SUPPLEMENTARY MATERIAL FILE 1: OPTIMISED GEOMETRIES

Energy (hartree) and optimized geometry (Å) at CCSD(T)/aug-cc-pVTZ computational level

N2···HF	CCSD(T)/aug-cc-pVTZ ENERGY=-209.73470476			
	F	0.0000000000	0.0000000000	-2.0858290437
	H	0.0000000000	0.0000000000	-1.1619279845
	N	0.0000000000	0.0000000000	0.9049135789
	N	0.0000000000	0.0000000000	2.0078763327
OC···HF	CCSD(T)/aug-cc-pVTZ ENERGY=-213.51811032			
	F	0.0000000000	0.0000000000	-2.1516496576
	H	0.0000000000	0.0000000000	-1.2247241088
	C	0.0000000000	0.0000000000	0.8566010138
	O	0.0000000000	0.0000000000	1.9890571491
C2H2···HF	CCSD(T)/aug-cc-pVTZ ENERGY=-177.54936116			
	F	0.0000000000	0.0000000000	-1.7591424757
	H	0.0000000000	0.0000000000	-0.8303906444
	C	0.0000000000	0.6057301677	1.3152329876
	C	0.0000000000	-0.6057301677	1.3152329876
	H	0.0000000000	1.6711494620	1.3211871766
	H	0.0000000000	-1.6711494620	1.3211871766
C2H4···HF	CCSD(T)/aug-cc-pVTZ ENERGY=-178.80121683			
	F	0.0000000000	0.0000000000	-1.8200456855
	H	0.0000000000	0.0000000000	-0.8905394907
	C	0.0000000000	0.6705591552	1.2640713743
	C	0.0000000000	-0.6705591552	1.2640713743
	H	-0.9253471086	1.2353829484	1.2674487646
	H	0.9253471086	1.2353829484	1.2674487646
	H	0.9253471086	-1.2353829484	1.2674487646
	H	-0.9253471086	-1.2353829484	1.2674487646
H2S···HF	CCSD(T)/aug-cc-pVTZ ENERGY=-499.29901207			
	F	0.0000000000	0.0044583416	-2.0495856850
	H	0.0000000000	-0.0131693414	-1.1180992170
	S	0.0000000000	-0.0564233089	1.1675378331
	H	-0.9699718963	0.8619083562	1.3069075652
	H	0.9699718963	0.8619083562	1.3069075652
H3P···HF	CCSD(T)/aug-cc-pVTZ ENERGY=-443.05387172			
	F	-0.0000000000	0.0000000000	-2.1312471905
	H	-0.0000000000	0.0000000000	-1.1997498823
	P	0.0000000000	0.0000000000	1.1611335654
	H	1.2084830291	0.0000000000	1.8965733846
	H	-0.6042415146	1.0465770033	1.8965733846
	H	-0.6042415146	-1.0465770033	1.8965733846
HCN···HF	CCSD(T)/aug-cc-pVTZ ENERGY=-193.64314061			
	F	0.0000000000	0.0000000000	-1.9617298337
	H	0.0000000000	0.0000000000	-1.0293899844
	N	0.0000000000	0.0000000000	0.8204567842
	C	0.0000000000	0.0000000000	1.9770155874
	H	0.0000000000	0.0000000000	3.0452914244
H2O···HF	CCSD(T)/aug-cc-pVTZ ENERGY=-176.70617748			
	F	0.0000000000	0.0064899277	-1.3001618619

	H	0.0000000000	-0.0147956575	-0.3631878075
	O	0.0000000000	-0.0536360711	1.3465354359
	H	-0.7644558226	0.3719268154	1.7477783818
	H	0.7644558226	0.3719268154	1.7477783818
H3N···HF	CCSD(T)/aug-cc-pVTZ ENERGY=-156.85043960			
	F	-0.0000000000	0.0000000000	-1.2742743506
	H	-0.0000000000	0.0000000000	-0.3216601242
	N	0.0000000000	0.0000000000	1.3737063455
	H	0.9423603730	0.0000000000	1.7502030813
	H	-0.4711801865	0.8161080225	1.7502030813
	H	-0.4711801865	-0.8161080225	1.7502030813
N2···HCl	CCSD(T)/aug-cc-pVTZ ENERGY=-569.72665685			
	Cl	0.0000000000	0.0000000000	-1.8390976253
	H	0.0000000000	0.0000000000	-0.5587167330
	N	0.0000000000	0.0000000000	1.7958636346
	N	0.0000000000	0.0000000000	2.8993665805
OC···HCl	CCSD(T)/aug-cc-pVTZ ENERGY=-573.50922646			
	Cl	0.0000000000	0.0000000000	-1.8824198772
	H	0.0000000000	0.0000000000	-0.5996741234
	C	0.0000000000	0.0000000000	1.7564688721
	O	0.0000000000	0.0000000000	2.8904158792
C2H2···HCl	CCSD(T)/aug-cc-pVTZ ENERGY=-537.54043942			
	Cl	0.0000000000	0.0000000000	-1.5398353414
	H	0.0000000000	0.0000000000	-0.2541303086
	C	0.0000000000	0.6055830392	2.1061445032
	C	0.0000000000	-0.6055830392	2.1061445032
	H	0.0000000000	1.6706976875	2.1103077592
	H	0.0000000000	-1.6706976875	2.1103077592
C2H4···HCl	CCSD(T)/aug-cc-pVTZ ENERGY=-538.79229119			
	Cl	0.0000000000	0.0000000000	-1.6101663216
	H	0.0000000000	0.0000000000	-0.3235085519
	C	0.0000000000	0.6700474352	2.0461806877
	C	0.0000000000	-0.6700474352	2.0461806877
	H	-0.9252108632	1.2351718715	2.0482249260
	H	0.9252108632	1.2351718715	2.0482249260
	H	0.9252108632	-1.2351718715	2.0482249260
	H	-0.9252108632	-1.2351718715	2.0482249260
H2S···HCl	CCSD(T)/aug-cc-pVTZ ENERGY=-859.28976671			
	Cl	0.0000000000	0.0017977459	-1.8405141407
	H	0.0000000000	-0.0179663439	-0.5512561774
	S	0.0000000000	-0.0559206772	1.9245940654
	H	-0.9692273626	0.8667135071	2.0362795614
	H	0.9692273626	0.8667135071	2.0362795614
H3P···HCl	CCSD(T)/aug-cc-pVTZ ENERGY=-803.04468043			
	Cl	-0.0000000000	0.0000000000	-1.9152712518
	H	-0.0000000000	0.0000000000	-0.6268666944
	P	0.0000000000	0.0000000000	1.9493888303
	H	1.2034045049	0.0000000000	2.6966069177
	H	-0.6017022524	1.0421788722	2.6966069177
	H	-0.6017022524	-1.0421788722	2.6966069177

HCN···HCl	CCSD(T)/aug-cc-pVTZ	ENERGY=-553.63216914		
	Cl	0.0000000000	0.0000000000	-1.7053328853
	H	0.0000000000	0.0000000000	-0.4170124769
	N	0.0000000000	0.0000000000	1.6549495447
	C	0.0000000000	0.0000000000	2.8130080461
	H	0.0000000000	0.0000000000	3.8812517710
H2O···HCl	CCSD(T)/aug-cc-pVTZ	ENERGY=-536.69441409		
	Cl	0.0000000000	0.0030013367	-1.0964372848
	H	0.0000000000	-0.0187343087	0.1966989064
	O	0.0000000000	-0.0507209881	2.0997080867
	H	-0.7629212766	0.3591394553	2.5198230048
	H	0.7629212766	0.3591394553	2.5198230048
H3N···HCl	CCSD(T)/aug-cc-pVTZ	ENERGY=-516.83721880		
	Cl	-0.0000000000	0.0000000000	-1.0412873520
	H	-0.0000000000	0.0000000000	0.2779902898
	N	0.0000000000	0.0000000000	2.0844348884
	H	0.9427412213	0.0000000000	2.4606321824
	H	-0.4713706106	0.8164378468	2.4606321824
	H	-0.4713706106	-0.8164378468	2.4606321824
N2···F2	CCSD(T)/aug-cc-pVTZ	ENERGY=-308.69569308		
	F	0.0000000000	0.0000000000	-2.4621473784
	F	0.0000000000	0.0000000000	-1.0426204053
	N	0.0000000000	0.0000000000	1.8249592298
	N	0.0000000000	0.0000000000	2.9288365091
OC···F2	CCSD(T)/aug-cc-pVTZ	ENERGY=-312.47728544		
	F	0.0000000000	0.0000000000	-2.5203454350
	F	0.0000000000	0.0000000000	-1.0993411115
	C	0.0000000000	0.0000000000	1.8064570016
	O	0.0000000000	0.0000000000	2.9420421201
C2H2···F2	CCSD(T)/aug-cc-pVTZ	ENERGY=-276.50759589		
	F	0.0000000000	0.0000000000	-2.2007025433
	F	0.0000000000	0.0000000000	-0.7778355210
	C	0.0000000000	0.6052620944	2.1733339011
	C	0.0000000000	-0.6052620944	2.1733339011
	H	0.0000000000	1.6695267224	2.1725695606
	H	0.0000000000	-1.6695267224	2.1725695606
C2H4···F2	CCSD(T)/aug-cc-pVTZ	ENERGY=-277.75953272		
	F	0.0000000000	0.0000000000	-2.2444064184
	F	0.0000000000	0.0000000000	-0.8191934508
	C	0.0000000000	0.6693425021	2.0747948960
	C	0.0000000000	-0.6693425021	2.0747948960
	H	-0.9249258605	1.2344265450	2.0742261334
	H	0.9249258605	1.2344265450	2.0742261334
	H	0.9249258605	-1.2344265450	2.0742261334
	H	-0.9249258605	-1.2344265450	2.0742261334
H2S···F2	CCSD(T)/aug-cc-pVTZ	ENERGY=-598.25631158		
	F	0.0000000000	0.0080109047	-2.5110235914
	F	0.0000000000	-0.0112966542	-1.0859911162
	S	0.0000000000	-0.0531713028	2.0046499493
	H	-0.9678775516	0.8765878723	2.0182042773

	H	0.9678775516	0.8765878723	2.0182042773
H3P···F2	CCSD(T)/aug-cc-pVTZ ENERGY=-542.01167539			
	F	-0.0000000000	0.0000000000	-2.5692079846
	F	-0.0000000000	0.0000000000	-1.1442271467
	P	0.0000000000	0.0000000000	2.0072099260
	H	1.1958500324	0.0000000000	2.7708324643
	H	-0.5979250162	1.0356365072	2.7708324643
	H	-0.5979250162	-1.0356365072	2.7708324643
HCN···F2	CCSD(T)/aug-cc-pVTZ ENERGY=-292.59702549			
	F	0.0000000000	0.0000000000	-2.3981754641
	F	0.0000000000	0.0000000000	-0.9756549523
	N	0.0000000000	0.0000000000	1.7732452558
	C	0.0000000000	0.0000000000	2.9329536405
	H	0.0000000000	0.0000000000	4.0006046026
H2O···F2	CCSD(T)/aug-cc-pVTZ ENERGY=-275.65823518			
	F	0.0000000000	0.0109083174	-1.8100878568
	F	0.0000000000	-0.0106781888	-0.3868378490
	O	0.0000000000	-0.0510440683	2.2745811790
	H	-0.7593443731	0.4029517588	2.6520158967
	H	0.7593443731	0.4029517588	2.6520158967
H3N···F2	CCSD(T)/aug-cc-pVTZ ENERGY=-255.79739985			
	F	-0.0000000000	0.0000000000	-1.7680640712
	F	-0.0000000000	0.0000000000	-0.3358270168
	N	0.0000000000	0.0000000000	2.2790069275
	H	0.9398087208	0.0000000000	2.6619323988
	H	-0.4699043604	0.8138982269	2.6619323988
	H	-0.4699043604	-0.8138982269	2.6619323988
N2···ClF	CCSD(T)/aug-cc-pVTZ ENERGY=-668.78053314			
	F	0.0000000000	0.0000000000	-2.4372338930
	Cl	0.0000000000	0.0000000000	-0.7883104825
	N	0.0000000000	0.0000000000	2.0988122173
	N	0.0000000000	0.0000000000	3.2023310384
OC···ClF	CCSD(T)/aug-cc-pVTZ ENERGY=-672.56373529			
	F	0.0000000000	0.0000000000	-2.4351857720
	Cl	0.0000000000	0.0000000000	-0.7809479405
	C	0.0000000000	0.0000000000	1.9925445015
	O	0.0000000000	0.0000000000	3.1263132370
C2H2···ClF	CCSD(T)/aug-cc-pVTZ ENERGY=-636.59498056			
	F	0.0000000000	0.0000000000	-2.1921030437
	Cl	0.0000000000	0.0000000000	-0.5325611702
	C	0.0000000000	0.6059505591	2.3238791470
	C	0.0000000000	-0.6059505591	2.3238791470
	H	0.0000000000	1.6708909861	2.3330373524
	H	0.0000000000	-1.6708909861	2.3330373524
C2H4···ClF	CCSD(T)/aug-cc-pVTZ ENERGY=-637.84824917			
	F	0.0000000000	0.0000000000	-2.2094784817
	Cl	0.0000000000	0.0000000000	-0.5393097725
	C	0.0000000000	0.6716306614	2.1771245744
	C	0.0000000000	-0.6716306614	2.1771245744

	H	-0.9253665413	1.2357104346	2.1821302489
	H	0.9253665413	1.2357104346	2.1821302489
	H	0.9253665413	-1.2357104346	2.1821302489
	H	-0.9253665413	-1.2357104346	2.1821302489
H2S···ClF	CCSD(T)/aug-cc-pVTZ	ENERGY=-958.34520751		
	F	0.0000000000	0.0143154508	-2.4183295332
	Cl	0.0000000000	-0.0101383765	-0.7453025391
	S	0.0000000000	-0.0519725650	2.1168149515
	H	-0.9695057081	0.8699454300	2.2335271125
	H	0.9695057081	0.8699454300	2.2335271125
HCN···ClF	CCSD(T)/aug-cc-pVTZ	ENERGY=-652.68578491		
	F	0.0000000000	0.0000000000	-2.3440194943
	Cl	0.0000000000	0.0000000000	-0.6846007798
	N	0.0000000000	0.0000000000	1.9482207121
	C	0.0000000000	0.0000000000	3.1061682221
	H	0.0000000000	0.0000000000	4.1743048951
H2O···ClF	CCSD(T)/aug-cc-pVTZ	ENERGY=-635.74733333		
	F	0.0000000000	0.0153516102	-1.8720922111
	Cl	0.0000000000	-0.0103328387	-0.2118676749
	O	0.0000000000	-0.0500245687	2.3537775746
	H	-0.7622013591	0.4340720368	2.6881947490
	H	0.7622013591	0.4340720368	2.6881947490
H3N···ClF	CCSD(T)/aug-cc-pVTZ	ENERGY=-615.89339691		
	F	-0.0000000000	0.0000000000	-1.8183062175
	Cl	-0.0000000000	0.0000000000	-0.1152923773
	N	0.0000000000	0.0000000000	2.2049237377
	H	0.9488371530	0.0000000000	2.5625432850
	H	-0.4744185765	0.8217170785	2.5625432850
	H	-0.4744185765	-0.8217170785	2.5625432850
N2···Cl2	CCSD(T)/aug-cc-pVTZ	ENERGY=-1028.82058163		
	Cl	0.0000000000	0.0000000000	-2.3369912531
	Cl	0.0000000000	0.0000000000	-0.3160067201
	N	0.0000000000	0.0000000000	2.8056726100
	N	0.0000000000	0.0000000000	3.9094520904
OC···Cl2	CCSD(T)/aug-cc-pVTZ	ENERGY=-1032.60270244		
	Cl	0.0000000000	0.0000000000	-2.3586723741
	Cl	0.0000000000	0.0000000000	-0.3354291219
	C	0.0000000000	0.0000000000	2.7616311969
	O	0.0000000000	0.0000000000	3.8966478762
C2H2···Cl2	CCSD(T)/aug-cc-pVTZ	ENERGY=-996.63363165		
	Cl	0.0000000000	0.0000000000	-2.1240454789
	Cl	0.0000000000	0.0000000000	-0.0973180265
	C	0.0000000000	0.6055263704	3.0244262370
	C	0.0000000000	-0.6055263704	3.0244262370
	H	0.0000000000	1.6701427427	3.0265855572
	H	0.0000000000	-1.6701427427	3.0265855572
C2H4···CL2	CCSD(T)/aug-cc-pVTZ	ENERGY=-997.88597852		
	Cl	0.0000000000	0.0000000000	-2.1666182227
	Cl	0.0000000000	0.0000000000	-0.1355774035

	C	0.0000000000	0.6700282405	2.9093307618
	C	0.0000000000	-0.6700282405	2.9093307618
	H	-0.9251519419	1.2349243042	2.9098453228
	H	0.9251519419	1.2349243042	2.9098453228
	H	0.9251519419	-1.2349243042	2.9098453228
	H	-0.9251519419	-1.2349243042	2.9098453228
H2S···Cl2	CCSD(T)/aug-cc-pVTZ ENERGY=-1318.38272503			
	Cl	0.0000000000	0.0089752042	-2.3878730305
	Cl	0.0000000000	-0.0138381860	-0.3561297018
	S	0.0000000000	-0.0498580905	2.8517758408
	H	-0.9684478855	0.8784539126	2.9045356932
	H	0.9684478855	0.8784539126	2.9045356932
H3P···Cl2	CCSD(T)/aug-cc-pVTZ ENERGY=-1262.13818065			
	Cl	-0.0000000000	0.0000000000	-2.4115599850
	Cl	-0.0000000000	0.0000000000	-0.3776995772
	P	0.0000000000	0.0000000000	2.8416934868
	H	1.2010780685	0.0000000000	3.5946872509
	H	-0.6005390342	1.0401641192	3.5946872509
	H	-0.6005390342	-1.0401641192	3.5946872509
HCN···Cl2	CCSD(T)/aug-cc-pVTZ ENERGY=-1012.72348834			
	Cl	0.0000000000	0.0000000000	-2.2584494531
	Cl	0.0000000000	0.0000000000	-0.2322273340
	N	0.0000000000	0.0000000000	2.6691252200
	C	0.0000000000	0.0000000000	3.8282630089
	H	0.0000000000	0.0000000000	4.8961852039
H2O···Cl2	CCSD(T)/aug-cc-pVTZ ENERGY=-995.78482080			
	Cl	0.0000000000	0.0093732999	-1.7960895317
	Cl	0.0000000000	-0.0130293116	0.2311612967
	O	0.0000000000	-0.0440483921	3.0381312218
	H	-0.7605454893	0.4138958808	3.4094906682
	H	0.7605454893	0.4138958808	3.4094906682
H3N···Cl2	CCSD(T)/aug-cc-pVTZ ENERGY=-975.92614239			
	Cl	-0.0000000000	0.0000000000	-1.7507469228
	Cl	-0.0000000000	0.0000000000	0.2966821949
	N	0.0000000000	0.0000000000	2.9603718048
	H	0.9428059776	0.0000000000	3.3354885680
	H	-0.4714029888	0.8164939274	3.3354885680
	H	-0.4714029888	-0.8164939274	3.3354885680