.2073636532

$E(Cl_3N\cdots HCN)$ = -1527.11835123 au

Cl_3N□HCCH

N	-0.0000000000	0.0000000000	-0.2610286405
Cl	1.6343606938	0.0000000000	-0.8886281980
Cl	-0.8171803469	-1.4153978798	-0.8886281980
Cl	-0.8171803469	1.4153978798	-0.8886281980
H	-0.0000000000	0.0000000000	2.1012755967
C	-0.0000000000	0.0000000000	3.1673931607
C	-0.0000000000	0.0000000000	4.3733729754
H	-0.0000000000	0.0000000000	5.4364888638

$E(Cl_3N\cdots HCCH)$ = -1511.02403895 au

Cl_3N□HCP

N	-0.0000000000	0.0000000000	-0.7988884766
Cl	1.6344486152	0.0000000000	-1.4265337079
Cl	-0.8172243076	-1.4154740220	-1.4265337079
Cl	-0.8172243076	1.4154740220	-1.4265337079
H	-0.0000000000	0.0000000000	1.5665116358
C	-0.0000000000	0.0000000000	2.6408458363
P	-0.0000000000	0.0000000000	4.1847144416

E(Cl_3N···HCP) = -1813.32009340 au

H_3P□HX

H_3P□HF

H	-0.0000000000	0.0000000000	1.1965328889
F	-0.0000000000	0.0000000000	2.1248138765
P	0.0000000000	0.0000000000	-1.1575390879
H	1.2047956360	0.0000000000	-1.8882984700
H	-0.6023978179	-1.0433836271	-1.8882984700
H	-0.6023978179	1.0433836271	-1.8882984700

E(H_3P□HF) = -443.08513383 au

H_3P□HCl

H	0.0000000000	0.0000000000	0.6253277561
Cl	0.0000000000	0.0000000000	1.9098488264
P	-0.0000000000	0.0000000000	-1.9437307194
H	1.1997267311	0.0000000000	-2.6861041897
H	-0.5998633656	-1.0389938268	-2.6861041897
H	-0.5998633656	1.0389938268	-2.6861041897

E(H_3P□HCl) = -803.06521136 au

H_3P□HBr

H	0.0000000000	0.0000000000	-0.1980265017
Br	0.0000000000	0.0000000000	1.2286725401
P	0.0000000000	0.0000000000	-2.8156413932
H	1.1988955113	0.0000000000	-3.5601494300
H	-0.5994477557	-1.0382739693	-3.5601494300
H	-0.5994477557	1.0382739693	-3.5601494300

E(H_3P□HBr) = -759.01769308 au

H_3P□HI

H	0.0000000000	0.0000000000	-0.6721024854
I	0.0000000000	0.0000000000	0.9475352584
P	0.0000000000	0.0000000000	-3.4502834965
H	1.1963043086	0.0000000000	-4.2005308017
H	-0.5981521543	-1.0360299219	-4.2005308017
H	-0.5981521543	1.0360299219	-4.2005308017

E(H_3P□HI) = -638.14114320 au

H_3P□HCN

P	-0.0000000000	0.0000000000	-1.9337058547

H	1.1978234865	0.0000000000	-2.6799233303
H	-0.5989117433	-1.0373455686	-2.6799233303
H	-0.5989117433	1.0373455686	-2.6799233303
H	-0.0000000000	0.0000000000	0.8855404657
C	0.0000000000	0.0000000000	1.9571163088
N	0.0000000000	0.0000000000	3.1126711628

E(H_3P□HCN) = -436.00824429 au

H_3P□HCCH

P	-0.0000000000	0.0000000000	-1.9811141630
H	1.1938912948	0.0000000000	-2.7360165704
H	-0.5969456474	-1.0339401906	-2.7360165704
H	-0.5969456474	1.0339401906	-2.7360165704
H	0.0000000000	0.0000000000	1.0056931972
C	0.0000000000	0.0000000000	2.0715226013
C	0.0000000000	0.0000000000	3.2774997979
H	0.0000000000	0.0000000000	4.3405260300

E(H_3P□HCCH) = -419.91364944 au

H_3P□HCP

CCSD(T)-F12C/CC-PVDZ-F12 ENERGY=-722.20992033

P	-0.0000000000	0.0000000000	-2.8604114618
H	1.1938714012	0.0000000000	-3.6154492908
H	-0.5969357006	-1.0339229622	-3.6154492908
H	-0.5969357006	1.0339229622	-3.6154492908
H	0.0000000000	0.0000000000	0.1258696523
C	0.0000000000	0.0000000000	1.1999975848
P	0.0000000000	0.0000000000	2.7439395781

E(H_3P□HCP) = -722.20965532 au

$(CH_3)_3P$□HX

$(CH_3)_3P$□HF

P	-0.0000000000	0.0000000000	-0.2415322601
C	1.6286930840	0.0000000000	-1.0822145636
C	-0.8143465420	-1.4104895857	-1.0822145636
C	-0.8143465420	1.4104895857	-1.0822145636
H	1.5160366340	0.0000000000	-2.1686499739
H	-0.7580183170	-1.3129262381	-2.1686499739
H	-0.7580183170	1.3129262381	-2.1686499739
H	2.1953090172	-0.8822072899	-0.7827191135
H	2.1953090172	0.8822072899	-0.7827191135
H	-1.8616684331	-1.4600897331	-0.7827191135
H	-0.3336405841	-2.3422970230	-0.7827191135
H	-0.3336405841	2.3422970230	-0.7827191135
H	-1.8616684331	1.4600897331	-0.7827191135
H	-0.0000000000	0.0000000000	1.9957895232
F	-0.0000000000	0.0000000000	2.9347821561

E[$(CH_3)_3P$□HF] = -560.86213184 au

$(CH_3)_3P\cdot HCl$

P	-0.0000000000	0.0000000000	-0.8237598225
C	1.6265094516	0.0000000000	-1.6726662432
C	-0.8132547258	-1.4085985046	-1.6726662432
C	-0.8132547258	1.4085985046	-1.6726662432
H	1.5104686607	0.0000000000	-2.7589922603
H	-0.7552343303	-1.3081042317	-2.7589922603
H	-0.7552343303	1.3081042317	-2.7589922603
H	2.1947300043	-0.8821607339	-1.3756305620
H	2.1947300043	0.8821607339	-1.3756305620
H	-1.8613386080	-1.4596115712	-1.3756305620
H	-0.3333913963	-2.3417723051	-1.3756305620
H	-0.3333913963	2.3417723051	-1.3756305620
H	-1.8613386080	1.4596115712	-1.3756305620
H	-0.0000000000	0.0000000000	1.5437191908
Cl	-0.0000000000	0.0000000000	2.8458003512

$E[(CH_3)_3P\cdot HCl]$ = -920.84071723 au

$(CH_3)_3P\cdot HBr$

P	-0.0000000000	0.0000000000	-1.6947232072
C	1.6273199557	0.0000000000	-2.5415432962
C	-0.8136599778	-1.4093004217	-2.5415432962
C	-0.8136599778	1.4093004217	-2.5415432962
H	1.5123064895	0.0000000000	-3.6280159720
H	-0.7561532448	-1.3096958382	-3.6280159720
H	-0.7561532448	1.3096958382	-3.6280159720
H	2.1950169514	-0.8822449279	-2.2438465489
H	2.1950169514	0.8822449279	-2.2438465489
H	-1.8615549957	-1.4598179777	-2.2438465489
H	-0.3334619558	-2.3420629057	-2.2438465489
H	-0.3334619558	2.3420629057	-2.2438465489
H	-1.8615549957	1.4598179777	-2.2438465489
H	-0.0000000000	0.0000000000	0.6508769258
Br	0.0000000000	0.0000000000	2.1019695883

$E[(CH_3)_3P\cdot HBr]$ = -876.79310152 au

$(CH_3)_3P\cdot HI$

P	-0.0000000000	0.0000000000	-2.3624377170
C	1.6253996932	0.0000000000	-3.2157962643
C	-0.8126998466	-1.4076374256	-3.2157962643
C	-0.8126998466	1.4076374256	-3.2157962643
H	1.5071921905	0.0000000000	-4.3020595184
H	-0.7535960952	-1.3052667253	-4.3020595184
H	-0.7535960952	1.3052667253	-4.3020595184
H	2.1943918012	-0.8822133725	-2.9202535314
H	2.1943918012	0.8822133725	-2.9202535314
H	-1.8612150928	-1.4592923594	-2.9202535314
H	-0.3331767084	-2.3415057319	-2.9202535314
H	-0.3331767084	2.3415057319	-2.9202535314
H	-1.8612150928	1.4592923594	-2.9202535314
H	-0.0000000000	0.0000000000	0.0879942361
I	-0.0000000000	0.0000000000	1.7306510867

$E[(CH_3)_3P\cdot HI]$ = -755.91550883 au

$(CH_3)_3P\square HCN$

P	-0.0000000000	0.0000000000	-0.7456630321
C	1.6222499077	0.0000000000	-1.6077869049
C	-0.8111249538	-1.4049096313	-1.6077869049
C	-0.8111249538	1.4049096313	-1.6077869049
H	1.4981803507	0.0000000000	-2.6933018276
H	-0.7490901754	-1.2974622432	-2.6933018276
H	-0.7490901754	1.2974622432	-2.6933018276
H	2.1936330239	-0.8821761627	-1.3164910724
H	2.1936330239	0.8821761627	-1.3164910724
H	-1.8608034795	-1.4586538439	-1.3164910724
H	-0.3328295444	-2.3408300066	-1.3164910724
H	-0.3328295444	2.3408300066	-1.3164910724
H	-1.8608034795	1.4586538439	-1.3164910724
H	-0.0000000000	0.0000000000	1.9581742012
C	-0.0000000000	0.0000000000	3.0352176288
N	0.0000000000	0.0000000000	4.1912353589

$E[(CH_3)_3P\square HCN]$ = -553.78261594 au

$(CH_3)_3P\square HCCH$

P	-0.0000000000	0.0000000000	-0.7608179464
C	1.6190604013	0.0000000000	-1.6331550291
C	-0.8095302006	-1.4021474378	-1.6331550291
C	-0.8095302006	1.4021474378	-1.6331550291
H	1.4915053199	0.0000000000	-2.7185755932
H	-0.7457526599	-1.2916814969	-2.7185755932
H	-0.7457526599	1.2916814969	-2.7185755932
H	2.1919214717	-0.8819585012	-1.3436801668
H	2.1919214717	0.8819585012	-1.3436801668
H	-1.8597592030	-1.4572804270	-1.3436801668
H	-0.3321622687	-2.3392389282	-1.3436801668
H	-0.3321622687	2.3392389282	-1.3436801668
H	-1.8597592030	1.4572804270	-1.3436801668
H	-0.0000000000	0.0000000000	2.1209457888
C	0.0000000000	0.0000000000	3.1898329521
C	0.0000000000	0.0000000000	4.3964484564
H	0.0000000000	0.0000000000	5.4594844115

$E[(CH_3)_3P\square HCCH]$ = -537.68646021 au

$(CH_3)_3P\square HCP$

P	-0.0000000000	0.0000000000	-1.4967150889
C	1.6190313621	0.0000000000	-2.3690417116
C	-0.8095156810	-1.4021222891	-2.3690417116
C	-0.8095156810	1.4021222891	-2.3690417116
H	1.4912235090	0.0000000000	-3.4544442193
H	-0.7456117545	-1.2914374415	-3.4544442193
H	-0.7456117545	1.2914374415	-3.4544442193
H	2.1919532411	-0.8819776751	-2.0797940888
H	2.1919532411	0.8819776751	-2.0797940888
H	-1.8597916928	-1.4572983531	-2.0797940888
H	-0.3321615483	-2.3392760282	-2.0797940888
H	-0.3321615483	2.3392760282	-2.0797940888

H	-1.8597916928	1.4572983531	-2.0797940888
H	-0.0000000000	0.0000000000	1.3774471479
C	-0.0000000000	0.0000000000	2.4544886598
P	-0.0000000000	0.0000000000	3.9994107922

E[$(CH_3)_3$P□HCP] = -839.98250356 au

Table S2. Energies (au) of monomers B and HX optimised at the CCSD(T)(F12c)/cc-pVDZ-F12 level

CO	-113.186968	FH	-100.37353
SC	-435.715480	ClH	-460.35645
SeC	-410.001593	BrH	-416.30951
H_3CNC	-132.524823	IH	-295.43406
HNC	-93.276342	NCH	-93.300098
FNC	-192.322881	HCCH	-77.207269
H_3CCN	-132.563405	HCP	-379.50326
HCN	-93.300098		
FCN	-192.436792		
N2	-77.207269		
PN	-395.573259		
OCO	-188.383340		
SCO	-510.965386		
HB	-25.233554		
FB	-124.537593		
H_3CB	-64.517248		
Oxirene	-152.277363		
$(CH_3)_2O$	-154.822753		
$H_2C=O$	-114.367526		
$H_2C=C=O$	-152.401232		
H_2O	-76.359838		
H_2S	-398.950517		
$(H_3C)_2S$	-477.444678		
$H_2C=S$	-436.958865		
Thiirene	-474.932964		
S_2	-795.452733		
$(CH_3)_3N$	-174.210473		
Azatetrahedrane	-170.436873		
H_3N	-56.492524		
Cl_3N	-1433.814294		
H_3P	-342.704240		
$(CH_3)_3P$	-460.475311		