

Electronic supplementary information -2 for

Anharmonicity and Vibrational Stark Fields in Phosphinic Acid Dimers

Manjusha Boda,[†] Arzoo and G. Naresh Patwari*

Department of Chemistry, Indian Institute of Technology Bombay, Mumbai 400076, India. Email: naresh@chem.iitb.ac.in

[†]Present address: School of Chemistry, University of Hyderabad, Hyderabad 500046, India

Cartesian coordinates of various hydrogen bonded phosphinic acid dimers considered in the present investigation at MP2/aug-cc-pVDZ level of theory. For the sake of convenience, the different possible dimers formed by different combinations of the monomeric units will be labelled with respect to only the R groups as R₁R₂ in the rest of the manuscript, i.e., dimer formed by combination of PA-2H and PA-BrCl will be labelled as (2H-BrCl) only.

2H-2H	2H-HF	2H-HCl
P 1.96450700 0.06215900 0.16139000	P 1.69058400 -0.03462200 - 0.34281300	P -1.35037000 0.20525000 0.69808400
O 1.11774800 1.34486300 0.23716200	O 0.76205900 -1.19988500 - 0.64268700	O -0.43790900 -0.88489700 1.25426500
H 2.32418100 -0.38872000 1.45479100	H 2.76799700 0.10797300 - 1.22867200	H -2.42430500 0.55963500 1.53240000
H 3.18992700 0.21744500 - 0.52213400	O 1.07576200 1.42936200 - 0.22262700	O -0.70604300 1.62151900 0.32314800
O 1.34665200 -1.21744800 - 0.61554500	H 0.07135800 1.41876800 - 0.01247300	H 0.22204900 1.50162300 - 0.09934700
H 0.38939100 -1.36540200 - 0.32723800	P -2.25778100 0.07841500 - 0.04484200	P 2.45337100 0.01225300 - 0.15025600
P -1.96454700 -0.06223100	O -1.42988700 1.33201500	O 1.60691600 1.17966400 -

0.16128800 O -1.11761000 -1.34481600 0.23736100 H -3.18967400 -0.21773600 - 0.52271600 H -2.32480500 0.38851800 1.45456400 O -1.34666100 1.21756300 - 0.61529700 H -0.38945400 1.36568600 - 0.32688800	0.28842000 H -3.51324000 0.05548100 0.59532300 H -2.53710400 -0.01532200 - 1.42976700 O -1.66753700 -1.36900500 0.38912400 H -0.73081500 -1.45275700 0.04460300 F 2.50295300 -0.25677100 1.03866400	0.68929900 H 3.58889000 -0.25908400 - 0.93971300 H 2.94803100 0.27654900 1.14983200 O 1.77522200 -1.45971900 - 0.07717100 H 0.91164300 -1.39605700 0.42848700 Cl -2.33510600 -0.44692700 - 0.98686000
2H-HBr P -0.76111600 0.97080700 0.55223100 O 0.14584600 0.41375400 1.64910800 H -1.70812500 1.91290300 0.99281700 O -0.08342000 1.71479400 - 0.69555700 H 0.74879900 1.20249800 - 1.00848900 P 2.83159600 -0.29959400 - 0.21441900 O 1.98607400 0.33904700 - 1.33117100 H 3.79918300 -1.20232500 - 0.69943000 H 3.55259600 0.67200500 0.52107500	2H-2F P -1.40381300 -0.06636000 0.03630500 O -0.48157700 -1.19302100 0.42485000 O -0.82137000 1.34386000 - 0.35690800 H 0.21398300 1.35616600 - 0.32237800 P 2.51011400 0.11059700 0.19892200 O 1.70418200 1.33221400 - 0.27887500 H 3.85831700 0.15055200 - 0.20643800 H 2.53020200 0.00998000 1.60995200 O 2.07565200 -1.35745600 - 0.34484400	2H-2Cl P 0.93946700 -0.08201800 - 0.03793300 O 0.04667800 -0.52082100 - 1.18649100 O 0.30823800 0.05586300 1.41759100 H -0.69346800 0.30995300 1.35147700 P -2.94845600 0.16455400 - 0.05031900 O -2.14997100 0.64239300 1.17662600 H -4.29488600 -0.13181700 0.24204800 H -2.98274500 1.14859200 - 1.06623800 O -2.48698600 -1.21360600 - 0.77478500

O 2.07987400 -1.22342800 0.88711900 H 1.31504900 -0.70800300 1.28152200 Br -2.05119100 -0.62567500 - 0.29230500	H 1.11494000 -1.49814600 - 0.13126100 F -2.40101600 -0.43541300 - 1.15255400 F -2.50198800 0.24798200 1.14899200	H -1.52365500 -1.13196400 - 1.01999200 Cl 1.81983200 1.71325400 - 0.45995600 Cl 2.52639800 -1.30992600 0.26895400
2H-2Br P 0.33269200 -0.15703300 - 0.03548800 O -0.53830400 -0.46352600 - 1.24683100 O -0.29676700 -0.33046600 1.42185900 H -1.30202700 -0.08036600 1.40210700 P -3.54070900 -0.05148400 - 0.02228100 O -2.76318600 0.25862600 1.27044500 H -4.88241000 -0.41629600 0.20829400 H -3.58873700 1.06948200 - 0.88410200 O -3.04205000 -1.29901400 - 0.93477200 H -2.08236200 -1.15371200 - 1.16527600 Br 2.14266900 -1.39186000 0.07061200 Br 1.08871000 1.91710800 -	2H-ClF P 1.14126500 -0.24662300 0.29469500 O 0.21956200 0.48039200 1.24916100 O 0.54461900 -1.34413300 - 0.67970200 H -0.46244700 -1.16995300 - 0.85265500 P -2.72517900 -0.07126200 - 0.00933500 O -1.90865400 -0.84520500 - 1.06084700 H -4.01156300 0.27701500 - 0.46444400 H -2.91796800 -0.82482100 1.17239700 O -2.17658000 1.37982900 0.47529500 H -1.25376500 1.25955100 0.82637900 F 2.30256400 -1.05398600 1.04240300 Cl 2.24998800 1.02031100 -	2H-BrF P -0.65166700 0.74640700 0.22618200 O 0.26189800 0.45025600 1.39757700 O -0.01889100 1.20312000 - 1.15565800 H 0.92130300 0.78477100 - 1.27303200 P 3.09283900 -0.18230000 - 0.08777000 O 2.26928900 0.12788700 - 1.35146300 H 4.25576500 -0.92781000 - 0.36195500 H 3.52710100 0.99565700 0.56448900 O 2.41364800 -1.10316600 1.06652300 H 1.56293200 -0.67075700 1.34835000 F -1.68143700 1.93705700 0.52120300 Br -2.03312300 -0.90005000 -

0.15004300	0.83617500	0.19144800
2H-BrCl P 0.62699200 0.57132000 - 0.08021900 O -0.27687000 0.66697800 - 1.30036500 O 0.01156800 0.91133700 1.35193300 H -0.96813900 0.57252700 1.39563500 P -3.20076500 0.11053000 0.04608900 O -2.37769800 0.05403000 1.34685700 H -4.45088000 -0.52802600 0.16145900 H -3.47685000 1.44122100 - 0.34793300 O -2.60644000 -0.62842900 - 1.27294400 H -1.70061200 -0.25477300 - 1.45781600 Br 1.52374200 -1.43905300 0.08277100 Cl 2.22750700 1.81628500 - 0.18472000	2H-HMe P -2.32631400 0.09178700 0.20397000 O -1.56392500 1.33785300 - 0.28044700 H -3.67043100 0.05665900 - 0.22389500 H -2.38702100 0.03072900 1.61833000 O -1.80689300 -1.36140500 - 0.28493100 H -0.80940000 -1.43675800 - 0.09699800 P 1.53132300 -0.08841300 - 0.27569100 O 0.72102600 -1.29021300 0.25303600 H 1.55676200 -0.07493900 - 1.69441900 O 1.01549600 1.38939700 0.15883100 H 0.01987400 1.46494400 0.00564100 C 3.25215100 -0.07750800 0.26159000 H 3.76646900 0.79450400 - 0.16771300 H 3.27129700 -0.01840000 1.35940200	2H-2Me P 1.37408900 -0.07791500 0.05098400 O 0.52356200 -1.16445900 0.75043600 O 0.76533400 0.51584900 - 1.34221800 H -0.16681400 0.84167200 - 1.16782000 P -2.49681400 0.10330000 0.09472900 O -1.63342800 1.23558600 - 0.49138500 H -2.80417200 0.35581300 1.45520500 H -3.75386600 -0.05164300 - 0.53140700 O -1.92412100 -1.40530900 0.02216600 H -0.94378100 -1.40525900 0.31610800 C 2.98908300 -0.68727200 - 0.48657500 C 1.63233700 1.34964200 1.14220000 H 2.82749900 -1.51870700 - 1.18760500 H 3.54819100 0.11668900 - 0.98674300

	H 3.73878100 -1.00736400 - 0.06598100	H 3.54658200 -1.05189800 0.38857000 H 2.06488600 1.01120500 2.09526100 H 2.29353900 2.08448200 0.65986200 H 0.64950100 1.80930500 1.32713300
2H-MeF P 1.41458200 0.06711100 0.03754500 O 0.52182500 1.25277800 0.38345600 O 0.76115800 -1.15180000 - 0.76565900 H -0.23666900 -1.24924100 - 0.58548100 P -2.56775900 -0.07766200 0.13687500 O -1.77045600 -1.31987700 - 0.29601200 H -3.87097600 -0.02485700 - 0.40112000 H -2.74512700 -0.03583500 1.54106300 O -2.00166400 1.37948400 - 0.29099200 H -1.02625800 1.43963400 - 0.04788300 C 2.93673900 0.44240900 -	2H-MeCl P 1.20592200 -0.38507700 0.05138400 O 0.33583200 -1.04608100 - 1.01785200 O 0.56718300 -0.17120600 1.50892000 H -0.38958900 0.17413800 1.44154000 P -2.64063200 0.27748200 - 0.06972500 O -1.85029500 0.67361500 1.18948900 H -4.02226700 0.10742400 0.15921600 H -2.54898900 1.27183200 - 1.07395600 O -2.27664600 -1.12754800 - 0.79063300 H -1.28276800 -1.17745500 - 0.94382700 Cl 1.74095900 1.51633800 -	2H-MeBr P -0.88702100 0.88224800 - 0.03198600 O -0.02929600 1.24649600 - 1.24404700 O -0.27375400 1.12601600 1.43316800 H 0.66292500 0.72525500 1.49058200 P 2.69076600 -0.39174800 0.05252500 O 2.07275600 0.05452400 1.38911600 H 4.09383700 -0.52768000 0.10105600 H 2.20332100 -1.65891600 - 0.35052500 O 2.52352700 0.58217100 - 1.23235500 H 1.56351000 0.86912500 - 1.32618800 C -2.50837100 1.66069300

0.83351300 H 2.68092700 0.87819100 - 1.80913100 H 3.51376300 1.16618200 - 0.24185600 H 3.51183900 -0.48302400 - 0.97292700 F 1.97364600 -0.60799200 1.40619700	0.58691900 C 2.78321200 -1.18703600 0.37396900 H 2.57547100 -2.19544400 0.76136900 H 3.34208800 -1.25254400 - 0.56948000 H 3.34253700 -0.59979900 1.11467800	0.03236800 H -2.35638400 2.74732000 0.11786400 H -3.04590100 1.42513000 - 0.89619700 H -3.05512600 1.27982200 0.90550600 Br -1.32622900 -1.32158200 - 0.09461300
HF-HF P -2.01005900 -0.06058600 0.39519800 O -1.09864500 -1.27433800 0.45020100 H -2.97207200 0.00773700 1.41169000 O -1.35754700 1.39457700 0.36760100 H -0.39667900 1.38197900 0.04705000 P 2.01065600 0.05960400 - 0.39527400 O 1.09802900 1.27206300 - 0.45782400 H 2.97542500 -0.01167000 - 1.40897200 O 1.35924400 -1.39573900 - 0.36256200 H 0.39653400 -1.38202200 - 0.04638500	HF-HCl P -2.16197500 -0.05418100 - 0.50522400 O -1.25493200 1.14898500 - 0.69840900 H -2.96592400 -0.37484300 - 1.60723900 O -1.51833000 -1.44705400 - 0.06988200 H -0.62513500 -1.33503200 0.39881100 P 1.66172000 0.11252800 0.74436600 O 0.75836300 -1.06155100 1.10964900 H 2.69089800 0.37182700 1.66413900 O 0.99537700 1.55712000 0.54318800 H 0.10981100 1.47691500 0.05957900	HF-HBr P -2.51891800 -0.60098800 - 0.15702500 O -1.63452400 -0.19516200 - 1.32355500 H -3.14536800 -1.84710000 - 0.29285900 O -1.89911700 -0.63195000 1.31236700 H -1.08564200 -0.03203300 1.40780000 P 1.07840600 1.10240800 0.23414000 O 0.17638700 0.91709500 1.45320900 H 2.02661500 2.13291400 0.35746700 O 0.39567300 1.43062700 - 1.18211500 H -0.40976400 0.83523400 - 1.32379300

F 2.97502100 0.10482300 0.90030000 F -2.97733400 -0.09968900 - 0.89825300	F -3.30669900 0.23274100 0.59882900 Cl 2.71827300 -0.27580800 - 0.97460300	F -3.81901900 0.35112400 - 0.03421500 Br 2.35101900 -0.68386600 - 0.08790400
HF-2F P 2.33797400 -0.06846000 - 0.30399300 O 1.41106300 -1.25872200 - 0.48276300 H 3.43008600 -0.02756000 - 1.17995800 O 1.71908000 1.40196100 - 0.37076200 H 0.72980600 1.40480300 - 0.19123500 P -1.74442000 0.06577400 0.05257700 O -0.85868400 1.28302000 0.08133200 O -1.12511200 -1.37522000 - 0.12995800 H -0.11553000 -1.34458500 - 0.26418700 F -2.89598400 0.14766300 - 1.04457100 F -2.67379900 -0.06973600 1.33734200 F 3.11217800 -0.12244800 1.10987600	HF-2Cl P -2.75951300 0.25615000 0.07397600 O -1.83629900 0.34019900 1.27787700 H -3.80420800 1.18938000 0.06170700 O -2.12747000 0.35321000 - 1.38873300 H -1.15144700 0.09701400 - 1.39990300 P 1.26063400 -0.13555300 - 0.05936600 O 0.39235500 -0.31949400 - 1.29165200 O 0.62559600 -0.42634800 1.37746500 H -0.35327200 -0.14375400 1.38635700 Cl 2.02643100 1.75551400 0.02871300 Cl 2.90471100 -1.31317600 - 0.06681800 F -3.60786300 -1.11687600 0.06453400	HF-2Br P -3.38037300 0.05266700 0.06460400 O -2.46689300 0.16951500 1.27332400 H -4.43624400 0.97274800 0.02881200 O -2.74158700 0.13186300 - 1.39617800 H -1.76329900 -0.12075800 - 1.40113700 P 0.62213900 -0.22739100 - 0.05026800 O -0.22165300 -0.52709900 - 1.28172000 O 0.00876000 -0.55800500 1.39280200 H -0.97584000 -0.29533800 1.40608000 Br 1.19851000 1.90484400 0.00313000 Br 2.51093600 -1.32454100 - 0.02691300 F -4.21230400 -1.33073100 0.07531000

HF-ClF P -2.55700400 -0.40516300 - 0.14129800 O -1.60454000 -0.27199400 - 1.31768200 H -3.52890700 -1.40470300 - 0.27767100 O -1.94550700 -0.62984800 1.31620900 H -0.97168700 -0.37735900 1.36233200 P 1.45836700 0.33719000 0.13493200 O 0.58833000 0.01165300 1.32759700 O 0.78224900 0.67821100 - 1.26083200 H -0.16931900 0.31671200 - 1.30887900 F -3.50736400 0.88889800 0.01558100 F 2.39196900 1.61274000 0.37096000 Cl 2.86022200 -1.07846900 - 0.21655800	HF-BrF P -2.91572500 -0.55818000 - 0.07731700 O -1.96114100 -0.48437100 - 1.25727500 H -3.73950100 -1.69086800 - 0.05247700 O -2.31677800 -0.46578900 1.39974600 H -1.39869000 -0.05116200 1.41289500 P 0.93991600 0.72645700 0.08889600 O 0.07324200 0.59082900 1.32242500 O 0.25370200 0.82432900 - 1.34286400 H -0.63192200 0.32159200 - 1.35145500 F -4.03529300 0.60214200 - 0.13468800 Br 2.47964500 -0.81972600 - 0.02361700 F 1.83834600 2.04971300 0.09776600	HF-BrCl P -3.24138800 0.06477400 0.06633000 O -2.34582100 0.26978600 1.27677100 H -4.39251200 0.86274400 0.03860400 O -2.61393900 0.22837300 - 1.39214500 H -1.61375400 0.08729100 - 1.39549200 P 0.79659700 0.17322000 - 0.04683300 O -0.03751900 -0.14594200 - 1.27769200 O 0.19309200 -0.16856500 1.39452700 H -0.81495400 -0.01391600 1.39350500 F -3.91532700 -1.40199700 0.06287800 Cl 1.29152300 2.15822100 0.00695600 Br 2.72024700 -0.85848600 - 0.02928400
HF-HMe P -1.87021900 -0.04948900 0.42711000 O -0.87475800 -1.18628400 0.60148200	HF-2Me P -2.23135400 -0.11618100 0.27511800 O -1.31223400 -1.32327300 0.15972200	HF-MeF P -2.34082600 -0.06366300 0.31974100 O -1.45758500 -1.28847100 0.48119200

O -1.31594800 1.42967900 0.24797000	H -3.30114700 -0.27328300 1.16943600	H -3.45392400 -0.01267800 1.17056800
H -0.33962900 1.43923800 - 0.10173800	O -1.60051300 1.29429000 0.63584000	O -1.68440500 1.38345300 0.43245300
P 1.94453500 0.12179700 - 0.40286900	H -0.58265100 1.35073200 0.38214500	H -0.67502600 1.36926100 0.28843000
O 1.07253100 1.38050400 - 0.59273700	P 1.67177400 0.09038300 - 0.06071700	P 1.73834300 0.06794700 - 0.04110800
H 3.11854700 0.17509000 - 1.18473800	O 0.82505900 1.38438200 0.01929100	O 0.86237800 1.30424100 0.11839500
O 1.32239400 -1.29335200 - 0.91972300	O 1.07612600 -1.09133300 - 1.01799800	O 1.15021200 -1.32892100 0.47759500
H 0.45983700 -1.43978400 - 0.44266800	H 0.15212700 -1.30518600 - 0.71168000	H 0.14158600 -1.34689500 0.46772200
C 2.45681100 -0.12652700 1.31527800	C 1.90758300 -0.65735200 1.57563700	F -3.09554700 -0.06193200 - 1.10988800
H 3.15273900 -0.97609300 1.37612900	H 2.56086600 -1.53893600 1.49993300	C 3.38603200 0.17934100 0.65372200
H 2.93383900 0.79019400 1.69112400	H 2.34242700 0.08581700 2.26008500	H 3.90377000 1.03516800 0.19957400
H 1.55537800 -0.34551000 1.90758400	H 0.91964700 -0.96704200 1.94913100	H 3.29715900 0.32855700 1.73849800
F -2.83680000 -0.29616300 - 0.84817500	C 3.28603900 0.39314600 - 0.80892700	H 3.92954300 -0.75177700 0.44310800
H -2.83886900 0.05248700 1.43665000	H 3.12564400 0.80269700 - 1.81647700	F 2.05256300 -0.19632900 - 1.61086900
	H 3.83435800 1.12618400 - 0.19969000	
	H 3.85161000 -0.54736200 - 0.87530300	
	F -3.06426900 0.12511700 - 1.09429800	

HF-MeCl	HF-MeBr	HCl-HCl
P 2.44959000 -0.28068300 0.11252300	P -2.69532500 0.20375600 0.10006300	P 1.80065500 0.74687200 - 0.34522900
O 1.58033200 -0.38866100 1.35316400	O -1.87503700 0.51721300 1.33913500	O 0.89766800 0.27100300 - 1.47981500
H 3.67634400 -0.95577400 0.18360100	H -4.02171300 0.65674100 0.13464800	H 2.68178600 1.78441100 - 0.69128500
O 1.84406100 -0.69601800 - 1.30104000	O -2.15481400 0.65515700 - 1.32903100	O 1.11900800 1.29836600 0.99743100
H 0.82296900 -0.72618500 - 1.30514700	H -1.15504900 0.86537100 - 1.33225400	H 0.32086100 0.72825500 1.25581400
P -1.54774100 -0.33413800 - 0.06157200	P 1.21073100 0.83420400 - 0.06654600	P -1.80064900 -0.74687300 0.34531000
O -0.72109800 -0.81763500 - 1.25434300	O 0.35247500 1.21974800 - 1.27482200	O -0.89789900 -0.27088300 1.48002000
O -1.01212900 -0.71303000 1.40787100	O 0.64415400 1.21563400 1.39292700	H -2.68183800 -1.78439000 0.69129400
H -0.01171200 -0.59483500 1.45887900	H -0.33038200 0.96462700 1.45703700	O -1.11878000 -1.29836300 - 0.99723200
F 2.98693300 1.22893500 - 0.10315600	F -2.95843900 -1.38452900 - 0.04958300	H -0.32064200 -0.72809600 - 1.25557200
C -3.26537600 -0.86202600 - 0.05598400	Br 1.47907800 -1.38155400 - 0.01910300	Cl -3.09813800 0.73588800 - 0.23706800
H -3.74002600 -0.51624500 - 0.98433600	C 2.88178100 1.49962000 - 0.07344700	Cl 3.09812500 -0.73595600 0.23679200
H -3.28160900 -1.96077200 - 0.00767500	H 3.38303800 1.17201700 - 0.99440300	
H -3.77064400 -0.43170200 0.81928300	H 2.80866700 2.59727500 - 0.04928300	
Cl -1.64956100 1.73190100 -	H 3.41766400 1.13000300	

0.07704600	0.81134100	
HCl-HBr P -1.21036900 1.09740600 0.23638700 O -0.31870700 0.80240700 1.44197700 H -2.02729200 2.23288500 0.37690700 O -0.51555600 1.35023900 - 1.18955800 H 0.20374000 0.65544600 - 1.35573400 P 2.18013700 -0.85497500 - 0.19442500 O 1.28735200 -0.51666600 - 1.38509600 H 2.93036200 -2.03357700 - 0.33860600 O 1.50015100 -1.04669200 1.24524300 H 0.77954100 -0.34924800 1.40023600 Br -2.68942400 -0.52424400 - 0.07016000 Cl 3.65123900 0.55836700 0.04957900	HCl-2F P 2.01738200 -0.66483900 0.15453800 O 1.10823500 -0.74942900 1.37776400 H 3.19254700 -1.42743900 0.24487900 O 1.42090700 -1.10874800 - 1.26900800 H 0.47893200 -0.77600200 - 1.36912400 P -1.91603700 0.09457700 - 0.07909100 O -1.02769400 -0.14339500 - 1.27132000 O -1.33877100 0.00475500 1.38761100 H -0.35884600 -0.28471800 1.40046000 F -3.21066200 -0.83379500 - 0.05797600 F -2.65661800 1.50320200 - 0.11819700 Cl 2.74537000 1.23482100 - 0.09545500	HCl-2Cl P -2.42691300 0.70823400 0.19224800 O -1.55947000 0.77804600 1.44595600 H -3.68379200 1.32318500 0.31077500 O -1.85858000 1.33893600 - 1.17015900 H -0.89471600 1.07694800 - 1.30114400 P 1.44301500 0.12490600 - 0.06327800 O 0.63631500 0.54133400 - 1.28055000 O 1.01761500 0.68013100 1.37259200 H 0.00055500 0.72048300 1.44606200 Cl 3.39306300 0.65241500 - 0.17883100 Cl 1.50432500 -1.90889600 0.10521600 Cl -2.92977800 -1.23324200 - 0.24008900
HCl-2Br P 3.09361000 0.53893100 - 0.07524600	HCl-ClF P 1.62699000 0.38931100 - 0.10503100	HCl-BrF P 1.10067800 0.74284300 - 0.10996600

O 2.19471200 0.69415800 - 1.29972400 H 4.21951400 1.37796000 - 0.06625700 O 2.45826500 0.79451700 1.37681200 H 1.54002800 0.37945200 1.43639500 P -0.77854300 -0.18235900 0.04836000 O 0.10526400 -0.34454200 1.27795400 O -0.12908900 -0.42299800 - 1.39642900 H 0.80074800 -0.00020300 - 1.42355700 Cl 3.94074900 -1.32767200 - 0.01175400 Br -1.67536800 1.83539900 - 0.00990200 Br -2.47641100 -1.55838300 0.03812000	O 0.75612000 0.10791500 - 1.30840800 O 0.96355200 0.54223600 1.32938100 H 0.06928500 0.05102000 1.37822200 P -2.19999000 -0.76011100 0.15670200 O -1.26893100 -0.72695000 1.36628200 O -1.56918700 -1.11153600 - 1.27747300 H -0.67124500 -0.67017400 - 1.38098500 Cl -3.18450600 1.02348300 - 0.07042600 F 2.44444700 1.75634700 - 0.23360300 H -3.25968000 -1.67545900 0.25824800 Cl 3.14945800 -0.93194400 0.08181600	O 0.22635800 0.51205400 - 1.32415300 O 0.42964700 0.85881600 1.32763000 H -0.38904500 0.25195100 1.38706900 P -2.52699500 -0.85515200 0.13882400 O -1.60099000 -0.72115100 1.34546000 O -1.86521800 -1.07451100 - 1.30798900 H -1.05126700 -0.49170400 - 1.41202600 Br 2.72576200 -0.71233400 0.03586400 Cl -3.75993600 0.77308100 - 0.03371200 F 1.91954300 2.11433700 - 0.18181600 H -3.44197500 -1.91699700 0.21871200
HCl-BrCl P -2.87851900 -0.79743200 0.18894100 O -2.03083700 -0.78435600 1.45804600 O -2.24591000 -1.41683400 - 1.14998000 H -1.29857700 -1.09451700 -	HCl-HMe P -1.50210900 0.63228400 0.46947200 O -0.53777900 0.00899100 1.47651600 H -2.45422000 1.50681100 1.02215700 O -0.88951700 1.47706200 -	HCl-2Me P 1.89464000 0.68574000 - 0.06998200 O 0.99076100 0.76790000 - 1.29872100 H 2.97116300 1.59057200 - 0.06937500 O 1.23793100 0.88334900

1.27071700 P 0.95062000 0.03606900 - 0.02233900 O 0.19065400 -0.46000800 - 1.24230700 O 0.53433000 -0.51532700 1.42005700 H -0.47995700 -0.62028900 1.47726400 Br 3.09016100 -0.39725900 - 0.10482600 Cl 0.85588400 2.07562200 0.10359700 Cl -3.50000900 1.09747900 - 0.29321600 H -4.09439200 -1.49119500 0.30034200	0.74071300 H -0.01992900 1.03129800 - 1.08907500 P 2.10812500 -0.38437700 - 0.40559800 O 1.23684100 0.30558500 - 1.47684900 H 3.16174500 -1.12349800 - 0.98500400 O 1.39994900 -1.55242200 0.48440300 H 0.62052200 -1.14844400 0.95673100 C 2.84610400 0.78735900 0.75986300 H 3.52402100 0.25552100 1.44340000 H 3.39028800 1.56402300 0.20325500 H 2.02840500 1.24752200 1.33544000 Cl -2.71139100 -0.80527700 - 0.37359000	1.36921200 H 0.29412800 0.42054200 1.40967900 P -1.87647800 -0.15321500 0.07801500 O -1.00531700 -0.23411500 1.35658800 O -1.20474400 -0.76167400 - 1.28099400 H -0.34175400 -0.28940000 - 1.44394600 C -2.33508300 1.55886100 - 0.30928300 H -2.99541900 1.58625800 - 1.18839600 H -2.83318900 2.01169300 0.56059500 H -1.40907300 2.11114600 - 0.53093600 C -3.37259100 -1.15143500 0.22685700 H -3.07263700 -2.19284500 0.41178400 H -3.96660200 -0.78591000 1.07698900 H -3.95797000 -1.09230800 - 0.70192400 Cl 2.89034900 -1.11975500 - 0.01877000
HCl-MeF	HCl-MeCl	HCl-MeBr

P 2.02105100 -0.69075800 0.09497800	P 2.14842800 -0.68917400 0.14605100	P 2.46221600 -0.63030600 0.17422600
O 1.16227800 -0.86933400 1.34281600	O 1.30183400 -0.87905800 1.40061300	O 1.62405900 -0.86654900 1.42663200
H 3.20965800 -1.43986100 0.08286700	H 3.42076100 -1.28336900 0.19623000	H 3.79407300 -1.06958300 0.26295900
O 1.37647700 -1.02003500 - 1.33353200	O 1.57170800 -1.19889000 - 1.25788600	O 1.97068100 -1.26013500 - 1.21319200
H 0.40955200 -0.70157400 - 1.37525800	H 0.56820300 -1.02752000 - 1.33015200	H 0.95362100 -1.23338300 - 1.29873700
P -1.91591100 0.08593100 - 0.07348600	P -1.74792600 -0.27421500 - 0.09492000	P -1.44756800 -0.79312900 - 0.10463500
O -1.06850000 -0.21213700 - 1.30417500	O -0.96987800 -0.77464900 - 1.31301500	O -0.60412200 -1.21098000 - 1.31255100
O -1.42069500 -0.49978600 1.33261600	O -1.31178700 -0.83960300 1.34689900	O -0.95515800 -1.28287300 1.34898000
H -0.41960400 -0.63000800 1.36882100	H -0.30583300 -0.86309700 1.43448400	H 0.03831200 -1.13405900 1.45288700
C -3.64874900 -0.35587200 - 0.18689900	C -3.52336000 -0.54612200 - 0.15568000	C -3.17411700 -1.29437400 - 0.16967400
H -4.08870000 0.16007600 - 1.05120900	H -3.91958100 -0.06474700 - 1.06011900	H -3.62162800 -0.88389700 - 1.08509800
H -3.72239100 -1.44349700 - 0.32345000	H -3.69802100 -1.63137600 - 0.19591100	H -3.20648600 -2.39407000 - 0.18984100
H -4.15901100 -0.05531900 0.73829900	H -3.98409800 -0.11612200 0.74395500	H -3.69164800 -0.91014900 0.71980000
F -1.99222200 1.68825100 0.17237800	Cl -1.55261600 1.78017600 0.05600800	Cl 2.71859600 1.38197800 - 0.16589300
Cl 2.74231900 1.23140600 - 0.02907400	Cl 2.63003800 1.29343600 - 0.11684700	Br -1.51260200 1.43467400 0.02666900

<p>HBr-HBr</p> <p>P 1.60859100 -1.09747100 0.19506000</p> <p>O 0.72757800 -0.77072300 1.40031800</p> <p>H 2.32542400 -2.30196700 0.30387800</p> <p>O 0.91623600 -1.24120800 - 1.24719400</p> <p>H 0.25927900 -0.48318300 - 1.39837900</p> <p>P -1.60856200 1.09737700 - 0.19551200</p> <p>O -0.72811300 0.77009600 - 1.40104100</p> <p>H -2.32542500 2.30183600 - 0.30447400</p> <p>O -0.91574000 1.24167900 1.24640300</p> <p>H -0.25932800 0.48342900 1.39813700</p> <p>Br -3.22234800 -0.40375700 0.03642400</p> <p>Br 3.22234600 0.40383000 - 0.03586000</p>	<p>HBr-2F</p> <p>P -1.46301100 1.13188600 0.12569900</p> <p>O -0.54055600 1.22531700 1.34102700</p> <p>H -2.57294100 1.99246400 0.17057100</p> <p>O -0.84632800 1.44893400 - 1.32630500</p> <p>H 0.03199700 0.97525000 - 1.42780900</p> <p>P 2.28692900 -0.18022100 - 0.07510900</p> <p>O 1.42026500 0.10383500 - 1.27306800</p> <p>O 1.76722200 0.11646000 1.38591000</p> <p>H 0.84058600 0.54891100 1.38686000</p> <p>F 3.71384100 0.52552100 - 0.14175700</p> <p>F 2.79143900 -1.68898700 - 0.00922800</p> <p>Br -2.38887900 -0.87076500 - 0.01571700</p>	<p>HBr-2Cl</p> <p>P 1.90768600 1.18258100 - 0.21046700</p> <p>O 1.02267100 1.26552500 - 1.45358100</p> <p>H 3.11279600 1.90028600 - 0.30185900</p> <p>O 1.31213700 1.69698000 1.19223800</p> <p>H 0.40064700 1.29644800 1.33812100</p> <p>P -1.82477800 0.09117700 0.06654300</p> <p>O -1.02905500 0.51312300 1.28894700</p> <p>O -1.50848800 0.78124700 - 1.33847700</p> <p>H -0.50859400 0.97082500 - 1.42469900</p> <p>Cl -3.81698700 0.39066400 0.26589900</p> <p>Cl -1.67334100 -1.92179400 - 0.23833300</p> <p>Br 2.59168500 -0.89427800 0.13044700</p>
<p>HBr-2Br</p> <p>P -2.55562000 1.07065800 0.09050800</p> <p>O -1.65077700 1.14576500 1.32092700</p>	<p>HBr-ClF</p> <p>P 1.62455400 -1.15334200 0.15311300</p> <p>O 0.69536600 -1.10815700 1.36647600</p>	<p>HBr-BrF</p> <p>P 1.95185600 -1.16502200 0.15757500</p> <p>O 1.03759300 -1.00139500 1.37206000</p>

H -3.61274000 1.99689900 0.08914800 O -1.89870000 1.30581500 - 1.35865400 H -1.05109300 0.76509600 - 1.43881600 P 1.16059700 -0.15074800 - 0.04326900 O 0.25364500 -0.18314600 - 1.26623100 O 0.49373200 -0.28445900 1.40729000 H -0.36633600 0.26817500 1.43826500 Br 2.35223300 1.70868400 - 0.00179100 Br 2.63177800 -1.76745500 - 0.03711800 Br -3.60194500 -0.87553200 - 0.00748600	H 2.62823400 -2.13439300 0.22449300 O 0.97616400 -1.43515000 - 1.29187600 H 0.14467600 -0.88161200 - 1.40226500 P -2.01571100 0.42346600 - 0.08444600 O -1.16132500 0.09660100 - 1.28807300 O -1.37056700 0.41709600 1.36634300 H -0.54223500 -0.18079800 1.40222500 Br 2.77778000 0.72353500 - 0.03590800 Cl -3.69616400 -0.70200400 0.00877300 F -2.65199100 1.88802100 - 0.15219600	H 2.82432700 -2.26433500 0.23014300 O 1.27251500 -1.36909300 - 1.28672800 H 0.52573600 -0.70676100 - 1.40680400 P -1.49735900 0.73150300 - 0.08847400 O -0.62879200 0.44914400 - 1.29587400 O -0.84204400 0.75680200 1.36087500 H -0.08320900 0.07615900 1.41998300 Br 3.33083000 0.55157600 - 0.03804700 F -2.18919900 2.17232400 - 0.14027600 Br -3.24785000 -0.57548600 0.00319000
HBr-BrCl P 2.09700700 -1.15095600 0.10452000 O 1.18566100 -1.08127100 1.33042200 H 3.01163900 -2.21798300 0.11998900 O 1.41855300 -1.30906100 - 1.34529200 H 0.65286500 -0.65962200 -	HBr-HMe P 0.90291100 1.06910200 - 0.31387800 O -0.03781200 0.67932800 - 1.45475100 O 0.25897600 1.46098500 1.09779800 H -0.51323100 0.80683500 1.32643900 P -2.47590500 -0.62830100	HBr-2Me P 1.30967000 1.09924100 - 0.07110400 O 0.41027400 1.09383600 - 1.30821600 H 2.29173600 2.10751500 - 0.06288700 O 0.62644900 1.24001400 1.36489000 H -0.23337900 0.63582000

1.43510800 P -1.41681900 0.56987700 - 0.05950800 O -0.51676100 0.45826500 - 1.28047100 O -0.74145600 0.63212600 1.38956500 H 0.03422900 -0.03203400 1.43189000 Br 3.40949400 0.62525300 - 0.01122900 Br -2.87192900 -1.08554200 0.00345700 Cl -2.55789900 2.24326300 - 0.07492400	0.29039200 O -1.62269900 -0.19265600 1.50103000 H -3.39519400 -1.64190800 0.63610500 O -1.69615000 -1.36220000 - 0.93916900 H -1.00803300 -0.73022300 - 1.28719400 C -3.41936100 0.73807000 - 0.42985900 H -4.07471200 0.35845700 - 1.22738100 H -4.01175000 1.22863700 0.35598400 H -2.69939700 1.45476200 - 0.85382900 H 1.74627900 2.16170400 - 0.58845300 Br 2.36710300 -0.55321000 0.08372900	1.41393900 P -2.28898300 -0.24816800 0.07795300 O -1.41072200 -0.22024400 1.35428400 O -1.54275500 -0.73798200 - 1.29014500 H -0.75972900 -0.14230100 - 1.45343700 C -2.98535800 1.38696600 - 0.28629400 H -3.64513900 1.33281800 - 1.16455900 H -3.53972800 1.75400900 0.58993200 H -2.14646700 2.06659900 - 0.50113200 C -3.62693100 -1.45118700 0.21676000 H -3.18036600 -2.44091300 0.38934600 H -4.26454600 -1.18398500 1.07185400 H -4.21724200 -1.46598500 - 0.71063500 Br 2.55406600 -0.74426700 - 0.00641300
HBr-MeF P -1.47807400 1.15298100 0.08678400 O -0.60935700 1.31880800	HBr-MeCl P -1.61874000 1.18502300 0.17151200 O -0.74070700 1.28704400	HBr-MeBr P -1.97174100 1.18429200 0.23863100 O -1.08301100 1.29679800

1.33187300 H -2.62750800 1.96266400 0.05816500 O -0.82191600 1.42816300 - 1.35101700 H 0.09151700 0.98247700 - 1.40514500 P 2.26603900 -0.15640800 - 0.07299900 O 1.48318500 0.27189500 - 1.30781200 O 1.87515500 0.51183600 1.32945900 H 0.91114300 0.81242800 1.36454500 C 4.04865300 -0.01256100 - 0.18464900 H 4.39712900 -0.60215100 - 1.04356600 H 4.30385700 1.04614700 - 0.32958500 H 4.49972300 -0.38674500 0.74443800 F 2.07181300 -1.74730700 0.18290600 Br -2.33571700 -0.89165400 - 0.00439700	1.41710100 H -2.80303700 1.94210000 0.22210900 O -0.99815500 1.60376900 - 1.24648500 H -0.04836500 1.24513800 - 1.34440800 P 2.15678700 0.16678200 - 0.11742100 O 1.41317400 0.69492100 - 1.34530300 O 1.83645800 0.85987100 1.29878500 H 0.84609400 1.02846500 1.40645200 C 3.95003400 0.20850700 - 0.23084900 H 4.25742600 -0.36731800 - 1.11441000 H 4.25794500 1.25915100 - 0.33660200 H 4.37835700 -0.22729500 0.68191900 Br -2.39705900 -0.87887400 - 0.07263100 Cl 1.71480000 -1.83603700 0.15341100	1.47578900 H -3.22519000 1.81207200 0.35406900 O -1.42579900 1.75289200 - 1.15767100 H -0.44191100 1.51686300 - 1.28928100 P 1.89723500 0.68963800 - 0.14868900 O 1.07690200 1.16168700 - 1.35259300 O 1.52464200 1.30766300 1.29157800 H 0.52407100 1.31056800 1.43133600 C 3.67219200 0.94998200 - 0.28553100 H 4.02965000 0.44167000 - 1.19142000 H 3.85029200 2.03319400 - 0.36120100 H 4.16368200 0.54019900 0.60729100 Br -2.54698200 -0.92752200 - 0.12609500 Br 1.67389600 -1.51864100 0.09056400
2F-2F P -2.05282000 -0.06464500 0.00038900	2F-2Cl P -2.47793300 -0.05169300 0.06044400	2F-2Br P -3.09873700 -0.24952600 0.05700500

O -1.14994200 -1.26963700 0.00558800 O -1.44002700 1.39321500 - 0.00586500 H -0.43070600 1.37348500 - 0.00180700 P 2.05283000 0.06464500 0.00011600 O 1.14991800 1.26960700 0.00524900 O 1.44000500 -1.39320700 - 0.00611800 H 0.43067400 -1.37342000 - 0.00180600 F 3.09400900 0.04897800 1.20127500 F 3.09382900 0.05772800 - 1.20123300 F -3.09402100 -0.04890200 1.20152700 F -3.09379100 -0.05779400 - 1.20099200	O -1.57620800 0.08251300 1.25915000 O -1.87004700 -0.31118100 - 1.37506900 H -0.85681500 -0.36311000 - 1.35199000 P 1.56006700 -0.13086400 - 0.04921700 O 0.70153800 -0.45379800 - 1.26033900 O 0.97582300 -0.45086700 1.40640500 H -0.01550400 -0.26189700 1.42015000 Cl 2.09772200 1.83465900 - 0.02912000 F -3.44326000 1.19704200 - 0.13851500 Cl 3.32184800 -1.11593800 - 0.04293700 F -3.59465300 -1.17351100 0.22154000	O -2.20814200 -0.16144600 1.26791000 O -2.47975100 -0.44385700 - 1.38404900 H -1.46807700 -0.53607900 - 1.35285100 P 0.90254000 -0.26798400 - 0.03448800 O 0.08032000 -0.69205100 - 1.24476700 O 0.35831000 -0.66004300 1.42526300 H -0.63615200 -0.49551200 1.45424200 F -4.06774300 1.00235400 - 0.10219000 F -4.21320300 -1.38077500 0.16638600 Br 2.90842400 -1.12140200 - 0.03153500 Br 1.19357000 1.91738000 - 0.01223000
2F-ClF P -2.29075600 -0.08050400 0.06382100 O -1.37279300 -0.26357500 1.24389100 O -1.71812100 0.41875800 - 1.32294000 H -0.70641000 0.40112300 -	2F-BrF P -2.71938000 -0.17351900 0.06460500 O -1.77862200 -0.27491300 1.23668600 O -2.22542500 0.44460500 - 1.30441900 H -1.21779600 0.54079000 -	2F-BrCl P -2.95686100 -0.16381600 0.05840200 O -2.07804400 0.04122900 1.26405900 O -2.32086000 -0.34293700 - 1.37706300 H -1.30606000 -0.31524700 -

1.33402000 P 1.77020300 0.32789600 - 0.05958500 O 0.86591100 0.32105000 - 1.27193600 O 1.12571000 0.44068500 1.39055400 H 0.15337100 0.16844300 1.37654300 F -3.50895600 0.90339100 0.33451400 Cl 3.03696000 -1.24197000 - 0.02964100 F -3.12842200 -1.39023600 - 0.27526000 F 2.80708500 1.54214600 - 0.05022100	1.32570300 P 1.25003000 0.70916000 - 0.06196300 O 0.35344600 0.63222900 - 1.28006100 O 0.58528700 0.80578800 1.38336100 H -0.33398300 0.38857300 1.38082200 F -4.05483900 0.63256600 0.36819100 F -3.37950000 -1.57056000 - 0.31675100 F 2.19774500 1.99675000 - 0.05393300 Br 2.72125400 -0.89584200 - 0.01019500	1.34708900 P 1.07270400 0.13532800 - 0.03971300 O 0.25067000 -0.28664800 - 1.24829000 O 0.51578200 -0.22570900 1.41955000 H -0.49015300 -0.13864500 1.42686700 F -4.03813200 0.98760300 - 0.13153900 F -3.96062900 -1.39044900 0.20084800 Br 3.07166300 -0.73089600 - 0.02286000 Cl 1.38816700 2.15298300 - 0.03822600
2F-HMe P -1.61109200 -0.08374500 0.00843800 O -0.64020500 -1.16989300 - 0.38296400 O -1.08701000 1.34720500 0.39435100 H -0.03897000 1.40755800 0.30734900 P 2.25761300 0.24990700 - 0.14601000 O 1.39462600 1.48575400 0.19325700	2F-2Me P -1.93440500 -0.00159100 0.04798000 O -1.03865800 0.56203900 1.12431000 O -1.32077900 -0.66461800 - 1.23270500 H -0.24720800 -0.73714900 - 1.17502500 P 1.95334000 -0.05011500 - 0.05105700 O 1.12970100 -0.84313300 - 1.10030200	2F-MeF P -2.04802800 0.06287700 - 0.01471400 O -1.18659500 1.29700400 0.03597000 O -1.39755500 -1.37199300 - 0.07745700 H -0.37274900 -1.32965500 - 0.14848400 P 2.04190600 -0.06245400 - 0.01268000 O 1.12649100 -1.24989100 - 0.28867000

H 3.55153800 0.62574300 - 0.56298500 O 1.79305300 -0.64153700 - 1.43036500 H 0.87153400 -0.96396800 - 1.25987100 C 2.44202100 -0.88410300 1.25020100 H 3.14227200 -1.68926000 0.98360400 H 2.80896500 -0.32791300 2.12496200 H 1.45289700 -1.31316900 1.47101600 F -2.75537800 0.16974400 - 1.07517600 F -2.55816600 -0.51408200 1.22007100	O 1.49809100 -0.25507000 1.50399300 H 0.54064700 -0.00716500 1.58061400 C 1.90124900 1.73331200 - 0.37036400 H 2.23159400 1.93028000 - 1.40083600 H 0.86059500 2.06930600 - 0.24667700 H 2.54302700 2.26487300 0.34742100 F -2.97378700 1.07948600 - 0.50630400 F -3.00346400 -1.04976800 0.60806500 C 3.66793600 -0.60529500 - 0.01449100 H 3.67647200 -1.67823500 0.22486000 H 4.11851300 -0.44762100 - 1.00502600 H 4.22565600 -0.04801400 0.75174200	O 1.43069100 1.40329400 - 0.23396300 H 0.43396500 1.41280200 - 0.12632600 C 3.60612500 -0.06763900 - 0.88269200 H 4.14728700 -0.98944200 - 0.62941600 H 3.40390100 -0.03610400 - 1.96203100 H 4.18880000 0.81316700 - 0.58033600 F -3.10394200 0.08195700 - 1.20963200 F -3.08688800 -0.03142300 1.18929100 F 2.50967800 -0.06148900 1.53885300
2F-MeCl P -2.16700700 0.01273300 0.06187200 O -1.30881000 0.12690700 1.29408800 O -1.53195800 0.10619600 -	2F-MeBr P -2.44904100 -0.02460800 0.06225200 O -1.61714400 0.21581600 1.29412700 O -1.84567700 0.18966700 -	2Cl-2Cl P -1.98196500 -0.15411900 0.06652100 O -1.11996400 -0.17950900 1.31797300 O -1.39956100 -0.79824700 -

1.37788500 H -0.52778800 0.33939100 - 1.34751800 P 1.81504600 0.37494300 - 0.06844600 O 0.92742800 0.70716000 - 1.27106500 O 1.24886600 0.76781300 1.38759400 H 0.27264700 0.54920800 1.44826600 C 3.45697600 1.09980100 - 0.11437900 H 3.96245000 0.76113000 - 1.02897700 H 3.34312800 2.19376100 - 0.12593000 H 4.01550400 0.78093200 0.77610600 F -3.37767800 1.05112300 0.04275000 F -3.03056100 -1.32561500 0.01804500 Cl 2.14479800 -1.66073800 0.01493600	1.37850300 H -0.88634900 0.56718400 - 1.34897100 P 1.41901600 0.86075600 - 0.06822200 O 0.50415800 1.13558300 - 1.26714900 O 0.83090400 1.20268100 1.39472000 H -0.10817900 0.86183900 1.46705200 C 2.99897700 1.71636900 - 0.11204800 H 3.52256500 1.43199100 - 1.03497300 H 2.79749500 2.79808800 - 0.10576200 H 3.58646700 1.42862900 0.77042800 F -3.81472800 0.79933800 0.05634600 F -3.07979700 -1.48706900 0.00560300 Br 1.93192300 -1.30538700 0.00317100	1.27675300 H -0.41085700 -0.58471800 - 1.35621500 P 1.98196400 -0.15411600 - 0.06649700 O 1.11987100 -0.17952000 - 1.31788300 O 1.39959700 -0.79822600 1.27681000 H 0.41089100 -0.58478800 1.35625500 Cl 2.53093800 1.75303000 0.39540300 Cl 3.74314900 -1.12255300 - 0.28417100 Cl -3.74318900 -1.12252000 0.28410800 Cl -2.53087300 1.75304600 - 0.39543300
2Cl-2Br P -1.27995600 -0.20244500 - 0.04053600 O -0.42969000 -0.53175500 - 1.26129800	2Cl-ClF P -2.21126800 0.29728400 0.06997900 O -1.32404300 0.27267500 1.29427100	2Cl-BrF P -1.70900200 0.75607900 0.06986100 O -0.81700900 0.77237200 1.29341000

O -0.69129000 -0.55359700 1.41102800 H 0.28524200 -0.28209100 1.43985400 P 2.65800900 -0.04120700 0.04523700 O 1.78791900 0.22321900 1.26258400 O 2.04563700 0.22868100 - 1.40756900 H 1.06844900 -0.04923600 - 1.42041000 Cl 3.34247300 -1.96248400 0.02813000 Br -1.78941700 1.94266600 0.00583600 Br -3.19292800 -1.25237600 - 0.03509000 Cl 4.34323200 1.07387100 0.02457200	O -1.55705900 0.47962900 - 1.36762600 H -0.59356300 0.16208100 - 1.36801000 P 1.78413200 -0.15706700 - 0.04695100 O 0.88386700 -0.36899100 - 1.25276700 O 1.18079700 -0.43213400 1.40927000 H 0.20332800 -0.17256300 1.42437100 Cl 2.53299100 1.73834700 - 0.00283500 F -3.27333600 1.48920200 0.09432100 Cl -3.44569500 -1.29982900 - 0.03423600 Cl 3.42969200 -1.32704900 - 0.07562600	O -1.05722900 0.94398000 - 1.37192200 H -0.14598900 0.50253100 - 1.39693700 P 2.15964200 -0.18184800 - 0.04868100 O 1.24087200 -0.25612500 - 1.25663000 O 1.52208000 -0.37352900 1.40689400 H 0.60550900 0.05384200 1.43246200 Br -2.99122700 -1.00868900 - 0.00836700 Cl 3.61573800 -1.58100900 - 0.07779500 Cl 3.17677100 1.58386100 0.00311400 F -2.78983700 1.93246700 0.07057600
2Cl-BrCl P -1.61803300 0.56071900 0.05385000 O -0.73518000 0.77349000 1.27486100 O -0.99760600 0.85170900 - 1.39525400 H -0.06095100 0.46656000 - 1.43061300 P 2.27217500 -0.07665700 -	2Cl-HMe P 1.14766900 -0.14271200 - 0.04259300 O 0.26177100 -0.46369000 - 1.23412400 O 0.66502100 -0.54734700 1.41503500 H -0.37412500 -0.41176100 1.48839500 P -2.64551100 -0.23380500	2Cl-2Me P 1.45290500 -0.16841100 - 0.03911300 O 0.62431000 -0.40572800 - 1.29094600 O 0.87503300 -0.58930900 1.37135000 H -0.19061500 -0.43996300 1.39562400 P -2.36032300 -0.08301000

0.04668800 O 1.36994300 -0.21903700 - 1.26100000 O 1.63590200 -0.27655900 1.40735600 H 0.69950700 0.11544300 1.42488500 Br -2.40507100 -1.49417700 - 0.00723800 Cl 3.80071100 -1.39836500 - 0.04192200 Cl -3.25990900 1.74108500 0.05849800 Cl 3.19698200 1.74059900 - 0.01987400	0.18830800 O -1.81945400 -0.20218800 1.49362500 H -3.99216700 -0.57764900 0.43244600 O -2.25294100 -1.38207500 - 0.90111300 H -1.30841800 -1.23956200 - 1.16941300 C -2.63736200 1.35407700 - 0.67738800 H -3.30266900 1.30435400 - 1.55182500 H -2.96542900 2.14467700 0.01305300 H -1.60622600 1.55478900 - 1.00619800 Cl 2.99960700 -0.96131300 - 0.16246200 Cl 1.53013800 1.87371500 0.01450700	0.06432100 O -1.57171700 -0.24623900 1.39118100 O -1.95981600 -1.12690900 - 1.12569400 H -0.99171700 -1.02102600 - 1.32197500 Cl 1.92597600 1.82959000 0.10143900 Cl 3.27614500 -1.06218200 - 0.10373600 C -2.16320500 1.58422500 - 0.62002700 H -2.47039800 2.32499700 0.13292800 H -1.09938900 1.72956200 - 0.86239000 H -2.76498300 1.69219400 - 1.53430400 C -4.11434600 -0.43249900 0.29406700 H -4.21409000 -1.46587700 0.65570400 H -4.52341000 0.25905800 1.04475100 H -4.64736900 -0.31845600 - 0.66075500
2Cl-MeF P -1.55469000 -0.12300100 - 0.05600900	2Cl-MeCl P 1.70117000 -0.09247200 - 0.05898000	2Cl-MeBr P -1.98804800 0.18365700 0.06079900

O -0.71553400 -0.36621800 - 1.29808100 O -0.91602900 -0.41558800 1.37502100 H 0.09398500 -0.22286700 1.36396200 P 2.48733900 -0.04355800 0.06541800 O 1.58906800 0.03833200 1.29481500 O 1.88091400 -0.73180800 - 1.24885900 H 0.88521700 -0.60701400 - 1.31460200 C 4.08491100 -0.81557700 0.30693200 H 4.61944300 -0.27739500 1.10159400 H 3.92494200 -1.86071400 0.60541000 H 4.65204800 -0.77231300 - 0.63282600 Cl -2.23632400 1.80096600 - 0.00043500 Cl -3.26054700 -1.21896900 - 0.01937400 F 2.89606900 1.44893800 - 0.41696500	O 0.84256300 -0.23199300 - 1.30395800 O 1.03700300 -0.33033000 1.37040900 H 0.07104800 0.03041100 1.37384100 P -2.23833300 0.34670200 0.06251300 O -1.33100600 0.60344600 1.26941000 O -1.62647100 0.66024900 - 1.39382600 H -0.67406100 0.34145300 - 1.44939100 Cl 2.58482800 1.75022900 0.02039300 Cl 3.27460300 -1.36832300 - 0.04198900 Cl -2.77901800 -1.64443300 0.00396500 C -3.79804100 1.23717300 0.08487600 H -4.34084000 0.96666400 1.00081700 H -3.57290600 2.31378200 0.08063300 H -4.38128000 0.96319700 - 0.80469400	O -1.19778300 0.51462200 1.31425100 O -1.53988500 0.81867700 - 1.33059700 H -0.51898900 0.95599800 - 1.35866300 P 1.85306600 0.90268300 - 0.11210600 O 0.98407400 1.18354000 - 1.34259000 O 1.28488300 1.38379200 1.31853900 H 0.32771900 1.09561100 1.41690900 C 3.50793200 1.60248700 - 0.17811800 H 4.01124900 1.22096100 - 1.07694100 H 3.40967200 2.69712100 - 0.23219200 H 4.05678800 1.30910700 0.72702600 Cl -2.07381800 -1.83633700 - 0.23500700 Br 2.16270000 -1.29486200 0.09798200 Cl -3.94113000 0.71435500 0.19124000
2Br-2Br P -1.94336400 -0.39061900	2Br-ClF P -1.11000200 -0.27704600 -	2Br-BrF P -1.49963200 -0.32617100 -

0.06420800 O -1.12524800 -0.55961400 1.33793400 O -1.41909000 -1.09634800 - 1.27841700 H -0.42388900 -0.92431700 - 1.37443900 P 1.94336600 -0.39065700 - 0.06416100 O 1.12529900 -0.55988200 - 1.33788200 O 1.41914000 -1.09624800 1.27856100 H 0.42389800 -0.92440000 1.37450600 Br 2.18650100 1.74814300 0.41634300 Br 3.97387000 -1.17576500 - 0.23760800 Br -3.97383400 -1.17583400 0.23758000 Br -2.18656100 1.74815900 - 0.41638200	0.04477400 O -0.29792400 -0.69678000 - 1.26336000 O -0.62639000 -0.78065900 1.40172400 H 0.37111200 -0.63591000 1.47732300 P 2.83208900 -0.55567200 0.15085900 O 1.93842300 -0.30060700 1.34424900 O 2.22704000 -1.24608000 - 1.14695100 H 1.23486500 -1.04884700 - 1.23092500 Br -1.24046500 1.92029400 0.07871800 Br -3.17554200 -0.97676900 - 0.11200200 Cl 3.79857100 1.11595600 - 0.44672800 F 4.06867600 -1.51400800 0.47070700	0.04610200 O -0.72384000 -0.80109100 - 1.26775800 O -1.15712000 -0.98462700 1.37876500 H -0.15456100 -0.97616600 1.50254800 P 2.33849700 -0.97356000 0.22479300 O 1.45136800 -0.82123900 1.44228000 O 1.73692000 -1.60717000 - 1.10710900 H 0.77139000 -1.32134500 - 1.22437600 Br -1.27132200 1.85210600 0.21452200 Br -3.64692000 -0.67271200 - 0.21021600 F 3.59722700 -1.92763600 0.46909700 Br 3.31728500 0.90218400 - 0.31144400
2Br-BrCl P 1.74254200 -0.19230800 0.04226200 O 0.92564400 -0.58807200 1.26606900 O 1.18034400 -0.59028300 - 1.40763700	2Br-HMe P 0.57098200 -0.28775300 - 0.01365700 O -0.25630800 -0.72237500 - 1.21548500 O 0.09481300 -0.70642100 1.44648500	2Br-2Me P 0.81593700 -0.28359600 - 0.03018900 O 0.01402500 -0.62279500 - 1.28012800 O 0.24642200 -0.68777000 1.39263800

H 0.18655400 -0.38773900 - 1.43641200	H -0.94945800 -0.59813000 1.51005800	H -0.81964800 -0.52901700 1.41623700
P -2.19325000 -0.32703100 - 0.03942900	P -3.20204900 -0.51389900 0.17390400	P -2.98504800 -0.26968900 0.06236000
O -1.34307300 0.01467700 - 1.25411100	O -2.39896900 -0.42627300 1.49136400	O -2.19705100 -0.32258000 1.39910100
O -1.60108900 -0.01992400 1.41689600	H -4.54178400 -0.89279600 0.40442400	O -2.55388800 -1.38208100 - 1.05233300
H -0.60510400 -0.22338100 1.42719900	O -2.75551300 -1.67487700 - 0.88021500	H -1.58855700 -1.26454300 - 1.25777800
Br -4.10179300 0.72862700 - 0.01438700	H -1.80990100 -1.51189000 - 1.13556300	Br 2.83661600 -1.14045700 - 0.04421200
Cl -2.70272600 -2.30621100 - 0.03455200	C -3.22669400 1.05328200 - 0.72838900	Br 1.15763000 1.91620000 0.03748700
Br 2.07729600 1.98708200 - 0.00606200	H -3.86566500 0.96001500 - 1.61869700	C -4.73050300 -0.64748800 0.31230800
Br 3.73395200 -1.08497700 0.03143200	H -3.60156700 1.84616500 - 0.06470200	H -4.80504900 -1.65769000 0.73961100
	H -2.19467200 1.28657000 - 1.03188600	H -5.15866700 0.08047400 1.01646600
	Br 2.64541300 -0.99010300 - 0.08165500	H -5.26361700 -0.60874900 - 0.64849300
	Br 0.73507300 1.92880900 0.00067800	C -2.82778000 1.35169600 - 0.73275000
		H -3.16206800 2.13263500 - 0.03369500
		H -1.76609800 1.51183300 - 0.97497800
		H -3.42461600 1.37987500 - 1.65613800

2Br-MeF	2Br-MeCl	2Br-MeBr
P -0.88899000 -0.25820500 - 0.05659800	P -1.04400200 -0.31332100 - 0.04747300	P 1.37202300 -0.32967400 - 0.04305300
O -0.09195700 -0.62269100 - 1.30118900	O -0.26554000 -0.72261500 - 1.28977600	O 0.58668900 -0.72922100 - 1.28420200
O -0.28953400 -0.63938800 1.37629200	O -0.53178200 -0.81322600 1.38202400	O 0.93510200 -0.93152200 1.37183800
H 0.72344300 -0.46685100 1.38276000	H 0.49718000 -0.79118000 1.41512500	H -0.09078300 -1.01193600 1.42556200
P 3.11772500 -0.23557600 0.06605100	P 2.85975000 -0.59554900 0.11596900	P -2.47171200 -1.02307000 0.17781400
O 2.22622000 -0.21438900 1.30266200	O 2.02138700 -0.77875200 1.38331200	O -1.60651400 -1.16045000 1.43518700
O 2.51702800 -0.88394100 - 1.27081100	O 2.30538200 -1.26529900 - 1.23948100	O -1.88116000 -1.62860500 - 1.19522500
H 1.51657100 -0.78937300 - 1.32434400	H 1.31908300 -1.09502100 - 1.33770700	H -0.92881200 -1.33152300 - 1.31918400
C 4.72990900 -0.98764300 0.27173300	C 4.55418300 -1.18025700 0.23296300	Br -2.83632100 1.13412800 - 0.24868100
H 5.26026500 -0.46758800 1.08112000	H 5.04378900 -0.66473600 1.07038200	Br 3.49132200 -0.87458100 - 0.16094800
H 4.58932000 -2.04483400 0.53550000	H 4.52525100 -2.26394700 0.41917700	Br 1.37861600 1.86760500 0.19360800
H 5.29019200 -0.90304900 - 0.66930800	H 5.07472300 -0.96600100 - 0.71022800	C -4.11009100 -1.75343000 0.30311100
Br -1.28929600 1.91429600 - 0.00191300	Br -1.18757600 1.88862100 0.08336600	H -3.98595400 -2.83478200 0.46471800
Br -2.86991500 -1.18965700 - 0.00834800	Cl 3.03598200 1.41749100 - 0.31402600	H -4.62893100 -1.29846200 1.15786600
F 3.49867200 1.28057900 - 0.36382100	Br -3.12295600 -1.00184200 - 0.07857000	H -4.65915100 -1.56347300 - 0.62908100

CIF-CIF P 1.99259100 0.29544500 0.02428300 O 1.08124100 0.22875800 1.23016000 O 1.40989400 -0.06424900 - 1.41064300 H 0.39719100 -0.09573200 - 1.39855000 P -2.04396300 -0.36008100 - 0.10057800 O -1.17708800 -0.11872800 - 1.31638300 O -1.35345500 -0.64752100 1.30262000 H -0.39843700 -0.31152200 1.31139900 F -3.01116400 -1.62211400 - 0.25314800 F 2.62960900 1.75403300 - 0.15504900 Cl 3.66341200 -0.81486800 0.19162100 Cl -3.39746600 1.10918700 0.18833800	CIF-BrF P -1.51046100 0.71753300 - 0.10756400 O -0.65322500 0.53105200 - 1.34218600 O -0.80179900 0.88087300 1.30971800 H 0.09943200 0.42009300 1.31136800 P 2.42455600 -0.33230000 - 0.00668700 O 1.49461100 -0.31417900 1.18685100 O 1.92107800 0.26145000 - 1.39303200 H 0.91430700 0.38075500 - 1.39780700 Br -3.03528000 -0.82708800 0.08492900 F 2.90629900 -1.81984000 - 0.35489300 F -2.41379000 2.03637500 - 0.15719200 Cl 4.19951500 0.56155200 0.31445000	CIF-BrCl P -2.67323200 -0.43856400 0.15448400 O -1.82393400 -0.04566500 1.34351800 O -1.97286500 -1.04610900 - 1.13698300 H -1.02064000 -0.70545500 - 1.22196400 P 1.28768100 0.18038700 - 0.02271300 O 0.43404600 -0.11186100 - 1.24825800 O 0.76190100 -0.32157300 1.40531900 H -0.24627100 -0.23102500 1.44992800 F -3.75550500 -1.56511100 0.48573600 Br 3.28557600 -0.69106800 - 0.12866400 Cl 1.61980600 2.18517100 0.16143600 Cl -3.87502100 1.06683900 - 0.45447700
CIF-HMe P 1.35735100 -0.35812800 - 0.10351600 O 0.39168000 -0.32031900 - 1.26845100	CIF-2Me P 1.66670800 -0.37556200 - 0.08296600 O 0.77074000 -0.26597500 - 1.29922000	CIF-MeF P -1.77143000 0.34873000 0.06713100 O -0.89711100 0.33413700 1.30072300

O 0.83279800 -0.73401900 1.33848600	O 1.04703800 -0.71257200 1.32380800	O -1.10908400 0.50863600 - 1.36415200
H -0.18955100 -0.51295500 1.42643600	H -0.01435200 -0.53363100 1.33981400	H -0.10376600 0.29557200 - 1.34196100
P -2.46719300 -0.04485400 0.20975800	P -2.17380200 0.04817000 0.07564500	P 2.28266800 -0.06876400 - 0.06758400
O -1.60671900 -0.18844200 1.48465400	O -1.38432000 -0.31271900 1.36192400	O 1.38147400 0.01197800 - 1.29461500
H -3.82525200 -0.33160400 0.46360200	O -1.84789300 -0.87286200 - 1.23316700	O 1.72169700 0.54868700 1.30151100
O -2.17470100 -1.10227000 - 0.99696800	H -0.87661300 -0.80335200 - 1.42514500	H 0.72111000 0.48664800 1.35615700
H -1.22803300 -0.99519700 - 1.27275700	C -1.88562300 1.76819700 - 0.41903200	C 3.92729700 0.61362600 - 0.25437200
C -2.38605600 1.61553700 - 0.50183300	H -2.50007900 2.01840800 - 1.29625200	H 4.42585300 0.10678400 - 1.09184200
H -3.08551700 1.69211300 - 1.34721100	H -2.12626000 2.43502400 0.42197800	H 3.83632800 1.68748800 - 0.46767500
H -2.63455000 2.35557200 0.27267700	H -0.82083400 1.87132700 - 0.67796800	H 4.48972600 0.45820500 0.67631700
H -1.35711900 1.78029600 - 0.85643200	C -3.94249800 -0.22516600 0.29420300	F -2.85130800 1.53056300 0.07451200
F 2.57031300 -1.38216000 - 0.30846900	H -4.09786400 -1.28465900 0.54306000	Cl -3.00192900 -1.25576300 - 0.02558000
Cl 2.38863000 1.38606600 0.06150000	H -4.30402600 0.40198400 1.12186400	F 2.59079600 -1.61895000 0.29095000
	H -4.47726700 0.02214300 - 0.63402700	
	F 2.82626500 -1.46962800 - 0.25203000	
	Cl 2.80420800 1.29794800 0.14746900	

ClF-MeCl	ClF-MeBr	BrF-BrF
P -1.90318200 0.38938900 0.09419700	P -2.16370600 0.42300000 0.08818700	P -1.83945400 0.77791400 - 0.08739200
O -1.02078000 0.43517900 1.32092300	O -1.33374400 0.67771300 1.32558300	O -0.94885000 0.59765400 - 1.29857800
O -1.31030400 0.78038900 - 1.32250700	O -1.63938500 0.89615200 - 1.33103500	O -1.17510400 0.88151600 1.35777000
H -0.28053500 0.74845400 - 1.32745800	H -0.61957300 1.04091400 - 1.33152200	H -0.33881400 0.31564900 1.39568900
P 2.06004700 0.31115000 - 0.09010000	P 1.71590400 0.81059300 - 0.08400700	P 1.84525400 -0.78597600 0.08004600
O 1.23025000 0.73004300 - 1.30616100	O 0.87922000 1.26319400 - 1.28532100	O 0.94637600 -0.62500600 1.28791900
O 1.58015600 0.85166200 1.34967000	O 1.23150000 1.29465000 1.37692100	O 1.18909200 -0.88527400 - 1.36909200
H 0.58738800 0.74354800 1.44131600	H 0.24993400 1.11791700 1.47515200	H 0.34663100 -0.32857700 - 1.40599400
C 3.79856700 0.75405200 - 0.16801600	C 3.44821500 1.28624300 - 0.14516400	Br -3.42471600 -0.71687300 0.02085200
H 4.23204100 0.30673800 - 1.07286200	H 3.88657200 0.88441000 - 1.06882500	F 2.70638400 -2.13089000 0.11872100
H 3.86589700 1.85083300 - 0.21714500	H 3.49597900 2.38560500 - 0.14780900	Br 3.41406900 0.72748700 - 0.00896000
H 4.30627300 0.37748600 0.73027600	H 3.96259100 0.88046200 0.73652100	F -2.68574700 2.13213900 - 0.13204100
F -3.18112900 1.34687400 0.20412800	F -3.61126400 1.10157500 0.15509400	
Cl 2.05142300 -1.74698800 0.08068100	Cl -2.69046400 -1.52504200 - 0.09878900	
Cl -2.81965000 -1.40357200 -	Br 1.71973700 -1.41636500	

0.12656600	0.02111900	
BrF-BrCl	BrF-HMe	BrF-2Me
P -1.99351000 0.89312200 - 0.22350000	P 0.89708000 -0.86467000 - 0.11133300	P 1.21415500 -0.86068300 - 0.08426500
O -1.06688300 0.82546300 - 1.41904300	O -0.03565400 -0.87223900 - 1.30365500	O 0.35347400 -0.91441500 - 1.32938900
O -1.47486300 1.55277900 1.13074300	O 0.34146000 -1.20257000 1.33138000	O 0.58515400 -1.15900200 1.33058200
H -0.49576600 1.33389800 1.27086500	H -0.61087800 -0.78260600 1.44463200	H -0.41682600 -0.78594900 1.37426600
P 1.87637800 0.55249700 0.12515900	P -2.72201300 0.20274800 0.20977800	P -2.46025000 0.12519700 0.07604100
O 1.03317700 0.91223900 1.33899100	O -1.93388400 -0.15007200 1.49052900	O -1.72793000 -0.27924400 1.38241300
O 1.51331300 1.22270400 - 1.28655100	H -4.10789900 0.29529000 0.45818200	O -2.33995800 -0.93840300 - 1.15776500
H 0.51944500 1.13022500 - 1.43815700	O -2.72262900 -0.91066400 - 0.98184300	H -1.37908800 -1.08153200 - 1.35975500
F -3.31454900 1.75261500 - 0.48823600	H -1.78350500 -1.07169200 - 1.25581300	C -1.86146600 1.71759300 - 0.55198100
Cl 3.82341300 1.05162300 0.33764600	C -2.19448200 1.77226800 - 0.51873800	H -2.42088300 2.00319500 - 1.45484400
Br 1.88232900 -1.62424500 - 0.20215800	H -2.83011600 2.01393900 - 1.38313800	H -1.97647800 2.48258900 0.23017300
Br -2.83866500 -1.05875500 0.26454100	H -2.26069100 2.56343700 0.24237500	H -0.79458100 1.61071200 - 0.80091700
	H -1.14891200 1.66342100 - 0.84529000	C -4.24494700 0.21227900 0.31810900
	Br 1.97210300 1.04905100 0.02441800	H -4.59538100 -0.77706900 0.64524100

	F 2.11832800 -1.89099800 - 0.24123500	H -4.46663800 0.95544100 1.09760400 H -4.73784800 0.48919200 - 0.62485300 F 2.46176300 -1.86497100 - 0.12854100 Br 2.25702400 1.07627800 0.05056600
BrF-MeF P -1.25675000 0.74119700 0.06842100 O -0.38712200 0.69442700 1.30675900 O -0.57661800 0.85909600 - 1.36162700 H 0.37885000 0.48197000 - 1.34972900 P 2.69952400 -0.16064100 - 0.06819200 O 1.79804600 -0.05042900 - 1.29281800 O 2.23937500 0.61192200 1.25922100 H 1.23929000 0.66789600 1.33153200 C 4.41378300 0.29707000 - 0.30794100 H 4.83380000 -0.32102000 - 1.11317000 H 4.45436900 1.35785700 -	BrF-MeCl P -1.42940000 0.87092600 0.10834600 O -0.55667200 0.96425800 1.34129500 O -0.82556800 1.23071500 - 1.31552300 H 0.18240200 1.02996200 - 1.34966900 P 2.42487400 0.21702200 - 0.10533400 O 1.67681700 0.74278200 - 1.33244300 O 2.08109500 0.89517200 1.31529200 H 1.08755600 0.97508700 1.42485700 C 4.21543700 0.30455800 - 0.21010100 H 4.54012800 -0.25187900 - 1.09987000 H 4.49670000 1.36401500 -	BrF-MeBr P -1.73834000 0.91048300 0.12426500 O -0.86394400 1.04949300 1.35165800 O -1.18311800 1.35216600 - 1.29618900 H -0.15602900 1.29698400 - 1.33116500 P 2.15077500 0.71359500 - 0.11843600 O 1.36269700 1.23111300 - 1.32614200 O 1.76189900 1.31188700 1.32877900 H 0.76760900 1.27204500 1.44983100 C 3.93030000 0.94764300 - 0.21840000 H 4.29446600 0.45797500 - 1.13185700 H 4.12614500 2.02957700 -

0.59091500 H 4.96520500 0.13288200 0.62779300 Br -2.67346100 -0.92094300 - 0.00916100 F 2.81674600 -1.71038700 0.39124300 F -2.26276000 1.98844800 0.04954100	0.30160900 H 4.65094700 -0.13165000 0.69901400 Br -2.40031700 -1.08225500 - 0.06488400 F -2.70547500 1.83647900 0.16627300 Cl 2.01014900 -1.79087800 0.14989600	0.26234400 H 4.40013800 0.50686100 0.67128100 Br -2.54462500 -1.11193700 - 0.09031700 F -3.09298300 1.76040500 0.21926700 Br 1.85936600 -1.48838800 0.07285900
BrCl-BrCl P -1.87707900 0.56247500 0.05134100 O -0.97068800 0.64101700 1.27096100 O -1.22248000 0.74937000 - 1.39979600 H -0.35127200 0.23126400 - 1.43507700 P 1.87749300 -0.56309500 - 0.05023600 O 0.97006500 -0.64395900 - 1.26894800 O 1.22422800 -0.74868400 1.40165200 H 0.35218100 -0.23198800 1.43669400 Br -2.97231900 -1.34634000 - 0.00131100 Br 2.97103500 1.34679600 - 0.00088200	BrCl-HMe P 0.67593100 0.10044800 - 0.00649300 O -0.16147900 -0.34418900 - 1.19613300 O 0.20783900 -0.29797600 1.45931300 H -0.84303500 -0.27268700 1.51169200 P -3.08878100 -0.41444500 0.17776600 O -2.29815400 -0.22507700 1.49196700 H -4.39007800 -0.90361700 0.42006500 O -2.54201100 -1.55751500 - 0.84886500 H -1.61736200 -1.31241300 - 1.11342600 C -3.25073500 1.12121200 - 0.76350200	BrCl-2Me P 1.13260700 -0.61857100 - 0.04966000 O 0.28685200 -0.82021900 - 1.29801200 O 0.52050400 -0.95552800 1.37142900 H -0.50892700 -0.64709500 1.40405200 P -2.62500600 -0.04181000 0.06704000 O -1.84689200 -0.24066500 1.39526200 O -2.36971400 -1.18057400 - 1.07515600 H -1.39834000 -1.20722700 - 1.28242800 C -2.23250100 1.55559200 - 0.69490400 H -2.82182900 1.69202500 - 1.61343100

Cl 3.31969200 -1.98133100 - 0.05142300 Cl -3.31799600 1.98204200 0.05304800	H -3.89042200 0.95286900 - 1.64225700 H -3.68090900 1.89911600 - 0.11605400 H -2.24424300 1.42520000 - 1.08935000 Cl 0.85042100 2.14942800 - 0.01512300 Br 2.75018600 -0.59851400 - 0.08434100	H -2.44488800 2.36198500 0.02263000 H -1.15973500 1.56246900 - 0.94104500 C -4.40620700 -0.16139100 0.32201500 H -4.62837600 -1.15782800 0.72988700 H -4.71844500 0.60746400 1.04344900 H -4.93181600 -0.02405300 - 0.63385500 Br 1.80905400 1.49701900 0.04276000 Cl 2.86986400 -1.67453000 - 0.08220000
BrCl-MeF P -1.21181900 -0.59251800 - 0.05930900 O -0.37111500 -0.82877300 - 1.30382000 O -0.56653600 -0.88469200 1.37225900 H 0.41112000 -0.57063400 1.38053800 P 2.75480900 -0.02030400 0.06681600 O 1.86340500 -0.10604300 1.30068200 O 2.25169100 -0.75788200 -	BrCl-MeCl P -1.37982300 -0.62873500 - 0.07873300 O -0.54763100 -0.90980200 - 1.31952200 O -0.82191000 -1.08331300 1.34652100 H 0.19448800 -0.93006900 1.39181900 P 2.52305800 -0.40446400 0.11821700 O 1.70568400 -0.71700900 1.37380100 O 2.07350700 -1.11997300 -	BrCl-MeBr P -1.71384400 -0.62782800 - 0.10266500 O -0.87227800 -0.90528500 - 1.33799800 O -1.23766000 -1.21125300 1.30496000 H -0.21105100 -1.17745100 1.37711300 P 2.17691500 -0.88811200 0.17136400 O 1.31260700 -1.15105000 1.40912900 O 1.68088900 -1.52472600 -

1.26422300 H 1.24816500 -0.79267000 - 1.32353900 C 4.45262600 -0.54686900 0.28359000 H 4.90534700 0.04706600 1.08926700 H 4.45469200 -1.61097600 0.55683100 H 4.99977400 -0.39604000 - 0.65690800 Cl -2.89704700 -1.72112100 - 0.01645500 F 2.92974100 1.52877600 - 0.37837300 Br -1.95477500 1.48331400 - 0.00041200	1.25276700 H 1.07497800 -1.07676700 - 1.36004600 C 4.27891200 -0.76194300 0.24357300 H 4.68945700 -0.19963800 1.09327800 H 4.39226300 -1.84277700 0.41339800 H 4.77391300 -0.46571700 - 0.69115300 Cl -3.20600000 -1.51142700 - 0.13531800 Br -1.83167200 1.52477500 0.08526200 Cl 2.43448300 1.62073600 - 0.28053200	1.22488300 H 0.70363600 -1.33369000 - 1.36065100 C 3.88531900 -1.43137000 0.31112200 H 4.33605900 -0.94003800 1.18417800 H 3.88234700 -2.52320700 0.44784800 H 4.42354600 -1.15930900 - 0.60696400 Cl -3.60632600 -1.34607800 - 0.25632700 Br -1.99164700 1.54231600 0.18011700 Br 2.30154900 1.30576500 - 0.20271300
HMe-HMe P 1.81631500 0.16936400 0.44230700 O 0.87458300 -0.64384700 1.35558100 O 1.23737400 1.58087800 - 0.12641700 H 0.40178100 1.37104600 - 0.65490600 P -1.81612800 -0.16939300 - 0.44239100 O -0.87515400 0.64534100 - 1.35504700	HMe-2Me P -2.18399900 0.27178600 0.12123100 O -1.33403800 0.54997100 1.37884300 O -1.61100100 0.84670400 - 1.28829900 H -0.69940800 0.42066100 - 1.43295900 P 1.56687500 -0.08790900 - 0.08403300 O 0.66719200 -0.39066900 - 1.30665700	HMe-MeF P -1.60335400 0.03501700 0.07396500 O -0.67017000 0.15724900 1.27303600 O -1.09508600 -0.79874300 - 1.18873000 H -0.07144000 -0.76585200 - 1.28580400 P 2.26578000 -0.26842300 - 0.10904500 O 1.44989900 -0.68335000 - 1.35053600

O -1.23579900 -1.58056700 0.12575100	O 1.00778300 -0.62996300 1.35045800	H 3.58572300 -0.76993600 - 0.14799600
H -0.40073600 -1.37001800 0.65502400	H 0.09183200 -0.23157800 1.49565100	O 1.77398200 -0.86297600 1.32587200
C 2.38852600 -0.77986700 - 0.99011300	C 1.83487300 1.69629300 0.11927000	H 0.83043300 -0.56413800 1.46594400
C -2.38982900 0.77839500 0.99039500	H 2.26118700 2.11273200 - 0.80532200	C 2.38454800 1.52845200 0.07713500
H 1.50955800 -1.00498200 - 1.61351000	H 0.85546700 2.16024900 0.31236400	H 3.04606200 1.77330200 0.92110500
H 3.10867000 -0.18389900 - 1.56957600	H 2.50388400 1.88698600 0.97110800	H 2.76880100 1.96771400 - 0.85484800
H 2.85000500 -1.71794300 - 0.64905400	C 3.17363500 -0.90993900 - 0.18987600	H 1.37271500 1.91313800 0.27741700
H -3.10955700 0.18131000 1.56923100	H 3.00257400 -1.99331000 - 0.26638100	C -3.26167400 -0.56298800 0.40800000
H -1.51135400 1.00409300 1.61427400	H 3.69882600 -0.55951100 - 1.09035300	H -3.72438700 0.08245300 1.16705600
H -2.85220700 1.71616500 0.64970600	H 3.76885800 -0.69112300 0.70835200	H -3.84794500 -0.54319700 - 0.52072500
H -2.96561000 -0.62721700 - 1.12545100	C -2.50303700 -1.49477300 - 0.12444200	H -3.19073600 -1.59203300 0.78663400
H 2.96643600 0.62627900 1.12488300	H -1.53589000 -1.98021600 - 0.32674600	F -1.90131700 1.52326900 - 0.51894900
	H -2.94746200 -1.91956000 0.78727600	
	H -3.17398500 -1.63785800 - 0.98408900	
	H -3.44134000 0.91654000 0.16866200	

HMe-MeCl	HMe-MeBr	2Me-2Me
P 1.41829700 -0.37602000 - 0.09812000	P 1.01183500 -0.89220400 - 0.10011700	P 1.90330000 -0.03084200 0.07356300
O 0.52024500 -0.66484400 - 1.30063200	O 0.07581400 -1.04331200 - 1.30067800	O 1.04019100 -0.00061100 1.35683100
O 0.90405600 -0.82651900 1.35003700	O 0.42941200 -1.22228400 1.35621000	O 1.35988100 -0.98775400 - 1.12768700
H -0.09798600 -0.61596700 1.46335900	H -0.50953800 -0.81251000 1.47112900	H 0.40761800 -0.71242200 - 1.32709700
P -2.39347400 -0.14012800 0.18979300	P -2.68357700 0.06284000 0.19692900	P -1.90321900 -0.03088700 - 0.07353700
O -1.58122100 -0.26868500 1.49534100	O -1.88956400 -0.17361700 1.49888900	O -1.04006800 -0.00053800 - 1.35678500
H -3.76673000 -0.40467900 0.38882800	H -4.07936200 0.04884500 0.41412700	O -1.35974100 -0.98758200 1.12776300
O -2.06197800 -1.21367600 - 0.98947200	O -2.56093400 -1.08216000 - 0.95478100	H -0.40736800 -0.71251500 1.32696500
H -1.09346200 -1.12638400 - 1.22140100	H -1.59510100 -1.18027700 - 1.19401800	C 3.56550400 -0.68949400 0.35190000
C -2.26900500 1.50987600 - 0.54403800	C -2.28053200 1.64630400 - 0.58131100	C 2.06089700 1.63431500 - 0.63706200
H -2.91769200 1.57410900 - 1.42992200	H -2.91505200 1.79950400 - 1.46648500	C -2.06144100 1.63425400 0.63698200
H -2.55898900 2.26289500 0.20322900	H -2.42952300 2.45699900 0.14690100	C -3.56530000 -0.68984300 - 0.35194300
H -1.22034300 1.67119700 - 0.83762800	H -1.22148500 1.61631700 - 0.88037900	H 2.43315000 2.33094900 0.12857900
C 3.09672600 -1.01604400 - 0.20193700	C 2.55232300 -1.82109200 - 0.18876800	H 2.73837900 1.61913000 - 1.50333500
H 3.56276100 -0.63035300 - 1.11890500	H 3.07599500 -1.54180800 - 1.11319100	H 1.05810900 1.94583400 - 0.96747600
H 3.66151800 -0.69528100	H 3.16562000 -1.58424100	H 3.46918400 -1.71379200

0.68384700 H 3.03616000 -2.11382500 - 0.24074100 Cl 1.69454500 1.68513600 0.04517000	0.69123300 H 2.29891300 -2.89196800 - 0.20366900 Br 1.69191700 1.24998000 0.01444300	0.73997400 H 4.12944600 -0.70238900 - 0.59203300 H 4.08179400 -0.06543600 1.09606900 H -2.73912000 1.61888700 1.50310800 H -1.05886500 1.94623900 0.96759000 H -2.43382000 2.33065500 - 0.12880500 H -4.12934800 -0.70271600 0.59193700 H -4.08156900 -0.06585500 - 1.09617700 H -3.46887100 -1.71416000 - 0.73992600
2Me-MeF P 1.94810200 -0.00159000 - 0.05290700 O 1.02693700 0.43478200 - 1.18795600 O 1.32831800 -0.06883000 1.41478700 H 0.30235600 -0.23751400 1.39526800 P -1.97328000 -0.01860900 0.07452800 O -1.16292500 -0.46813100 1.31345500	2Me-MeCl P 1.71666000 0.36792100 - 0.04823400 O 0.81288600 0.60578600 - 1.26088000 O 1.08079700 0.61536100 1.39976900 H 0.09865100 0.26784600 1.43037400 P -2.13115500 -0.04785900 0.07513800 O -1.29295800 -0.23854300 1.36250600	2Me-MeBr P 1.26423800 0.84673400 - 0.04919500 O 0.34448300 0.96334500 - 1.26958900 O 0.59658100 1.03689800 1.39501300 H -0.31710100 0.53527000 1.43443400 P -2.45995100 -0.13934900 0.07510500 O -1.60256200 -0.19592400 1.36298600

O -1.42869900 -0.55376400 - 1.36868500	O -1.50564200 -0.69223200 - 1.28846700	O -1.74343400 -0.68296700 - 1.28768100
H -0.47585300 -0.26629000 - 1.46202900	H -0.59626000 -0.30001700 - 1.42771700	H -0.90772200 -0.15309100 - 1.43198700
C -2.04452300 1.79069100 - 0.05692400	Cl 2.35629400 -1.60706600 - 0.03983900	Br 2.19415900 -1.19149100 - 0.01449800
H -2.43728800 2.21313800 0.87961000	C -2.40932100 1.70967200 - 0.28361400	C -3.90505200 -1.21650500 0.18479100
H -1.01810500 2.15205300 - 0.22237900	H -2.86713900 2.19636400 0.59007200	H -3.55331000 -2.24399200 0.35622700
H -2.67630600 2.08658200 - 0.90724700	H -1.42798300 2.16525000 - 0.48648100	H -4.52890900 -0.89808900 1.03252800
F 2.50406600 -1.50598500 - 0.32964700	H -3.05315500 1.82153700 - 1.16828100	H -4.48024500 -1.17191200 - 0.75113800
C -3.65723700 -0.67101900 0.09786800	C -3.72550100 -0.88918300 0.18146100	C -3.00403700 1.55394000 - 0.28727900
H -3.59925500 -1.76848700 0.12869900	H -3.53736500 -1.95922700 0.34994500	H -3.53071400 1.96680800 0.58562300
H -4.17302100 -0.30745000 0.99844100	H -4.29344200 -0.48046100 1.02977100	H -2.10387600 2.15376500 - 0.49163000
H -4.19681500 -0.35270500 - 0.80568400	H -4.28611900 -0.75338600 - 0.75454200	H -3.65755600 1.56391600 - 1.17187400
C 3.47936300 0.92298700 0.10329100	C 3.25368800 1.30596600 - 0.04178000	C 2.67797400 1.96458400 - 0.04754000
H 4.03211300 0.85717800 - 0.84378100	H 3.81176000 1.07060700 - 0.95829200	H 3.26156400 1.79081300 - 0.96193800
H 3.23344200 1.97168300 0.31969300	H 2.99854800 2.37566300 - 0.01776100	H 2.29475500 2.99597500 - 0.03099100
H 4.07515600 0.50025000 0.92370400	H 3.83907400 1.03333100 0.84678800	H 3.28939700 1.76902600 0.84387000

MeF-MeF	MeF-MeCl	MeF-MeBr
P 2.04566800 0.06552400 - 0.02815800	P -1.81789900 -0.36381000 0.07261100	P 2.50378900 -0.05619000 - 0.06491100
O 1.17217800 1.30052500 - 0.20745300	O -0.95240800 -0.62651600 1.30573200	O 1.59643700 0.02809400 - 1.28614100
O 1.40493900 -1.35645200 - 0.38577100	O -1.18483400 -0.70913200 - 1.36283300	O 1.81632100 -0.07400800 1.37987000
H 0.39387200 -1.35647000 - 0.29937200	H -0.20644100 -0.43750900 - 1.39374600	H 0.90361900 0.37359900 1.38441600
P -2.04567400 -0.06551600 - 0.02820200	P 2.19242900 0.00077400 - 0.06495800	P -1.39437800 0.85273200 0.07309100
O -1.17222400 -1.30046500 - 0.20805900	O 1.28505100 0.04503900 - 1.28822800	O -0.50829200 1.05530500 1.30501500
O -1.40497100 1.35657800 - 0.38539000	O 1.51240400 0.14726400 1.37592500	O -0.73637700 1.13197500 - 1.36758900
H -0.39391600 1.35660300 - 0.29887100	H 0.54212100 -0.15572800 1.38079900	H 0.19519500 0.72819000 - 1.40598000
C 3.63222600 0.09973000 - 0.86252400	C 3.55686900 1.16352500 - 0.06988400	C -2.91344600 1.81748300 0.05887800
H 3.45519000 0.16744900 - 1.94465800	H 4.16691700 0.98990100 - 0.96678800	H -3.48819200 1.57605800 0.96334300
H 4.19302400 0.97996300 - 0.51979500	H 3.14434900 2.18159800 - 0.08925900	H -2.63656700 2.88246100 0.05628100
H 4.18410600 -0.82033700 - 0.62670500	H 4.15952500 1.01722900 0.83683400	H -3.48838900 1.56747300 - 0.84306300
C -3.63233100 -0.09938700 - 0.86239000	C -3.41416200 -1.19102300 0.06756100	F 3.49678800 1.22837400 - 0.01148400
H -3.45542600 -0.16670100 - 1.94457100	H -3.23230700 -2.27575000 0.08233300	Br -2.08919300 -1.27286400 - 0.00724400
H -4.19309700 -0.97974400 - 0.51992700	H -3.96866600 -0.88724400 0.96582900	C 3.66474500 -1.42209700 - 0.05783200
H -4.18417300 0.82059600 -	H -3.96395500 -0.90686400 -	H 3.09373200 -2.36073400 -

0.62615700 F 2.49306900 -0.08262700 1.52598300 F -2.49287300 0.08206900 1.52605300	0.83990400 Cl -2.30076400 1.65024900 - 0.02383700 F 2.96839500 -1.42473100 0.00928000	0.06119100 H 4.28912600 -1.36096600 - 0.95956700 H 4.28846300 -1.36255300 0.84442900
MeCl-MeCl P 1.96575100 -0.38872800 - 0.09244600 O 1.15631600 -0.74603200 - 1.33970800 O 1.42723900 -0.92742500 1.32242900 H 0.41557300 -0.85333400 1.38072600 P -1.96574600 -0.38873100 0.09244600 O -1.15630900 -0.74602600 1.33970800 O -1.42722800 -0.92742200 - 1.32242800 H -0.41556000 -0.85333500 - 1.38071700 C 3.69207200 -0.89075300 - 0.12977200 H 3.72373100 -1.98794100 - 0.20101900 H 4.16838300 -0.43978800 - 1.01093100 H 4.18536300 -0.55174000 0.79123700	MeCl-MeBr P 2.25180100 -0.46468400 - 0.06775000 O 1.34130200 -0.46139200 - 1.29719500 O 1.55350000 -0.57832000 1.37483400 H 0.71290800 -0.00678800 1.41641500 P -1.46567900 0.86476000 0.07596500 O -0.56179900 0.90775300 1.31155800 O -0.76695600 1.02979800 - 1.36341700 H 0.07756200 0.46433700 - 1.41173100 C -2.78990700 2.08351000 0.06220200 H -3.39982200 1.94592700 0.96540300 H -2.32834200 3.08240500 0.06269000 H -3.39867200 1.94173500 - 0.84103300	MeBr-MeBr P 1.96084800 -0.85124300 - 0.15435500 O 1.10734800 -1.15391200 - 1.38879500 O 1.46261400 -1.44138400 1.25684700 H 0.45803000 -1.32989100 1.36243600 P -1.96088500 -0.85122500 0.15435700 O -1.10740000 -1.15392900 1.38879800 O -1.46266600 -1.44138600 - 1.25684300 H -0.45808300 -1.32989200 - 1.36243300 Br -2.08851400 1.35941800 - 0.14709600 Br 2.08857000 1.35939600 0.14709700 C 3.67867200 -1.37781500 - 0.26543800 H 3.69059600 -2.47276100 - 0.37379100

C -3.69206400 -0.89077100 0.12977000	Br -2.52286200 -1.10362400 - 0.01043100	H 4.13255100 -0.90319300 - 1.14603800
H -3.72371300 -1.98795900 0.20101900	C 3.50659700 -1.75234800 - 0.05485300	H 4.20496400 -1.07596400 0.65029800
H -4.16838000 -0.43980900 1.01092800	H 2.99169900 -2.72434900 - 0.05311000	C -3.67873000 -1.37772900 0.26543000
H -4.18535600 -0.55176400 - 0.79124000	H 4.12152300 -1.65079300 - 0.95940100	H -3.69069800 -2.47267500 0.37377500
Cl 2.05177600 1.67035300 0.11385600	H 4.12490600 -1.64451900 0.84653400	H -4.13259600 -0.90309400 1.14602900
Cl -2.05179400 1.67035000 - 0.11385700	Cl 3.33988500 1.29694500 - 0.00201400	H -4.20500300 -1.07585200 - 0.65030800

Cartesian coordinates of various hydrogen bonded phosphinic acid dimers considered in the present investigation at B3LYP-D3/aug-cc-pVDZ level of theory. For the sake of convenience, the different possible dimers formed by different combinations of the monomeric units will be labelled with respect to only the R groups as R_1R_2 in the rest of the manuscript, i.e., dimer formed by combination of PA-2H and PA-BrCl will be labelled as (2H-BrCl) only.

2H-2H	2H-HF	2H-HCl
P 1.98871100 0.05999100 0.14867600	P 1.71114900 -0.04193500 - 0.32163100	P -1.38384300 0.19200400 0.67684500
O 1.13786300 1.33237100 0.22151600	O 0.80453700 -1.22075700 - 0.60424600	O -0.48678100 -0.91275800 1.21177400
H 2.41242800 -0.34668800 1.44653800	H 2.79591000 0.09761400 - 1.20923300	H -2.44122100 0.55655800 1.53784300
H 3.18770600 0.20912100 -	O 1.07105100 1.40572500 -	O -0.71004800 1.58824000

0.59740800 O 1.34114900 -1.23968400 - 0.55252000 H 0.37494600 -1.36734100 - 0.27797400 P -1.98877500 -0.06002200 0.14846100 O -1.13792200 -1.33240000 0.22131000 H -3.18765100 -0.20908900 - 0.59782700 H -2.41270200 0.34651500 1.44629900 O -1.34113200 1.23973100 - 0.55250800 H -0.37496600 1.36737600 - 0.27782600	0.22441600 H 0.06053700 1.40474200 - 0.02996500 P -2.28015700 0.08211700 - 0.05152500 O -1.43267200 1.32561600 0.24017000 H -3.49769900 0.05767800 0.67390600 H -2.65293700 0.00864900 - 1.42406100 O -1.65488400 -1.35918300 0.32197800 H -0.70899400 -1.43152400 - 0.00629100 F 2.51850600 -0.23509100 1.06756700	0.30507100 H 0.23204400 1.48044300 - 0.09175800 P 2.48977900 0.01914000 - 0.13973700 O 1.63270000 1.19069000 - 0.63281400 H 3.57783000 -0.27202300 - 1.00012000 H 3.07007200 0.28856900 1.13254400 O 1.78587000 -1.42907100 - 0.01396200 H 0.90674800 -1.35939300 0.46703200 Cl -2.42075900 -0.43259100 - 1.00914700
2H-HBr P -0.80145800 0.95047000 0.54645900 O 0.08927300 0.36696600 1.63427600 H -1.71739800 1.92464600 1.00309700 O -0.09343000 1.67135900 - 0.69013200 H 0.75869600 1.18278600 - 0.99062900 P 2.87453200 -0.29022100 - 0.21241400 O 2.02664400 0.37872700 -	2H-2F P -1.43039000 -0.08023700 0.00590600 O -0.54318400 -1.23469200 0.37170100 O -0.81154800 1.31993000 - 0.33610100 H 0.22746900 1.34000800 - 0.28348000 P 2.54398000 0.11689700 0.20367300 O 1.69943100 1.32706400 - 0.21493300 H 3.85124000 0.14188700 -	2H-2Cl P 0.96803000 0.07746200 - 0.07920700 O 0.08394300 -0.22826700 - 1.26906900 O 0.30644800 0.75783300 1.19105900 H -0.71595500 0.57635700 1.25145400 P -2.99310400 -0.03606000 0.03544200 O -2.17177200 0.28859200 1.28977000 H -4.25570400 -0.60202400

1.30034100 H 3.78976100 -1.24100200 - 0.72945800 H 3.66713000 0.65719200 0.49629800 O 2.10900700 -1.16306900 0.91058900 H 1.32274500 -0.66094500 1.28290500 Br -2.17033800 -0.61012600 - 0.30814900	0.34102600 H 2.71143600 0.05670000 1.61554400 O 2.03476800 -1.34683400 - 0.25488400 H 1.06483200 -1.45877900 - 0.04953000 F -2.41511500 -0.39909300 - 1.20732200 F -2.53529400 0.21810500 1.11621600	0.33789000 H -3.26174200 1.12870600 - 0.73693500 O -2.39213000 -1.12902700 - 0.99289600 H -1.44343200 -0.90711400 - 1.21330800 Cl 2.51311700 1.33384100 - 0.55883100 Cl 1.92274700 -1.61584200 0.60561300
2H-2Br P 0.38286600 -0.13559500 - 0.03080800 O -0.49022000 -0.41676400 - 1.23888400 O -0.30133800 -0.15655300 1.40390300 H -1.32493100 0.01222200 1.36091600 P -3.60431200 -0.10242400 - 0.00848500 O -2.79537500 0.22103900 1.25373500 H -4.88243300 -0.64803500 0.27023300 H -3.84490000 1.06498500 - 0.78577200 O -3.00243600 -1.20876100 - 1.02108300 H -2.04053600 -1.01662700 -	2H-ClF P 1.18463100 -0.20931600 0.27319700 O 0.29301800 0.57778100 1.19903100 O 0.54105800 -1.28285200 - 0.68690400 H -0.47870400 -1.13874700 - 0.82977100 P -2.77440400 -0.08861000 - 0.00137400 O -1.92746600 -0.88487900 - 1.00230900 H -4.01277200 0.33324600 - 0.54366300 H -3.09441100 -0.85948100 1.15126800 O -2.17288000 1.30924600 0.54427300 H -1.23328500 1.18259100	2H-BrF P -0.70146000 0.71410500 0.22815200 O 0.17682900 0.35738500 1.40238000 O -0.01992200 1.15700800 - 1.12748000 H 0.93650800 0.76730600 - 1.23674100 P 3.14438500 -0.17485700 - 0.09221800 O 2.29890600 0.17771100 - 1.32271200 H 4.24248700 -1.01347600 - 0.40292400 H 3.69811600 0.98488700 0.51907100 O 2.43173500 -1.01162700 1.09359900 H 1.56115600 -0.59050500

1.21419600 Br 2.06589700 -1.57620300 0.17559600 Br 1.36523600 1.86417600 - 0.23063100	0.85578500 F 2.28593000 -1.05668200 1.06878300 Cl 2.39112700 0.97881800 - 0.87114300	1.34048700 F -1.66676100 1.95358200 0.54669300 Br -2.18232100 -0.86044800 - 0.24530900
2H-BrCl P 0.67731600 0.52980300 - 0.08495400 O -0.21583500 0.55890500 - 1.30873300 O 0.01635000 0.83918300 1.32622300 H -0.98137400 0.55190200 1.35934800 P -3.25466800 0.13216900 0.04995200 O -2.40931700 0.12499600 1.32989800 H -4.46413500 -0.59205300 0.18666000 H -3.62991300 1.45170200 - 0.32889400 O -2.62284100 -0.55207400 - 1.27161500 H -1.69910200 -0.20683600 - 1.43111800 Br 1.71203300 -1.43875500 0.11506400 Cl 2.20304200 1.89500500 - 0.20108600	2H-HMe P -2.35196200 0.09510600 0.22617600 O -1.57815800 1.33500000 - 0.23481500 H -3.68485700 0.05638500 - 0.25921900 H -2.47194900 0.04647000 1.64553900 O -1.79847000 -1.34851300 - 0.22807500 H -0.79249200 -1.41735100 - 0.07230600 P 1.55117400 -0.08984700 - 0.30803100 O 0.74048100 -1.29389700 0.19492400 H 1.60656500 -0.06912600 - 1.73204100 O 1.00708300 1.37135000 0.12261500 H 0.00788100 1.44637500 - 0.00641700 C 3.26576500 -0.08025800 0.26543300 H 3.78435200 0.79733700 -	2H-2Me P 1.39252700 -0.05833500 0.06228900 O 0.54354300 -1.13697600 0.76019200 O 0.74945500 0.56431300 - 1.29368500 H -0.19427500 0.85864400 - 1.12561800 P -2.55751200 0.07742100 0.05529600 O -1.69390900 1.19904900 - 0.53304200 H -2.99436100 0.41167900 1.37074300 H -3.75678700 -0.16927700 - 0.66664200 O -1.91831600 -1.39526500 0.13934900 H -0.92752400 -1.36045100 0.40829100 C 2.98796200 -0.68981200 - 0.52207300 C 1.70359500 1.34761000 1.17599000 H 2.79643000 -1.51112000 -

	0.13994000 H 3.26302400 -0.03655700 1.36160100 H 3.76075700 -1.00160100 - 0.06471700	1.22268000 H 3.54496400 0.10694900 - 1.02963400 H 3.56160200 -1.06743200 0.33306200 H 2.15205000 0.98600900 2.10944100 H 2.36439500 2.07783400 0.69315900 H 0.73777000 1.82024100 1.39446300
2H-MeF P 1.42090400 0.08565900 0.01745000 O 0.53866500 1.28515400 0.31061200 O 0.76040400 -1.14732200 - 0.74417300 H -0.24309700 -1.23997400 - 0.58619400 P -2.58701900 -0.08412400 0.14181600 O -1.77223500 -1.29279000 - 0.32966600 H -3.88348600 -0.01843600 - 0.43126600 H -2.80265500 -0.11720500 1.54939900 O -2.01273000 1.38519700 - 0.19560800 H -1.02450300 1.43940900	2H-MeCl P 1.23199900 -0.37769700 0.04332900 O 0.35863500 -1.05058500 - 1.00625000 O 0.57580100 -0.11502300 1.47809800 H -0.38924500 0.20664200 1.41388700 P -2.67822200 0.26762300 - 0.06089400 O -1.86280400 0.65266300 1.17749200 H -4.04261000 -0.00174500 0.22090300 H -2.69568800 1.32043800 - 1.02007900 O -2.24877000 -1.06708100 - 0.85908600 H -1.24879900 -1.11496000 -	2H-MeBr P -0.94117500 0.82272200 - 0.03398100 O -0.07213400 1.12759200 - 1.24691300 O -0.28531300 1.04343700 1.40989600 H 0.65028100 0.64192800 1.46597700 P 2.75722500 -0.36506900 0.05469300 O 2.06558900 -0.00745000 1.37400600 H 4.17306500 -0.33940100 0.13745700 H 2.42739900 -1.68481200 - 0.36714200 O 2.49586100 0.59285900 - 1.21774200 H 1.51920600 0.82098900 -

0.00215000 C 2.96159200 0.42804400 - 0.84415600 H 2.72261000 0.83761800 - 1.83249300 H 3.53332300 1.16255100 - 0.26575300 H 3.53150700 -0.50189200 - 0.95014100 F 1.95229000 -0.54638800 1.41858500	0.98299100 Cl 1.81931300 1.51017300 - 0.64776300 C 2.79238100 -1.21236900 0.39708300 H 2.55602500 -2.20477900 0.80075100 H 3.35730100 -1.30874900 - 0.53628800 H 3.35670100 -0.62591300 1.12998000	1.31489500 C -2.50776600 1.71935400 0.03264300 H -2.27421400 2.78944000 0.10270800 H -3.06786200 1.51266700 - 0.88542700 H -3.07183200 1.39165200 0.91220800 Br -1.53976900 -1.36703500 - 0.07721400
HF-HF P -2.00569600 -0.06037800 0.39489000 O -1.09888400 -1.27085900 0.44745300 H -2.97205800 0.00428800 1.41627100 O -1.34600600 1.38396400 0.36328800 H -0.38154100 1.38320300 0.04288600 P 2.00604500 0.05977500 - 0.39464100 O 1.09786600 1.26901800 - 0.45234400 H 2.97430500 -0.00643900 - 1.41411200 O 1.34801300 -1.38525500 - 0.36000200 H 0.38259400 -1.38455000 -	HF-HCl P -2.18051900 -0.04896300 - 0.49130100 O -1.27739500 1.14930600 - 0.68765600 H -2.99248100 -0.36821600 - 1.59601200 O -1.53126700 -1.43004300 - 0.05069600 H -0.62184600 -1.33303800 0.39438100 P 1.67532600 0.10874900 0.73163800 O 0.77454900 -1.07295200 1.05213400 H 2.65969800 0.37415300 1.70660000 O 0.98836200 1.53258500 0.50506400 H 0.09531600 1.45567300	HF-HBr P -2.54951500 -0.58498900 - 0.15772100 O -1.67048100 -0.18789900 - 1.32364800 H -3.19474600 -1.82838000 - 0.29626900 O -1.91850600 -0.61621100 1.29981100 H -1.08376000 -0.04424000 1.40033100 P 1.09961100 1.08879700 0.23275200 O 0.20149300 0.85311100 1.43878100 H 1.98205200 2.18266100 0.37034000 O 0.39629100 1.37058500 - 1.17617100 H -0.41970600 0.78516500 -

0.04280100 F 2.96959900 0.10838900 0.90197600 F -2.97166600 -0.10441600 - 0.90009400	0.03002200 F -3.31992500 0.24574800 0.61644000 Cl 2.83162900 -0.26135500 - 0.94741000	1.31302500 F -3.83644000 0.38476500 - 0.03136200 Br 2.50945500 -0.62506100 - 0.08030200
HF-2F P 2.33067400 -0.06878600 - 0.30406000 O 1.40870400 -1.25665600 - 0.48101700 H 3.42910700 -0.03257200 - 1.18225400 O 1.70461200 1.39123800 - 0.37083000 H 0.71282000 1.40744900 - 0.19137200 P -1.73861200 0.06536000 0.05219400 O -0.85903800 1.28062400 0.08081300 O -1.11188200 -1.36423000 - 0.13329600 H -0.09634400 -1.34620800 - 0.26532200 F -2.88963600 0.15288900 - 1.04478900 F -2.66309200 -0.06532000 1.34074400 F 3.09934500 -0.12729800 1.11288900	HF-2Cl P -2.78769100 0.20423400 0.07436100 O -1.87372200 0.31237600 1.27625300 H -3.86925100 1.10444500 0.06899700 O -2.14849400 0.32265800 - 1.37628000 H -1.15544500 0.13444700 - 1.39117000 P 1.28580400 -0.08323500 - 0.05571900 O 0.39919300 -0.16161500 - 1.27924400 O 0.61513900 -0.28963600 1.37108400 H -0.38050200 -0.05800400 1.36522300 Cl 2.28241500 1.71510900 0.03414400 Cl 2.78868500 -1.46627300 - 0.08531800 F -3.58647600 -1.19824200 0.06182600	HF-2Br P -3.41872300 -0.01305900 0.06649600 O -2.51509200 0.14656200 1.27024300 H -4.52619700 0.85467800 0.03663800 O -2.77709800 0.09530300 - 1.38398700 H -1.78017900 -0.07383400 - 1.39394400 P 0.65527200 -0.15797100 - 0.04712100 O -0.22138600 -0.33778600 - 1.27162500 O -0.01013100 -0.40448600 1.38158100 H -1.00980600 -0.19411600 1.37547100 Br 1.52569000 1.89965200 0.01772600 Br 2.39599000 -1.52858600 - 0.04294000 F -4.17618800 -1.43858200 0.07930700
HF-ClF	HF-BrF	HF-BrCl

P -2.55841600 -0.39461200 - 0.14021500 O -1.62325600 -0.23719800 - 1.32041800 H -3.54590000 -1.38487700 - 0.29467900 O -1.92688800 -0.66223700 1.29403200 H -0.95498400 -0.39745300 1.35720200 P 1.45637800 0.33604600 0.13247000 O 0.58067400 0.02593200 1.31850900 O 0.78287700 0.62374500 - 1.26887100 H -0.18306300 0.29186900 - 1.31850500 F -3.49040900 0.90788200 0.05569700 F 2.35704700 1.63700600 0.36190100 Cl 2.90275000 -1.06823500 - 0.17243400	P -2.93178900 -0.53783900 - 0.07773200 O -1.99200600 -0.45636500 - 1.26178200 H -3.76981900 -1.66804600 - 0.06377500 O -2.31341200 -0.46514200 1.38524000 H -1.38607700 -0.06697300 1.40811200 P 0.95068600 0.70961500 0.08667600 O 0.08193300 0.54592000 1.30898000 O 0.26267800 0.75391700 - 1.33977200 H -0.64217300 0.27976800 - 1.34862500 F -4.03867700 0.63555500 - 0.11553000 Br 2.58936400 -0.76717200 - 0.00360900 F 1.77509400 2.08172900 0.10385200	P -3.27063700 -0.02497500 0.06723300 O -2.39094100 0.21742800 1.27490400 H -4.47686800 0.69975800 0.05618400 O -2.64786500 0.19241700 - 1.37892800 H -1.63762100 0.15662800 - 1.38545200 P 0.82297600 0.26504600 - 0.04098700 O -0.05964800 0.09976300 - 1.26074700 O 0.16142000 0.06026700 1.39231700 H -0.85967200 0.11565300 1.36435700 F -3.84691200 -1.53262300 0.04811100 Cl 1.68827200 2.13540400 0.00805100 Br 2.54373900 -1.12926200 - 0.04691800
HF-HMe P -1.92011600 -0.06007000 0.39411100 O -0.96325600 -1.22576500 0.53464000 O -1.32064600 1.39782300 0.24798600	HF-2Me P -2.25945700 -0.11327300 0.24723600 O -1.36695600 -1.32900200 0.10073200 H -3.32539700 -0.27225600 1.15583800	HF-MeF P -2.33620300 -0.06305000 0.31443300 O -1.45857800 -1.28200000 0.49661100 H -3.46361000 -0.00666300 1.15667100

H -0.33642500 1.41528500 - 0.08963900 P 1.95175800 0.11759900 - 0.38465600 O 1.07235900 1.36731200 - 0.54992700 H 3.10251900 0.17199800 - 1.21019400 O 1.30189400 -1.28956700 - 0.86317800 H 0.42397900 -1.42374700 - 0.40766900 C 2.52618800 -0.11183300 1.32204800 H 3.21306600 -0.96577600 1.37169000 H 3.02426900 0.80269700 1.66659400 H 1.64751900 -0.31084200 1.94934400 F -2.89563700 -0.24828300 - 0.88484800 H -2.88708600 0.03895400 1.41437700	O -1.59693100 1.27279800 0.61418200 H -0.56962900 1.33423300 0.37607200 P 1.68088500 0.08310300 - 0.04334900 O 0.82927400 1.36607500 0.04749500 O 1.06002900 -1.09346500 - 0.97791100 H 0.12924600 -1.29900600 - 0.68649900 C 1.94648500 -0.65698400 1.59724500 H 2.60081400 -1.53348700 1.51725400 H 2.38651500 0.08838600 2.27086800 H 0.96879400 -0.96848700 1.98594000 C 3.28472800 0.39696100 - 0.81912400 H 3.10702100 0.81010500 - 1.81897500 H 3.83973200 1.12611200 - 0.21669700 H 3.85118100 -0.53845100 - 0.89994500 F -3.10524300 0.15943800 - 1.10911300	O -1.67452300 1.37484200 0.41304800 H -0.65789000 1.37165200 0.29076500 P 1.73124200 0.06814700 - 0.02794500 O 0.86386400 1.30096900 0.15248500 O 1.13765400 -1.32186600 0.48124700 H 0.12749600 -1.35050000 0.48081900 F -3.07455800 -0.08359700 - 1.12422300 C 3.39159900 0.17811800 0.64831000 H 3.89961900 1.03721800 0.19573100 H 3.31574500 0.31860100 1.73279400 H 3.93420000 -0.74740000 0.42489900 F 2.01821600 -0.17716800 - 1.60651100
HF-MeCl	HF-MeBr	HCl-HCl

P 2.46029500 -0.30802700 0.11492700 O 1.59259900 -0.38162600 1.35195800 H 3.67056100 -1.02463400 0.19016300 O 1.83249100 -0.70484600 - 1.28669000 H 0.80808000 -0.70705300 - 1.30195900 P -1.56124200 -0.29199300 - 0.06004700 O -0.72326200 -0.74571400 - 1.24922000 O -0.99656000 -0.65777700 1.39456700 H 0.00541100 -0.54923100 1.44853100 F 3.04351500 1.18470000 - 0.10163100 C -3.26243600 -0.88878800 - 0.05880100 H -3.74994000 -0.55537300 - 0.98121600 H -3.23315500 -1.98473400 - 0.01979300 H -3.78276100 -0.48794300 0.81769000 Cl -1.74326300 1.78617000 - 0.07345600	P -2.72385800 0.24303700 0.10304100 O -1.88960700 0.49663000 1.33914000 H -4.03051200 0.76705000 0.14622700 O -2.15295100 0.67830000 - 1.31166700 H -1.14123700 0.83620200 - 1.32680300 P 1.24220800 0.77141100 - 0.06425100 O 0.36971000 1.10750100 - 1.26977100 O 0.63708300 1.13401100 1.37734600 H -0.34049400 0.89293800 1.44100400 F -3.06831200 -1.32885400 - 0.05747900 Br 1.64799900 -1.44793300 - 0.00549400 C 2.87609400 1.53914700 - 0.07739900 H 3.39909700 1.22995000 - 0.98856300 H 2.73265400 2.62709500 - 0.07070800 H 3.42895500 1.21879800 0.81205700	P 1.83753800 0.72795300 - 0.34043700 O 0.94193100 0.22335700 - 1.46016400 H 2.67783600 1.80127300 - 0.70373900 O 1.14081200 1.24672600 0.99991800 H 0.32019400 0.70208400 1.24648100 P -1.83757700 -0.72781700 0.34052600 O -0.94207300 -0.22319500 1.46032600 H -2.67821600 -1.80084700 0.70388600 O -1.14067800 -1.24713400 - 0.99954200 H -0.32011600 -0.70252700 - 1.24622500 Cl -3.21272100 0.71256100 - 0.23094200 Cl 3.21322700 -0.71219800 0.23037000
HCl-HBr	HCl-2F	HCl-2Cl

P -1.25325600 1.07995800 0.23479200 O -0.36746200 0.74969800 1.42779900 H -2.01368200 2.26033800 0.38598400 O -0.54576100 1.29076100 - 1.18450100 H 0.20225400 0.62275100 - 1.34016800 P 2.22680900 -0.83684200 - 0.19407600 O 1.34647200 -0.47089200 - 1.37800600 H 2.93933000 -2.04462800 - 0.34810100 O 1.53142400 -1.00335800 1.23429500 H 0.78299500 -0.33330600 1.38307700 Br -2.83954200 -0.47545200 - 0.05883100 Cl 3.76159400 0.53232100 0.05448500	P 2.02870000 -0.64893000 0.15562700 O 1.11652700 -0.67165200 1.37281700 H 3.15867100 -1.48549300 0.26203300 O 1.39723100 -1.06735100 - 1.25321800 H 0.45371700 -0.73346600 - 1.35416500 P -1.93351700 0.07616600 - 0.08121400 O -1.04965800 -0.13732200 - 1.27452700 O -1.34635400 -0.02635000 1.37304500 H -0.35119900 -0.27544500 1.39605500 F -3.21400400 -0.87106700 - 0.07021400 F -2.68873200 1.47702600 - 0.11225700 Cl 2.88336400 1.21287400 - 0.10890200	P -2.46997700 0.76880200 0.18835900 O -1.58320000 0.72456600 1.42268900 H -3.61976100 1.57480000 0.32132200 O -1.82067400 1.28790900 - 1.17770800 H -0.87605000 0.95457300 - 1.29292700 P 1.49291000 0.07531300 - 0.05485600 O 0.60696700 0.34103200 - 1.25199100 O 0.96893300 0.51148500 1.38120600 H -0.05110100 0.58399400 1.42156400 Cl 3.31754800 0.98930600 - 0.19408100 Cl 1.96283700 -1.92142100 0.08569700 Cl -3.28679400 -1.08788000 - 0.21047500
HCl-2Br P 3.14978800 0.47617200 - 0.07670400 O 2.25422200 0.62366900 - 1.29697200 H 4.27839800 1.32183700 - 0.07857300	HCl-ClF P 1.65240900 0.36549700 - 0.10324300 O 0.78235000 0.07189700 - 1.29744100 O 0.98962100 0.47004300 1.32838900	HCl-BrF P 1.14401700 0.70993100 - 0.10780000 O 0.27930100 0.42502600 - 1.31060100 O 0.47045200 0.75624900 1.32546700

O 2.50015900 0.74212900 1.36036900 H 1.55285600 0.39900400 1.41351900 P -0.83391600 -0.11468000 0.04587300 O 0.06357400 -0.18169200 1.26658600 O -0.14963000 -0.26983000 - 1.38670600 H 0.81224200 0.07988800 - 1.39087600 Cl 4.01273400 -1.40081200 0.00377200 Br -1.96714100 1.81136700 - 0.01016400 Br -2.37980700 -1.70279400 0.04464700	H 0.06665400 0.02729300 1.37344700 P -2.22428700 -0.73468700 0.15564300 O -1.30189400 -0.65776600 1.36283200 O -1.56476200 -1.07618200 - 1.26081000 H -0.65664100 -0.65265800 - 1.36273100 Cl -3.28696000 1.01977400 - 0.09531100 F 2.41672100 1.76374800 - 0.23631300 H -3.25260100 -1.69257300 0.27123800 Cl 3.23570300 -0.91024800 0.05902600	H -0.38618200 0.19790500 1.37254300 P -2.57332600 -0.82287200 0.13846600 O -1.65833500 -0.66389900 1.34310200 O -1.88867200 -1.03527700 - 1.29154200 H -1.04825100 -0.48876100 - 1.38990900 Br 2.90268900 -0.62031400 0.02086900 Cl -3.85539200 0.78682700 - 0.05329300 F 1.84912800 2.14473800 - 0.19209900 H -3.46886700 -1.90832100 0.22869400
HCl-BrCl P -2.83563500 -1.07082800 0.16313400 O -1.92475400 -0.99689000 1.37873600 O -2.14975000 -1.23426000 - 1.27238700 H -1.29157700 -0.70832900 - 1.34231400 P 0.94527600 0.27983000 - 0.00520100 O 0.05243700 0.16389200 - 1.22358400	HCl-HMe P -1.56864400 0.60223200 0.45827300 O -0.63514100 -0.05828600 1.46085700 H -2.49034500 1.51005700 1.02423600 O -0.91416100 1.42448900 - 0.73668900 H -0.02495200 1.00197700 - 1.07143000 P 2.13048600 -0.36732200 - 0.39117300	HCl-2Me P 1.93986400 0.65973000 - 0.07267700 O 1.05332100 0.70259200 - 1.30809000 H 2.97638400 1.61922300 - 0.06525400 O 1.24804400 0.82580900 1.34619100 H 0.28835500 0.38749800 1.38609900 P -1.89817500 -0.13600600 0.07647700

O 0.24746400 0.37107700 1.42407100 H -0.62365000 -0.16385300 1.45337100 Br 2.39017500 -1.41528600 0.10265000 Cl 2.11785600 1.95493600 - 0.05262000 Cl -4.07016400 0.58335100 0.04258800 H -3.76423000 -2.13168400 0.19641900	O 1.25783100 0.33971500 - 1.44080500 H 3.15765400 -1.13539500 - 0.99383800 O 1.39846500 -1.49992900 0.51126600 H 0.59775500 -1.10671600 0.95869000 C 2.92555500 0.79532600 0.75407400 H 3.59543300 0.25153800 1.43154500 H 3.48346000 1.54766900 0.18325300 H 2.13498800 1.28697100 1.33592400 Cl -2.84733000 -0.78988800 - 0.40377600	O -1.02574300 -0.20621100 1.34708300 O -1.20482900 -0.72473400 - 1.27169000 H -0.32880100 -0.27541300 - 1.42611400 C -2.37930300 1.57623600 - 0.30560000 H -3.04223500 1.59923400 - 1.17892200 H -2.87680200 2.02192400 0.56432200 H -1.46362600 2.13772400 - 0.52982900 C -3.38543400 -1.15452500 0.22824000 H -3.07492100 -2.18757600 0.42411700 H -3.98774100 -0.78930700 1.06873100 H -3.96532400 -1.11194500 - 0.70143500 Cl 3.03508100 -1.10884800 - 0.00425800
HCl-MeF P 2.03204300 -0.68401500 0.09322100 O 1.16259600 -0.83235800 1.33034000 H 3.18398700 -1.49932400 0.08301700	HCl-MeCl P 2.17188700 -0.71117700 0.14578900 O 1.30835600 -0.82971500 1.39004400 H 3.39154500 -1.41876600 0.20610700	HCl-MeBr P 2.48217900 -0.64948200 0.17335200 O 1.63848800 -0.88526200 1.41433300 H 3.79998200 -1.14828700 0.25412300

O 1.36659600 -0.96406300 - 1.32876200 H 0.39160200 -0.66113600 - 1.36849700 P -1.92798500 0.08087700 - 0.07421600 O -1.08534200 -0.22101400 - 1.29996900 O -1.41565500 -0.48787400 1.32543400 H -0.41371400 -0.61313300 1.36987500 C -3.66258300 -0.37257700 - 0.18628400 H -4.10358800 0.13433600 - 1.05200700 H -3.72934100 -1.45892000 - 0.31653800 H -4.17469000 -0.07096100 0.73439000 F -2.00632900 1.68589300 0.15467800 Cl 2.86795400 1.21175200 - 0.00898900	O 1.54888500 -1.16760600 - 1.24957200 H 0.54847500 -0.97120300 - 1.32076400 P -1.77225900 -0.22975500 - 0.09152900 O -0.97371500 -0.69404300 - 1.30299600 O -1.29748200 -0.77951000 1.33713700 H -0.29167600 -0.80012900 1.42472400 C -3.53714600 -0.59256900 - 0.15911200 H -3.95522800 -0.12675600 - 1.05794100 H -3.65316800 -1.68239500 - 0.20780400 H -4.02021900 -0.19563900 0.74017700 Cl -1.67914000 1.84923800 0.06082900 Cl 2.83875600 1.23569600 - 0.11538100	O 1.95503900 -1.22514200 - 1.21768300 H 0.93682400 -1.20129100 - 1.29935200 P -1.46664700 -0.76461100 - 0.10351000 O -0.61328700 -1.18355300 - 1.29614000 O -0.94961300 -1.22421600 1.34503400 H 0.04622600 -1.09797700 1.44709200 C -3.18253900 -1.32253400 - 0.16791100 H -3.63961100 -0.93855900 - 1.08607300 H -3.17546400 -2.41987000 - 0.17582600 H -3.71403400 -0.94789600 0.71330200 Cl 2.82669400 1.37492200 - 0.12085500 Br -1.59600800 1.48692300 - 0.00735500
HBr-HBr P 1.66201800 -1.08163000 0.19466200 O 0.79156600 -0.72190900 1.39017500 H 2.32458900 -2.32329700 0.31220100	HBr-2F P -1.48326100 1.11690800 0.12736500 O -0.55718800 1.14506000 1.33669700 H -2.52500600 2.06795700 0.17804500	HBr-2Cl P 1.94311500 1.23289100 - 0.20282100 O 1.03950800 1.23887900 - 1.42834200 H 3.04308700 2.11375900 - 0.28884700

O 0.95707200 -1.18991600 - 1.23805000 H 0.26689400 -0.46006800 - 1.38001300 P -1.66218800 1.08155200 - 0.19502900 O -0.79169700 0.72206600 - 1.39057300 H -2.32535700 2.32289400 - 0.31263500 O -0.95701100 1.19032300 1.23755600 H -0.26648800 0.46076600 1.37940800 Br -3.36844100 -0.35294500 0.03346800 Br 3.36898100 0.35210200 - 0.03341000	O -0.82980300 1.38391000 - 1.31146200 H 0.05306400 0.91332500 - 1.40585000 P 2.31855100 -0.15997400 - 0.08006500 O 1.45766500 0.10126000 - 1.28043200 O 1.77628400 0.12555600 1.36735000 H 0.83194100 0.52794400 1.37999300 F 3.72525200 0.58499500 - 0.14178600 F 2.85790400 -1.65641800 - 0.01757200 Br -2.58483900 -0.82191700 - 0.01120900	O 1.28775300 1.62368400 1.20588200 H 0.39094800 1.18112300 1.32628600 P -1.87319400 0.05472500 0.05861000 O -1.01191600 0.38772700 1.25671100 O -1.44888500 0.63255300 - 1.36016600 H -0.45261900 0.86361000 - 1.41124800 Cl -3.80875600 0.68145300 0.27000200 Cl -2.04834600 -1.98029300 - 0.18083400 Br 2.92568200 -0.75732800 0.06954600
HBr-2Br P -2.62355200 1.01504900 0.09137000 O -1.71941900 1.07557100 1.31540400 H -3.67132100 1.96121500 0.10031300 O -1.94810800 1.25039700 - 1.34241800 H -1.06040800 0.77759000 - 1.41176800 P 1.23081300 -0.08867500 - 0.04127800	HBr-ClF P 1.65829200 -1.12762600 0.15295400 O 0.73704500 -1.03501100 1.36273900 H 2.61484900 -2.16238800 0.23528900 O 0.97871800 -1.38532500 - 1.27503900 H 0.13117200 -0.85261900 - 1.37844400 P -2.05341200 0.39800900 - 0.08488200	HBr-BrF P 2.00760200 -1.13547900 0.15643700 O 1.09253200 -0.95770800 1.36112500 H 2.85211300 -2.26382500 0.23469900 O 1.31595000 -1.31130900 - 1.27831800 H 0.52751200 -0.69509800 - 1.38464800 P -1.55419300 0.69694200 - 0.08870700

O 0.32532000 -0.02947300 - 1.25629000 O 0.54192900 -0.13693500 1.39664000 H -0.36363600 0.34019900 1.40491100 Br 2.63315500 1.65156900 0.00019400 Br 2.52879900 -1.88549300 - 0.04312700 Br -3.71879900 -0.93126200 - 0.02117900	O -1.20522400 0.05580800 - 1.28178300 O -1.41048900 0.34868000 1.35871100 H -0.54520100 -0.19991400 1.39285400 Br 2.92464100 0.70225500 - 0.05278400 Cl -3.78686500 -0.67469100 - 0.00551000 F -2.63474500 1.88608500 - 0.15744600	O -0.71491700 0.34174900 - 1.29055200 O -0.88742700 0.66647700 1.34823400 H -0.09143100 0.02516500 1.39668500 Br 3.45812000 0.55501400 - 0.02600900 F -2.11857800 2.19346600 - 0.16129500 Br -3.43287900 -0.45997500 0.01997000
HBr-BrCl P 2.16330100 -1.11296900 0.10482300 O 1.25466700 -1.02387000 1.32376500 H 3.05570700 -2.20660700 0.12891400 O 1.46666100 -1.25835700 - 1.33073100 H 0.65876800 -0.66103300 - 1.41020000 P -1.48569000 0.52805400 - 0.05803400 O -0.59867200 0.34079300 - 1.27153800 O -0.79730800 0.51914900 1.37865200 H 0.02442300 -0.08977700 1.40318200	HBr-HMe P 0.97761200 1.04264200 - 0.31271300 O 0.06952900 0.61461200 - 1.45755100 O 0.29303900 1.40397500 1.08056300 H -0.50443000 0.77504000 1.30105100 P -2.50920100 -0.61013500 0.28269200 O -1.65815200 -0.15569800 1.47955700 H -3.40313200 -1.65029800 0.63902000 O -1.71237400 -1.30828400 - 0.94677900 H -0.99590800 -0.69589400 - 1.27391400	HBr-2Me P 1.36930600 1.07321100 - 0.07148700 O 0.48740000 1.02518700 - 1.31214800 H 2.29329300 2.14330800 - 0.05651400 O 0.65416400 1.16973600 1.34486400 H -0.22890800 0.59376800 1.38909500 P -2.31907400 -0.23113200 0.07542300 O -1.44015600 -0.19200900 1.34290400 O -1.55580900 -0.69949100 - 1.28221900 H -0.75229700 -0.13029900 - 1.43524700

Br 3.54090900 0.64378400 - 0.01912700 Br -3.10325800 -1.00551500 0.00722500 Cl -2.47492500 2.31866200 - 0.08362200	C -3.49869900 0.73869100 - 0.42233000 H -4.14485600 0.35013300 - 1.21911600 H -4.09989300 1.20385200 0.36841200 H -2.80485900 1.47951900 - 0.84077200 H 1.77287500 2.17784700 - 0.59021000 Br 2.53947300 -0.51661900 0.10905200	C -3.03930200 1.40021800 - 0.28409400 H -3.70107100 1.34000200 - 1.15652300 H -3.59270400 1.75978300 0.59190900 H -2.21319100 2.08892000 - 0.50160500 C -3.64602800 -1.45228200 0.21815900 H -3.19092400 -2.43294900 0.40028500 H -4.29037000 -1.18647800 1.06476300 H -4.23006600 -1.48140500 - 0.70942100 Br 2.74658800 -0.70630000 0.00599200
HBr-MeF P -1.50141200 1.14422000 0.08558200 O -0.62082300 1.24348400 1.32204500 H -2.57839700 2.05809700 0.05988500 O -0.81343900 1.35562400 - 1.34067100 H 0.10701000 0.91728900 - 1.38723900 P 2.29073800 -0.15739400 - 0.07357700	HBr-MeCl P -1.63554200 1.19505900 0.16879700 O -0.74509600 1.28206000 1.39892000 H -2.78057600 2.02127200 0.21542000 O -0.99273800 1.55120400 - 1.24972900 H -0.03739600 1.20282200 - 1.34133500 P 2.17241700 0.14909700 - 0.11696400	HBr-MeBr P -1.98643600 1.19700600 0.23520800 O -1.08981800 1.34394800 1.45502100 H -3.22663500 1.86607300 0.33616100 O -1.42409400 1.69497800 - 1.17483800 H -0.43222000 1.48665700 - 1.29608000 P 1.91015300 0.67757700 - 0.14958300

O 1.50713700 0.25983600 - 1.30446500 O 1.87553500 0.50035600 1.31949600 H 0.90577100 0.78077600 1.36466500 C 4.07528000 0.01480200 - 0.18701700 H 4.43062900 -0.56575100 - 1.04588300 H 4.31290900 1.07528800 - 0.33011800 H 4.53325200 -0.35285000 0.73815300 F 2.11385400 -1.75194700 0.17374600 Br -2.56240200 -0.83125600 0.00439700	O 1.42621900 0.68441000 - 1.33228300 O 1.82215000 0.81851000 1.29680400 H 0.83467500 0.99939400 1.40349700 C 3.97003900 0.23306700 - 0.22965500 H 4.29065500 -0.32405300 - 1.11649600 H 4.25030200 1.28956100 - 0.32364800 H 4.40763000 -0.20023400 0.67609200 Br -2.54293700 -0.84759500 - 0.02845100 Cl 1.76521000 -1.88332800 0.12221100	O 1.09228100 1.18227400 - 1.33359900 O 1.51484000 1.25538600 1.29475000 H 0.51515800 1.29165700 1.42932400 C 3.68767400 0.96723600 - 0.27938000 H 4.05302700 0.48716500 - 1.19339100 H 3.84494200 2.05215700 - 0.32972400 H 4.18409300 0.54720900 0.60181300 Br -2.63012900 -0.93422900 - 0.04280400 Br 1.70509200 -1.56374000 0.02389700
2F-2F P -2.04568400 -0.06362500 0.00031600 O -1.14785700 -1.26592600 0.00497500 O -1.42677600 1.38420600 - 0.00535100 H -0.41346900 1.37782600 - 0.00161800 P 2.04564000 0.06365100 0.00005600 O 1.14787900 1.26601600 0.00464800	2F-2Cl P -2.50198200 -0.10971400 0.06547300 O -1.61493200 0.08790400 1.25951800 O -1.87204500 -0.38263000 - 1.35064300 H -0.85605800 -0.32852100 - 1.34717100 P 1.58023400 -0.06591700 - 0.04975400 O 0.68628700 -0.23105700 - 1.26032500	2F-2Br P -3.13629900 -0.32504900 0.06407100 O -2.25802400 -0.14817300 1.26750400 O -2.49773900 -0.55421800 - 1.35591100 H -1.48082900 -0.50421600 - 1.34570100 P 0.93417400 -0.17838200 - 0.03658800 O 0.05974200 -0.42057100 - 1.25321400

O 1.42680000 -1.38419000 - 0.00556500 H 0.41352300 -1.37789900 - 0.00163200 F 3.08403900 0.05466400 1.20318000 F 3.08390500 0.06274800 - 1.20318500 F -3.08409500 -0.05460200 1.20342700 F -3.08394800 -0.06281600 - 1.20292800	O 0.94238400 -0.32763200 1.38703300 H -0.05672400 -0.16764500 1.38779300 Cl 2.40341800 1.81281800 0.01618600 F -3.51396800 1.09742300 - 0.15595400 Cl 3.19546800 -1.31001400 - 0.08288200 F -3.56950500 -1.27366200 0.25122800	O 0.31180900 -0.52713600 1.39472200 H -0.68912100 -0.38616900 1.40444100 F -4.16029500 0.87646200 - 0.13380700 F -4.19310900 -1.50416200 0.21583500 Br 2.79693300 -1.36904500 - 0.07616700 Br 1.58411700 1.95171600 0.06351000
2F-CIF P -2.29549400 -0.07221200 0.06113600 O -1.38729600 -0.22950800 1.24544500 O -1.70433400 0.34426200 - 1.33722500 H -0.68908600 0.36390300 - 1.34322500 P 1.77150400 0.33407800 - 0.05327400 O 0.86527100 0.35643700 - 1.25749600 O 1.12331900 0.37368200 1.39185900 H 0.13946000 0.13573800 1.37945900 F -3.48404200 0.95512600 0.30138000	2F-BrF P -2.72960600 -0.16484800 0.06097900 O -1.80339300 -0.23688200 1.23949400 O -2.20361100 0.36323000 - 1.32570300 H -1.19730200 0.50077500 - 1.33675800 P 1.25391800 0.71574700 - 0.05303500 O 0.34781600 0.67129300 - 1.25924200 O 0.59329100 0.73526400 1.39046800 H -0.34311500 0.35303800 1.38526300 F -4.03985600 0.69395600 0.32888100	2F-BrCl P -2.97999800 -0.25619900 0.06494000 O -2.12455300 0.01160300 1.26814500 O -2.31739000 -0.44462900 - 1.34996600 H -1.31503600 -0.26852700 - 1.34052000 P 1.09145400 0.23961100 - 0.03914800 O 0.19957000 0.02079500 - 1.24500200 O 0.46422900 -0.03133600 1.40284200 H -0.54779000 -0.01255000 1.38680600 F -4.10853800 0.84526600 - 0.14630800

Cl 3.08487900 -1.21707700 - 0.08540400 F -3.16655500 -1.37254400 - 0.22182200 F 2.77615700 1.57532100 - 0.01511400	F -3.42711300 -1.55888300 - 0.25640200 F 2.16476000 2.03030900 - 0.01649300 Br 2.78243000 -0.86737200 - 0.07681200	F -3.92491800 -1.52494200 0.22630800 Br 2.90506500 -1.02331600 - 0.07355100 Cl 1.80615200 2.16702100 0.01040300
2F-HMe P -1.62660900 -0.08284000 - 0.01085100 O -0.68614900 -1.16962900 - 0.44881100 O -1.07260300 1.32016000 0.40422300 H -0.01807900 1.39941400 0.31758600 P 2.26303600 0.24374900 - 0.14735000 O 1.39534400 1.47144600 0.18441000 H 3.55437700 0.62940700 - 0.58084500 O 1.77752300 -0.65659800 - 1.40877500 H 0.84957000 -0.96641700 - 1.24757800 C 2.46131300 -0.87445100 1.26619900 H 3.15983100 -1.67979000 1.00766700 H 2.82866100 -0.30895900 2.13116000	2F-2Me P -1.94349100 -0.01126300 0.05917000 O -1.07418700 0.52380200 1.16373500 O -1.30350300 -0.65948700 - 1.20561900 H -0.21449400 -0.73608100 - 1.16430200 P 1.95898000 -0.04509600 - 0.05271000 O 1.13556100 -0.83430600 - 1.09850100 O 1.47779000 -0.24578800 1.48714300 H 0.51849900 -0.00472700 1.56585300 C 1.90668100 1.74113600 - 0.38106500 H 2.23007100 1.93543300 - 1.41078500 H 0.86904400 2.07425600 - 0.25308300 H 2.54880200 2.27560400 0.32929900	2F-MeF P -2.04209300 0.06190700 - 0.01183200 O -1.18940600 1.29556300 0.03871600 O -1.38140900 -1.35950100 - 0.08656100 H -0.34920400 -1.32859000 - 0.15954000 P 2.03485500 -0.05914900 - 0.01632200 O 1.12640000 -1.24527800 - 0.29332200 O 1.41458500 1.39472000 - 0.24100200 H 0.41689000 1.41727400 - 0.13083400 C 3.60727600 -0.07133800 - 0.88057700 H 4.14380700 -0.99099700 - 0.62130000 H 3.41019100 -0.04482900 - 1.95851000 H 4.18920800 0.80765900 - 0.58124400

H 1.47639100 -1.30214500 1.49498800 F -2.78241200 0.21539400 - 1.07056500 F -2.55649600 -0.54049900 1.20442100	F -2.95300100 1.09794700 - 0.49675300 F -3.03698800 -1.05369500 0.58175500 C 3.67385400 -0.61107600 - 0.01367500 H 3.67673700 -1.68164400 0.22254900 H 4.12670900 -0.45333800 - 0.99981400 H 4.23145600 -0.06015600 0.75300100	F -3.10391900 0.08922600 - 1.20131700 F -3.07023900 -0.03427300 1.20117100 F 2.48614600 -0.06138300 1.54018500
2F-MeCl P -2.17876300 0.03890600 0.06360900 O -1.32655500 0.11825700 1.29588500 O -1.53297700 0.14767500 - 1.36246300 H -0.51319300 0.33174800 - 1.34298400 P 1.83212000 0.33051600 - 0.06567300 O 0.94086600 0.62107000 - 1.26954400 O 1.23254000 0.71912800 1.37102800 H 0.25499300 0.50558600 1.43461000 C 3.44913900 1.12241000 - 0.11989700	2F-MeBr P -2.47457900 0.00926600 0.06581100 O -1.64057900 0.20399500 1.29753200 O -1.85887800 0.23043200 - 1.36087300 H -0.87371400 0.54995300 - 1.34343000 P 1.45136700 0.80337300 - 0.06738900 O 0.53321800 1.02717700 - 1.26750900 O 0.82222300 1.13066600 1.37462300 H -0.11975800 0.79651600 1.44615900 C 2.98763600 1.74762200 - 0.11628300	2Cl-2Cl P -2.03358000 -0.16012200 0.04780200 O -1.14811400 -0.11473000 1.27479600 O -1.37990500 -0.63398600 - 1.32515600 H -0.38332400 -0.44039100 - 1.35239100 P 2.03359600 -0.16023800 - 0.04780000 O 1.14812700 -0.11481600 - 1.27479300 O 1.37988300 -0.63426100 1.32509500 H 0.38338400 -0.44029400 1.35243300 Cl 2.88474200 1.67306800 0.31264100

H 3.96811300 0.79458000 - 1.02700600 H 3.28917500 2.20744000 - 0.14470000 H 4.01751100 0.83895600 0.77245600 F -3.36879600 1.10068100 0.06052800 F -3.06299900 -1.28536800 0.00495300 Cl 2.24186900 -1.70684000 0.03865600	H 3.53206900 1.47952100 - 1.02794000 H 2.72305100 2.81255300 - 0.12911200 H 3.58212600 1.50947700 0.77214500 F -3.81178000 0.87816600 0.07526400 F -3.14803400 -1.43331600 - 0.00537100 Br 2.08622200 -1.35452300 0.02444400	Cl 3.63414000 -1.40978400 - 0.25870400 Cl -3.63404900 -1.40979000 0.25881400 Cl -2.88490000 1.67310300 - 0.31262000
2Cl-2Br P -1.33798500 -0.11332600 - 0.03879800 O -0.46329200 -0.36373000 - 1.25321900 O -0.70348300 -0.41305200 1.39728900 H 0.29520100 -0.23566100 1.39934900 P 2.71727800 -0.12837800 0.04459300 O 1.83540300 0.07638300 1.25719600 O 2.07251400 0.09706900 - 1.39418700 H 1.07102900 -0.07451600 - 1.38597700 Cl 3.53636400 -2.01367500 0.01720400	2Cl-ClF P -2.24932300 0.23811000 0.06875700 O -1.35896800 0.20555600 1.28377900 O -1.58945700 0.40280100 - 1.36124000 H -0.59951400 0.17460300 - 1.35616500 P 1.82214400 -0.09385600 - 0.04287500 O 0.90942800 -0.20109800 - 1.24575100 O 1.17707800 -0.29757800 1.39932200 H 0.18215300 -0.10525600 1.39458900 Cl 2.78721000 1.71830200 0.01560000	2Cl-BrF P -1.76883100 0.68382200 0.07099500 O -0.88626400 0.61036900 1.29244800 O -1.08556700 0.85560100 - 1.35092900 H -0.14265800 0.48072800 - 1.36225900 P 2.22178300 -0.11362300 - 0.04577700 O 1.29408200 -0.13265300 - 1.24176700 O 1.56754400 -0.20536600 1.40379800 H 0.60400300 0.10976400 1.40100200 Br -3.19455100 -0.99237200 - 0.06399500

Br -2.04287500 2.00332500 0.01977500 Br -3.17062100 -1.35192700 - 0.04645900 Cl 4.33814700 1.11073300 0.03557100	F -3.29286700 1.44718400 0.11018500 Cl -3.51753800 -1.35150200 - 0.03323500 Cl 3.33949700 -1.45568200 - 0.08880400	Cl 3.55776900 -1.65468900 - 0.06893600 Cl 3.40498600 1.56535800 - 0.03062900 F -2.76197800 1.93699300 0.11203300
2Cl-BrCl P -1.68113800 0.48738300 0.05242300 O -0.78723000 0.63504500 1.26740600 O -1.02580300 0.73794400 - 1.38133900 H -0.05822200 0.43513400 - 1.39416600 P 2.33651000 -0.00309600 - 0.04540100 O 1.42914600 -0.07504300 - 1.25435100 O 1.67253300 -0.14282800 1.39561100 H 0.70139500 0.15524200 1.39157200 Br -2.62036800 -1.52949500 - 0.02295200 Cl 3.76626600 -1.45862300 - 0.05132900 Cl -3.24821800 1.79615500 0.07219100 Cl 3.41359900 1.74699300 - 0.01280400	2Cl-HMe P 1.98610000 0.00622500 0.33851700 O 1.08905600 1.21687100 0.48213600 O 1.31974800 -1.42563300 0.28358200 H 0.29166500 -1.39622500 0.03676500 P -1.98168700 -0.10640300 - 0.05271700 O -1.09710200 -1.34043100 - 0.30508200 H -2.27056100 0.03737100 1.33371000 O -1.36531700 1.31773500 - 0.51550400 H -0.42695100 1.41398000 - 0.19046900 C -3.56387800 -0.18051000 - 0.91623900 H -4.10404100 -1.08064900 - 0.59902500 H -4.15013400 0.71741500 - 0.68530400	2Cl-2Me P 1.83960500 0.04682600 0.43646900 O 0.95068200 1.27186700 0.36538900 O 1.22144200 -1.35701000 0.09740000 H 0.14237300 -1.33279000 - 0.10754700 P -2.02030200 -0.03709900 - 0.11337300 O -1.17850800 -1.31061400 - 0.37026800 O -1.44884900 1.31048600 - 0.82044200 H -0.51861200 1.46706100 - 0.51154900 Cl 3.50527100 0.22744300 - 0.76250600 Cl 2.65746700 -0.14061300 2.32649200 C -2.14855600 0.32346500 1.66261900 H -2.79879000 1.19114600 1.82639900

	H -3.36582000 -0.22971400 - 1.99407400 Cl 3.34735400 -0.12708000 1.86992400 Cl 3.18195600 0.14891400 - 1.33760400	H -2.54205300 -0.55471700 2.18851300 H -1.13995400 0.55122700 2.02952100 C -3.67154300 -0.19648400 - 0.82808600 H -3.56435800 -0.37506100 - 1.90442100 H -4.18247800 -1.04925400 - 0.36526600 H -4.24122200 0.72508800 - 0.65924600
2Cl-MeF P -1.55666600 0.00297400 - 0.06198500 O -0.68038800 -0.08097400 - 1.29203000 O -0.88322200 0.40346500 1.31738400 H 0.12964900 0.19998300 1.33214500 P 2.52264700 -0.08268900 0.10697100 O 1.59170100 -0.12760700 1.30682200 O 1.90049000 -0.48441400 - 1.30702400 H 0.90677300 -0.33531700 - 1.35570500 C 4.04066200 -1.02628500 0.27212000	2Cl-MeCl P 1.75090100 -0.03809800 - 0.05452600 O 0.87652700 -0.05682900 - 1.28843200 O 1.05551200 -0.14445900 1.36738400 H 0.06314900 0.14614700 1.34654600 P -2.26872200 0.31811300 0.05816300 O -1.36831100 0.58232800 1.26081900 O -1.64473400 0.64892000 - 1.38214100 H -0.67446400 0.39302400 - 1.43299300 Cl 2.92375500 1.65554300 0.00837500	2Cl-MeBr P -2.02971100 0.16815800 0.05339200 O -1.18905600 0.43650800 1.28116000 O -1.47970700 0.63248200 - 1.36027300 H -0.46511900 0.82995600 - 1.35493500 P 1.89875600 0.87249100 - 0.10966400 O 1.00274900 1.14373000 - 1.31549700 O 1.29756400 1.27112700 1.32600400 H 0.34014600 0.98198900 1.40877100 C 3.50560100 1.69100300 - 0.16985200

H 4.58634000 -0.66385100 1.15062800 H 3.77900700 -2.08249200 0.40428800 H 4.64503100 -0.89752100 - 0.63289800 Cl -3.07761500 1.35571500 - 0.27438600 Cl -2.54353500 -1.77479900 0.27585600 F 3.06993600 1.42702700 - 0.11618500	Cl 3.11894900 -1.56124300 - 0.04460400 Cl -2.78939500 -1.69648700 - 0.01324700 C -3.84299100 1.19420000 0.09046300 H -4.38326100 0.90752900 0.99908800 H -3.62708700 2.26973500 0.10021000 H -4.42056800 0.92733200 - 0.80108800	H 4.02696200 1.36890800 - 1.07747700 H 3.32610300 2.77328300 - 0.19688700 H 4.07947900 1.41843900 0.72222000 Cl -2.45123100 -1.83782100 - 0.13684200 Br 2.36212700 -1.32861200 0.02175100 Cl -3.88623400 1.02977000 0.16866100
2Br-2Br P -2.01923900 -0.38701500 0.04260100 O -1.15120000 -0.41127300 1.28676700 O -1.37969500 -0.94267400 - 1.31248100 H -0.38385900 -0.74987100 - 1.35690700 P 2.01923800 -0.38679000 - 0.04253500 O 1.15109200 -0.41099300 - 1.28662300 O 1.37972900 -0.94221200 1.31266300 H 0.38379600 -0.74980500 1.35695700 Br 2.71283900 1.68877300 0.38853200	2Br-ClF P -1.15836400 -0.22096900 - 0.03335700 O -0.27577100 -0.50103400 - 1.23583800 O -0.57073600 -0.58383100 1.40832900 H 0.43565600 -0.46906400 1.43533700 P 2.88171200 -0.61801000 0.14712800 O 2.00149500 -0.27346800 1.32090300 O 2.21019200 -1.15823000 - 1.18117000 H 1.22514900 -0.91356800 - 1.24170000 Br -1.72816300 1.93312200 0.03824500	2Br-BrF P -1.56089400 -0.25568500 - 0.03160700 O -0.67261900 -0.53839800 - 1.22907300 O -1.07017900 -0.79619800 1.39086200 H -0.05943200 -0.78625500 1.45987800 P 2.39757200 -1.04332000 0.21747800 O 1.52390400 -0.74218800 1.41029600 O 1.70758200 -1.52612200 - 1.12773200 H 0.76583500 -1.15873600 - 1.22071200 Br -1.88604200 1.93770900 0.20142000

Br 3.86210500 -1.59715000 - 0.24993200 Br -3.86232100 -1.59704700 0.24978400 Br -2.71239800 1.68867500 - 0.38858400	Br -3.06806700 -1.33844700 - 0.08668400 Cl 4.12143600 0.91086000 - 0.37106100 F 3.94591200 -1.76348800 0.47870900	Br -3.58127400 -1.13888700 - 0.22446700 F 3.43640300 -2.22962000 0.48916800 Br 3.75843400 0.62027300 - 0.27051100
2Br-BrCl P 1.80045200 -0.08178200 0.04037300 O 0.95707500 -0.41087100 1.25794600 O 1.19665200 -0.45146900 - 1.39254700 H 0.18567700 -0.36651500 - 1.39282100 P -2.25247500 -0.43918300 - 0.03693100 O -1.37295100 -0.19373000 - 1.24575400 O -1.61098100 -0.21512200 1.40577300 H -0.59686500 -0.28490000 1.38462700 Br -4.04890600 0.84975200 - 0.02080600 Cl -2.99604900 -2.36012900 - 0.02804000 Br 2.28965000 2.09485200 - 0.03088900 Br 3.74801800 -1.13044100 0.05033800	2Br-HMe P 0.61478800 -0.27168200 - 0.01173200 O -0.21825200 -0.72818300 - 1.19327000 O 0.07305200 -0.56435300 1.44824800 H -0.98241300 -0.53074700 1.48971500 P -3.22145100 -0.54718000 0.15749000 O -2.42349900 -0.48813100 1.47233900 H -4.55606500 -0.96660400 0.37823000 O -2.73412400 -1.65439700 - 0.92632400 H -1.78451900 -1.48678500 - 1.15908100 C -3.27740400 1.05427400 - 0.69178500 H -3.91467900 0.98214900 - 1.58163500 H -3.66146600 1.81673200 - 0.00326000	2Br-2Me P 0.85686300 -0.27011100 - 0.03106900 O 0.04348800 -0.65969100 - 1.25092300 O 0.23301500 -0.49892200 1.39817200 H -0.85589800 -0.43984100 1.40087200 P -3.00533000 -0.28491100 0.05331100 O -2.21904000 -0.37894700 1.38240900 O -2.54599900 -1.34783800 - 1.08765000 H -1.57601600 -1.24191300 - 1.27006200 Br 2.83038300 -1.29742900 0.05025500 Br 1.36355900 1.92469900 - 0.15288600 C -4.74978000 -0.68846600 0.29551200 H -4.81376200 -1.70606000 0.69840000

	H -2.25329500 1.31346500 - 0.99079800 Br 2.66225300 -1.13281800 0.00093700 Br 0.92077500 1.95458300 - 0.13241100	H -5.18510200 0.01686200 1.01347000 H -5.28230200 -0.63370700 - 0.66143300 C -2.85769600 1.36925200 - 0.68435900 H -3.18804800 2.12275800 0.04083000 H -1.80196800 1.54067900 - 0.92949100 H -3.45832600 1.42984400 - 1.59984300
2Br-MeF P -0.92324600 -0.17930600 - 0.04813800 O -0.05092300 -0.40583100 - 1.26706600 O -0.25628100 -0.34607600 1.38635800 H 0.77376300 -0.27982800 1.35640800 P 3.16431500 -0.25154100 0.07126500 O 2.27111400 -0.22476000 1.29926700 O 2.52721400 -0.81771300 - 1.27837100 H 1.53270400 -0.67593800 - 1.33062900 C 4.73603400 -1.09626500 0.26820700	2Br-MeCl P -1.08528400 -0.27432100 - 0.03874300 O -0.24623500 -0.60618800 - 1.25649300 O -0.48760400 -0.61273000 1.39663000 H 0.54392000 -0.65972200 1.39682200 P 2.90391000 -0.58287900 0.11294000 O 2.04597700 -0.76370400 1.36008400 O 2.31229800 -1.17907500 - 1.25407500 H 1.32911800 -0.99426700 - 1.34135300 C 4.56482100 -1.27152500 0.23195000	2Br-MeBr P 1.40049900 -0.31061800 - 0.03693500 O 0.59819900 -0.74217900 - 1.24800000 O 0.89126600 -0.76682000 1.40056400 H -0.12570800 -0.94052600 1.42393400 P -2.49644500 -1.02660900 0.17879900 O -1.61063200 -1.22043700 1.40643200 O -1.90072300 -1.54922400 - 1.21926900 H -0.94036300 -1.27861600 - 1.32687300 Br -2.90926400 1.16736200 - 0.12859500

H 5.28406500 -0.63047300 1.09501000 H 4.53680100 -2.14919500 0.49885500 H 5.30807000 -1.01522300 - 0.66296300 Br -1.82021500 1.86686000 - 0.08048500 Br -2.66641800 -1.56061000 0.01702800 F 3.62265800 1.25758800 - 0.30496200	H 5.07407300 -0.80887200 1.08416300 H 4.46745200 -2.35285700 0.38940100 H 5.10619500 -1.06664800 - 0.69786700 Br -1.59681200 1.90230800 0.00047400 Cl 3.19910600 1.44629700 - 0.25376700 Br -3.04608100 -1.32145200 - 0.04510800	Br 3.49649400 -1.04560900 - 0.09842700 Br 1.57253200 1.91793400 0.04497400 C -4.12131000 -1.80269800 0.29418800 H -3.96585300 -2.88327300 0.40585700 H -4.63812400 -1.39999800 1.17173300 H -4.68624600 -1.58768500 - 0.61905000
CIF-CIF P 2.00652500 0.30891900 0.02214100 O 1.11871600 0.17207200 1.23197700 O 1.34076000 0.36480700 - 1.41352200 H 0.36534900 0.08713100 - 1.39792700 P -2.03845400 -0.42485600 - 0.08351600 O -1.13330100 -0.34301000 - 1.28555900 O -1.39592800 -0.37201100 1.36257800 H -0.40496200 -0.15533600 1.33958100 F -2.88516700 -1.78088700 - 0.05964200	CIF-BrF P -1.49750700 0.78996000 - 0.08246500 O -0.60420700 0.73705200 - 1.29734700 O -0.82553800 0.75951200 1.35506600 H 0.09065500 0.32803600 1.33412500 P 2.42785400 -0.37219900 - 0.01778300 O 1.50267700 -0.34471100 1.17141800 O 1.83303300 -0.08604800 - 1.45706200 H 0.87333400 0.24197700 - 1.42344400 Br -3.08634000 -0.73545500 - 0.11556800	CIF-BrCl P -2.70056900 -0.48775700 0.14320600 O -1.85991300 -0.08587600 1.32775800 O -1.97606100 -0.93497700 - 1.19191500 H -1.02006100 -0.59223200 - 1.24117400 P 1.31955400 0.21483100 - 0.00632600 O 0.42590300 -0.02115500 - 1.20785400 O 0.72423600 -0.12500700 1.43427100 H -0.29016900 -0.11037000 1.43670700 F -3.65084500 -1.73617900 0.44783400

F 2.88307600 1.64491000 0.05915200 Cl 3.47121400 -1.09968300 - 0.05617200 Cl -3.53546300 0.95055300 - 0.10502100	F 3.13842100 -1.79349800 - 0.19292700 F -2.35836200 2.13665400 - 0.01741900 Cl 4.05122400 0.83499700 0.19136000	Br 3.19914600 -0.94796200 - 0.07917200 Cl 1.92958000 2.17714600 0.07389100 Cl -4.07925700 0.92550300 - 0.34986300
CIF-HMe P 1.39174200 -0.35717700 - 0.09821400 O 0.43610200 -0.34115100 - 1.26441700 O 0.83157100 -0.57402600 1.35490900 H -0.21425700 -0.42834900 1.41839400 P -2.48435000 -0.07013300 0.18932400 O -1.63209300 -0.23554100 1.46013800 H -3.84087000 -0.39861600 0.42895300 O -2.14309700 -1.07703200 - 1.03865400 H -1.19099600 -0.96504100 - 1.29221000 C -2.43052600 1.61869500 - 0.46894400 H -3.12372800 1.71103700 - 1.31408500 H -2.69399700 2.32849800 0.32455000	CIF-2Me P 1.68573500 -0.37793100 - 0.08312900 O 0.80117000 -0.29833800 - 1.30318500 O 1.04110600 -0.58544600 1.32823200 H -0.04303300 -0.46561700 1.33926300 P -2.18436000 0.04577400 0.06936700 O -1.39568700 -0.32932500 1.34625900 O -1.82552000 -0.84677400 - 1.24147600 H -0.85297400 -0.77978600 - 1.42550500 C -1.90390200 1.78028700 - 0.39421400 H -2.52372500 2.04636100 - 1.25886200 H -2.13618000 2.43036000 0.45790400 H -0.84485600 1.88760600 - 0.66061400	CIF-MeF P -1.77655300 0.34378500 0.06240700 O -0.89683500 0.38630500 1.28465200 O -1.11457100 0.40208800 - 1.36877200 H -0.09141900 0.25982400 - 1.34836300 P 2.28394300 -0.05167000 - 0.07581900 O 1.39036600 0.09009200 - 1.29599100 O 1.71649500 0.50738100 1.30757300 H 0.71344300 0.47625000 1.35968400 C 3.93935400 0.62169700 - 0.24093200 H 4.43040200 0.14181800 - 1.09501000 H 3.85847500 1.70095700 - 0.41473200 H 4.50033800 0.42846100 0.68039100

H -1.40519400 1.81021500 - 0.81160500 F 2.52286500 -1.48462200 - 0.23363500 Cl 2.56291000 1.32288000 - 0.05302800	C -3.95331100 -0.25158900 0.28396300 H -4.09682500 -1.31234900 0.52091400 H -4.32236900 0.36146700 1.11488500 H -4.48875400 -0.00159600 - 0.63966200 F 2.77937000 -1.54746300 - 0.19592800 Cl 2.92764200 1.25143600 0.05174700	F -2.82955900 1.55078300 0.02380100 Cl -3.05069200 -1.24925900 0.06621100 F 2.56913600 -1.62093600 0.21442100
ClF-MeCl P -1.92685300 0.41400700 0.09312200 O -1.04188900 0.40748500 1.31197500 O -1.29114500 0.67845800 - 1.32660000 H -0.25714200 0.65162700 - 1.32488500 P 2.08915800 0.25635600 - 0.08956400 O 1.23583300 0.64525800 - 1.29224700 O 1.56079700 0.74168800 1.34543300 H 0.56587700 0.63880500 1.42558000 C 3.79871200 0.81999200 - 0.16458300	ClF-MeBr P -2.21399200 0.45756900 0.09052300 O -1.34354200 0.56632300 1.31477900 O -1.61704500 0.82474000 - 1.32348600 H -0.58726000 0.91751500 - 1.32311000 P 1.77183100 0.71793600 - 0.08351700 O 0.90006900 1.07816200 - 1.28415300 O 1.21481600 1.16189300 1.35679600 H 0.23531000 0.96460800 1.44274200 C 3.44652700 1.38605500 - 0.14593400	BrF-BrF P -1.89205500 0.73322300 - 0.08510700 O -1.00677600 0.51218200 - 1.28685000 O -1.22182300 0.77918500 1.35283900 H -0.34017800 0.28089600 1.37552200 P 1.89852400 -0.73904200 0.07887100 O 1.01787500 -0.51158500 1.28278400 O 1.22236600 -0.79690300 - 1.35593300 H 0.34476000 -0.29174300 - 1.38065800 Br -3.58811400 -0.67043400 0.01132400

H 4.26008500 0.41565000 - 1.07193600 H 3.78764800 1.91640800 - 0.20038500 H 4.33124200 0.47080300 0.72655700 F -3.08578600 1.51681900 0.18484900 Cl 2.22150000 -1.81739700 0.04301500 Cl -3.05157500 -1.28072000 - 0.06995500	H 3.93228200 1.02413300 - 1.05829300 H 3.36695500 2.48040200 - 0.16454200 H 3.99672200 1.05538700 0.74139300 F -3.51864400 1.38276900 0.18290500 Cl -3.08372000 -1.37963500 - 0.09280200 Br 2.03120500 -1.51683500 0.03280500	F 2.66152100 -2.14325200 0.14145100 Br 3.59099900 0.66782500 - 0.03328200 F -2.65197800 2.13940900 - 0.14202200
BrF-BrCl P -2.05502200 0.94304600 - 0.21634400 O -1.12759800 0.75556100 - 1.39176700 O -1.44817200 1.46003000 1.15600900 H -0.47758100 1.18546100 1.26634700 P 1.93983100 0.51212200 0.11270800 O 1.01897200 0.71405100 1.29948800 O 1.44849200 1.05586600 - 1.30592800 H 0.44589700 0.95582100 - 1.40713500 F -3.19828300 2.02814600 - 0.49077500	BrF-HMe P 0.96211800 -0.87474400 - 0.09960600 O 0.02472300 -0.79173300 - 1.27888200 O 0.36585400 -1.07084200 1.34543000 H -0.60998700 -0.67999700 1.43013800 P -2.74567900 0.18653900 0.19834700 O -1.94600300 -0.13890000 1.47209400 H -4.14017500 0.18965700 0.44540000 O -2.65674000 -0.90403500 - 1.00233000 H -1.70813200 -1.02271500 - 1.26404300	BrF-2Me P 1.25634500 -0.86592000 - 0.07559400 O 0.38307400 -0.86953600 - 1.30696100 O 0.59856800 -1.01642700 1.34052900 H -0.43261800 -0.68226900 1.36620900 P -2.47849600 0.13333600 0.06962300 O -1.74157500 -0.26562400 1.36905300 O -2.30452700 -0.91251100 - 1.16368900 H -1.34038200 -1.03794800 - 1.35807500 C -1.91290800 1.74999900 - 0.53870300

Cl 3.74926200 1.43221500 0.34220300 Br 2.42481100 -1.64186100 - 0.15652500 Br -3.25678900 -0.85629100 0.20201800	C -2.30354200 1.79881200 - 0.50471300 H -2.95687300 2.02588800 - 1.35611000 H -2.39562100 2.57131700 0.26836100 H -1.26155000 1.74045100 - 0.84577600 Br 2.33831000 0.86635300 - 0.03401600 F 2.01160500 -2.08140800 - 0.21404400	H -2.48570500 2.04231800 - 1.42696100 H -2.02662300 2.49946800 0.25381200 H -0.85230800 1.65872200 - 0.80490200 C -4.26857400 0.16694500 0.31262900 H -4.58977300 -0.83055800 0.63476000 H -4.51140700 0.89846300 1.09262000 H -4.76839400 0.43279500 - 0.62640200 F 2.36368300 -2.02755200 - 0.09811200 Br 2.56091500 0.93750900 - 0.02715000
BrF-MeF P -1.26694300 0.73888900 0.06123500 O -0.38101600 0.74516400 1.28193200 O -0.59840900 0.75702900 - 1.37150600 H 0.38420600 0.44204900 - 1.35720400 P 2.70716900 -0.14785000 - 0.07707700 O 1.82009400 0.02103700 - 1.29829900	BrF-MeCl P -1.46559100 0.89815700 0.10572600 O -0.58260400 0.85948600 1.32759200 O -0.80849800 1.13847300 - 1.31225100 H 0.19620100 0.90260200 - 1.33512100 P 2.45957100 0.13538200 - 0.09900200 O 1.66530200 0.59020100 - 1.31844600	BrF-MeBr P -1.76522800 0.94578100 0.12656500 O -0.88972900 1.05649600 1.34910300 O -1.17048400 1.33580000 - 1.28625700 H -0.14351500 1.24941000 - 1.32517600 P 2.17337000 0.65340400 - 0.11692800 O 1.36090100 1.13890000 - 1.31443400

O 2.23116500 0.56437700 1.27033300 H 1.23236000 0.65214200 1.33510600 C 4.42973600 0.30762500 - 0.29353100 H 4.84816400 -0.28102000 - 1.11772200 H 4.47774600 1.37563200 - 0.53565900 H 4.97514300 0.10602000 0.63531500 Br -2.74140200 -0.90595700 0.09199600 F 2.80463300 -1.71822700 0.31319600 F -2.24037100 2.01243400 0.00284200	O 2.04293900 0.78529400 1.30772100 H 1.04625900 0.84434200 1.40671900 C 4.23842300 0.39701700 - 0.21520100 H 4.61161100 -0.13038200 - 1.09964200 H 4.41174200 1.47565500 - 0.31525100 H 4.71771500 0.01411700 0.69214700 Br -2.76573000 -0.88207500 - 0.05396500 F -2.56217500 2.06601600 0.17684000 Cl 2.24350800 -1.91997000 0.15767400	O 1.73750600 1.22712000 1.31975300 H 0.74218300 1.19794400 1.43470700 C 3.94186000 0.99465800 - 0.22035000 H 4.33447100 0.52506900 - 1.12849600 H 4.06753000 2.08373900 - 0.26965400 H 4.43707300 0.59004600 0.66870300 Br -2.69588400 -1.05034900 - 0.06780200 F -3.06525600 1.87916100 0.21485300 Br 2.00955800 -1.58727900 0.05850000
BrCl-BrCl P -1.95015000 0.50212700 0.05016200 O -1.04128900 0.52101800 1.26266300 O -1.26931300 0.63915700 - 1.38699100 H -0.35590300 0.19791200 - 1.40063900 P 1.95071100 -0.50242900 - 0.04925700 O 1.04242900 -0.52066700 - 1.26219400	BrCl-HMe P 0.75170300 0.31107400 - 0.00628200 O -0.12938300 0.07921800 - 1.21816200 O 0.04260100 0.57205200 1.38488900 H -0.92714600 0.14588000 1.42538200 P -3.02929000 -0.58978000 0.11084200 O -2.23820500 -0.43016800 1.42201100	BrCl-2Me P 1.17064000 -0.61653200 - 0.04995000 O 0.31021100 -0.85897900 - 1.27335400 O 0.52978400 -0.79586900 1.37756500 H -0.53181400 -0.56239600 1.39177300 P -2.64516400 -0.05015600 0.05995500 O -1.87345000 -0.27984000 1.38058600

O 1.26924400 -0.64137500 1.38744000 H 0.35632900 -0.19914400 1.40145700 Br -3.18699000 -1.34803300 - 0.00880800 Br 3.18633000 1.34846500 0.01204400 Cl 3.30122000 -2.03448500 - 0.06196100 Cl -3.29975600 2.03502100 0.06210800	H -4.21769400 -1.33140000 0.31577700 O -2.32012900 -1.47731200 - 1.05080300 H -1.44787400 -1.06500100 - 1.28117900 C -3.48118100 1.00123500 - 0.63270600 H -4.11827600 0.83458000 - 1.50993100 H -4.00152400 1.61772700 0.11023100 H -2.55201000 1.49767400 - 0.94169400 Cl 1.97725600 1.94510700 - 0.24551700 Br 2.16832000 -1.38904600 0.30240200	O -2.35534400 -1.15112100 - 1.10075600 H -1.38176500 -1.18838100 - 1.28952200 C -2.25799200 1.57508700 - 0.65504500 H -2.84683100 1.73788500 - 1.56570300 H -2.46984000 2.35817800 0.08298400 H -1.18953300 1.59195100 - 0.90437500 C -4.42906800 -0.19436700 0.30871600 H -4.64131400 -1.19725700 0.69739900 H -4.75156500 0.55663900 1.03977400 H -4.95231700 -0.04673600 - 0.64351600 Br 1.99625800 1.47523400 - 0.12060900 Cl 2.84530700 -1.80627500 - 0.00809000
BrCl-MeF P -1.24334700 -0.55356800 - 0.05295100 O -0.36344200 -0.71219100 - 1.27517900 O -0.56872400 -0.69957100 1.37880900	BrCl-MeCl P -1.41834100 -0.61700300 - 0.07225200 O -0.55018400 -0.83902100 - 1.29267600 O -0.80346200 -0.94143600 1.35729200	BrCl-MeBr P -1.74078000 -0.62635700 - 0.09843700 O -0.89043700 -0.94229900 - 1.31043700 O -1.21821300 -1.09053200 1.32970500

H 0.43195000 -0.45080900 1.36440200 P 2.78727200 -0.02798600 0.07160600 O 1.89886800 -0.12275000 1.29967400 O 2.25065800 -0.70887100 - 1.26884000 H 1.24674000 -0.72483000 - 1.32730300 C 4.47287800 -0.60966900 0.27913600 H 4.93909200 -0.05067600 1.09832500 H 4.44300900 -1.67734900 0.52556600 H 5.02595200 -0.45271900 - 0.65378700 Cl -2.76702700 -1.92576000 0.00349200 F 3.00065400 1.52882800 - 0.32825600 Br -2.28445400 1.41855500 - 0.06774900	H 0.22159400 -0.82632000 1.37803800 P 2.55845200 -0.38008100 0.11551300 O 1.72429700 -0.68987900 1.35336400 O 2.06642600 -1.03888300 - 1.26219800 H 1.06808000 -0.99285000 - 1.35938800 C 4.29824400 -0.83150200 0.24289800 H 4.73262000 -0.30773800 1.10118400 H 4.35198500 -1.91680600 0.39375500 H 4.81152500 -0.54698700 - 0.68188700 Cl -3.13238700 -1.74205900 - 0.11069100 Br -2.14639000 1.49028300 0.01570400 Cl 2.57124800 1.67415800 - 0.23085900	H -0.18872800 -1.12276200 1.37801400 P 2.19835400 -0.88191100 0.17237700 O 1.32323600 -1.19357900 1.38332300 O 1.68745800 -1.44927300 - 1.24170000 H 0.70424100 -1.29020500 - 1.36399700 C 3.90013000 -1.46721100 0.30345600 H 4.35489000 -1.01952900 1.19347800 H 3.86902100 -2.55991400 0.39997800 H 4.44904200 -1.17615000 - 0.59841100 Cl -3.60797700 -1.46630800 - 0.20663000 Br -2.13052800 1.56544900 0.05320700 Br 2.36035300 1.34926600 - 0.10029900
HMe-HMe P 1.86649100 0.13620900 0.41565600 O 0.93756800 -0.69812700 1.31082300 O 1.25180100 1.52234200 - 0.15641800	HMe-2Me P -2.22299000 0.23127700 0.12216000 O -1.37552700 0.48384100 1.37808000 O -1.61429600 0.77838100 - 1.27436800	HMe-MeF P -1.61521000 0.02088700 0.10421200 O -0.70757800 0.07369600 1.31911800 O -1.08478200 -0.74653500 - 1.18286100

H 0.39331300 1.32751900 - 0.65552400	H -0.68496400 0.38436100 - 1.40944000	H -0.05763300 -0.74421000 - 1.27073900
P -1.86712300 -0.13666800 - 0.41568800	P 1.60919800 -0.04937200 - 0.09252100	P 2.27977500 -0.26988300 - 0.09465200
O -0.93834900 0.69761400 - 1.31106400	O 0.72058100 -0.32941900 - 1.31935000	O 1.45645300 -0.71290400 - 1.31334900
O -1.25251000 -1.52300400 0.15599500	O 1.01617000 -0.58433700 1.32278600	H 3.60215300 -0.78080700 - 0.13077500
H -0.39403700 -1.32832600 0.65513200	H 0.08789700 -0.21545400 1.46310800	O 1.78097800 -0.81996000 1.34776100
C 2.48446800 -0.80192500 - 1.01221500	C 1.90365700 1.73443500 0.12218000	H 0.82698200 -0.55193200 1.48290600
C -2.48440700 0.80137800 1.01253900	H 2.33804600 2.15007700 - 0.79520700	C 2.40447100 1.53683200 0.03763600
H 1.62264100 -1.05020700 - 1.64538800	H 0.93335200 2.20970900 0.31341000	H 3.06419400 1.80602100 0.87173900
H 3.19473000 -0.19048600 - 1.58231000	H 2.56975500 1.91145100 0.97522400	H 2.78784300 1.94696700 - 0.90456800
H 2.96356800 -1.72569800 - 0.66545100	C 3.20791800 -0.89746900 - 0.19229600	H 1.39621600 1.92886800 0.22549000
H -3.19470000 0.19004900 1.58271300	H 3.02169200 -1.97349300 - 0.29025300	C -3.28908900 -0.57442400 0.38681100
H -1.62231900 1.04925500 1.64551500	H 3.74996800 -0.54049900 - 1.07639200	H -3.75580900 0.03992600 1.16501300
H -2.96331200 1.72537100 0.66609200	H 3.79342700 -0.70510700 0.71474700	H -3.85992700 -0.50840600 - 0.54622600
H -3.00138500 -0.61872800 - 1.11898600	C -2.60107800 -1.53048400 - 0.11689200	H -3.23376500 -1.61736700 0.71995200
H 3.00043600 0.61857000 1.11926400	H -1.65242300 -2.04942700 - 0.30659700	F -1.88343700 1.54219000 - 0.41793900
	H -3.06595600 -1.93416900 0.79084800	

	H -3.26698200 -1.65691000 - 0.97943600 H -3.46461700 0.91812200 0.16426600	
HMe-MeCl P 1.44715800 -0.41214700 - 0.12722700 O 0.57089500 -0.81014900 - 1.30479500 O 0.91105500 -0.75056700 1.33639900 H -0.10136000 -0.58267600 1.43463900 P -2.41126100 -0.14406100 0.16296200 O -1.59468200 -0.31960000 1.45215500 H -3.78337200 -0.44721700 0.35479600 O -2.04894700 -1.14601600 - 1.05939400 H -1.06899200 -1.10223300 - 1.25566600 C -2.32430400 1.55021200 - 0.48329300 H -2.95921200 1.64409900 - 1.37286300 H -2.64623600 2.25238800 0.29554200 H -1.27953100 1.75854800 - 0.74905300	HMe-MeBr P 1.04591400 -0.93829900 - 0.12898500 O 0.10888400 -1.20868900 - 1.29782700 O 0.46193500 -1.14034400 1.34303300 H -0.49564500 -0.76994900 1.43977900 P -2.70025800 0.06473700 0.16787500 O -1.90279200 -0.21146800 1.45154100 H -4.10036900 -0.00982800 0.38240200 O -2.52185900 -1.00862400 - 1.03377700 H -1.55081700 -1.15368600 - 1.22846000 C -2.35607800 1.70972000 - 0.51750600 H -2.98182700 1.88433000 - 1.40139700 H -2.55194700 2.46950300 0.24916700 H -1.29542700 1.74593900 - 0.79898300	2Me-2Me P 1.95732800 -0.00391300 0.05455700 O 1.10131800 0.03631600 1.33307000 O 1.33252700 -0.85450400 - 1.17595600 H 0.37117400 -0.57774000 - 1.32997200 P -1.95744000 -0.00424600 - 0.05462000 O -1.10149900 0.03591900 - 1.33318100 O -1.33251700 -0.85469300 1.17594000 H -0.37121600 -0.57774700 1.32993300 C 3.56876300 -0.80015800 0.30345300 C 2.25032500 1.67887200 - 0.58052100 C -2.25049100 1.67857700 0.58032800 C -3.56883500 -0.80061800 - 0.30335900 H 2.68286600 2.30355400 0.21058200

C 3.13790300 -1.04297400 - 0.16790700 H 3.60857200 -0.72462000 - 1.10420500 H 3.68960700 -0.65244700 0.69384400 H 3.08529800 -2.13799000 - 0.12375700 Cl 1.70083800 1.67825600 - 0.14536700	C 2.59466900 -1.86985100 - 0.14843700 H 3.11170800 -1.66979800 - 1.09282600 H 3.21042200 -1.56087300 0.70282800 H 2.34045200 -2.93477400 - 0.07186100 Br 1.72019600 1.23727000 - 0.21010200	H 2.91848800 1.64815800 - 1.44968700 H 1.28052500 2.09181200 - 0.88503100 H 3.39492300 -1.82208600 0.66075100 H 4.12486200 -0.82923900 - 0.64139700 H 4.13517600 -0.24235900 1.05918100 H -2.91863100 1.64791700 1.44951300 H -1.28069400 2.09157200 0.88477500 H -2.68307100 2.30317400 - 0.21082100 H -4.12488200 -0.82962800 0.64152500 H -4.13532600 -0.24293800 - 1.05911700 H -3.39495000 -1.82257500 - 0.66055000
2Me-MeF P 1.97805600 -0.02640600 - 0.05929200 O 1.08374400 0.38936700 - 1.21454300 O 1.32743100 -0.06360200 1.38857600 H 0.29735900 -0.21830500 1.37834500	2Me-MeCl P 1.76677300 0.32089900 - 0.05513900 O 0.87764600 0.53493200 - 1.27430400 O 1.09683200 0.55951400 1.37146800 H 0.10305400 0.24568100 1.40274900	2Me-MeBr P 1.33019200 0.79599500 - 0.05548100 O 0.42584100 0.88217800 - 1.28108400 O 0.62588300 0.96783700 1.36626400 H -0.30576600 0.50087000 1.40407300

P -1.98581300 0.01101700 0.07395100	P -2.15401800 -0.01688100 0.07152000	P -2.49134300 -0.11231300 0.07119800
O -1.16449900 -0.41699400 1.30515300	O -1.30669300 -0.19112100 1.34683400	O -1.62745000 -0.15511300 1.34664500
O -1.40545300 -0.49244000 - 1.35790300	O -1.50340900 -0.62971200 - 1.28593100	O -1.75750000 -0.62516600 - 1.28538000
H -0.44578200 -0.22300300 - 1.44234400	H -0.58066600 -0.26577200 - 1.41259200	H -0.89992200 -0.12816500 - 1.41566900
C -2.11571600 1.82320700 - 0.04178700	Cl 2.46449200 -1.65504200 - 0.02722200	Br 2.35081700 -1.22817100 0.00166800
H -2.52383900 2.22475900 0.89371000	C -2.48114800 1.74026200 - 0.27347000	C -3.91886400 -1.21970100 0.18489300
H -1.10451800 2.21905300 - 0.19914800	H -2.94682400 2.20817400 0.60240100	H -3.54968700 -2.23678300 0.36180700
H -2.75183200 2.10637900 - 0.88915700	H -1.51698100 2.22337900 - 0.47604800	H -4.54975000 -0.90952300 1.02657200
F 2.52612200 -1.54075600 - 0.29890400	H -3.12981900 1.84216500 - 1.15191300	H -4.49165300 -1.19130100 - 0.74974000
C -3.65259800 -0.69579700 0.09256200	C -3.73077600 -0.89950600 0.18192000	C -3.07578700 1.57588000 - 0.27796000
H -3.56153000 -1.78776900 0.12900100	H -3.51757900 -1.96052000 0.35753300	H -3.60551300 1.97155300 0.59713700
H -4.18341900 -0.34452600 0.98561300	H -4.30963400 -0.50007300 1.02338200	H -2.19412000 2.19640100 - 0.48214400
H -4.19591900 -0.39974300 - 0.81278200	H -4.29166100 -0.78458700 - 0.75330700	H -3.73264800 1.57825500 - 1.15621500
C 3.51579400 0.89664000 0.09799200	C 3.28356300 1.30262100 - 0.03995200	C 2.70421900 1.97292000 - 0.04521500
H 4.07989600 0.80718100 - 0.83724100	H 3.85816100 1.07442200 - 0.94403900	H 3.30725900 1.81501700 - 0.94559800
H 3.27207900 1.94869800 0.28606200	H 2.99782100 2.36180200 - 0.03015700	H 2.27734400 2.98392400 - 0.04546500

H 4.09698000 0.49201100 0.93424100	H 3.86318400 1.05669400 0.85620300	H 3.30713000 1.81316000 0.85493100
MeF-MeF P 2.03969700 0.06640700 - 0.03767400 O 1.17265400 1.29455400 - 0.24446800 O 1.39574700 -1.34977800 - 0.38040700 H 0.38108000 -1.35978000 - 0.31311600 P -2.03973000 -0.06639600 - 0.03759500 O -1.17270400 -1.29446300 - 0.24491500 O -1.39578000 1.34991600 - 0.37977800 H -0.38109800 1.35989900 - 0.31256600 C 3.64185000 0.09709200 - 0.85222000 H 3.47919300 0.15208400 - 1.93488400 H 4.19313500 0.98132600 - 0.51289300 H 4.19285400 -0.81601500 - 0.60012700 C -3.64191600 -0.09674800 - 0.85209000 H -3.47930600 -0.15131700 - 1.93478200	MeF-MeCl P -1.84311300 -0.32221100 0.06900400 O -0.97184100 -0.54668900 1.29803000 O -1.18123500 -0.64580600 - 1.35105900 H -0.19984900 -0.38155900 - 1.38338500 P 2.19594200 -0.00274400 - 0.06508300 O 1.29401300 0.06171000 - 1.28394600 O 1.50921000 0.14163600 1.36535300 H 0.52878500 -0.13036300 1.37699800 C 3.58394400 1.13923500 - 0.06919900 H 4.18768000 0.95827400 - 0.96563400 H 3.18914500 2.16173300 - 0.08570200 H 4.18431100 0.98210300 0.83396100 C -3.40495700 -1.22480100 0.07147400 H -3.17040000 -2.29623200 0.09711600	MeF-MeBr P 2.51092000 -0.05470300 - 0.06623300 O 1.60469300 0.00055800 - 1.28229600 O 1.81681300 -0.07630000 1.36793700 H 0.88521700 0.33210200 1.37909100 P -1.43838300 0.80025600 0.07104200 O -0.54613300 0.95153600 1.29820300 O -0.74690000 1.04481300 - 1.35282700 H 0.18940700 0.64916500 - 1.38916000 C -2.89761100 1.86492800 0.06195100 H -3.49096700 1.65299700 0.95760800 H -2.54852700 2.90528500 0.07293700 H -3.48075500 1.66541700 - 0.84329300 F 3.46452500 1.26042200 - 0.02364300 Br -2.27614600 -1.30054500 - 0.01631100

H -4.19319700 -0.98110800 - 0.51308400 H -4.19290000 0.81626700 - 0.59961700 F 2.45949800 -0.05553800 1.52705400 F -2.45948900 0.05493500 1.52719400	H -3.97295200 -0.93983800 0.96350200 H -3.96486300 -0.97764100 - 0.83680800 Cl -2.41954700 1.68554200 - 0.03531500 F 2.94235000 -1.44507500 - 0.00184000	C 3.71244000 -1.39142800 - 0.05815700 H 3.16876900 -2.34329100 - 0.05867200 H 4.33199200 -1.31535300 - 0.95880300 H 4.33402800 -1.31352700 0.84094900
MeCl-MeCl P 1.98647600 -0.35774600 - 0.08850700 O 1.16375600 -0.68479000 - 1.32748400 O 1.41347500 -0.87180500 1.31496200 H 0.40238400 -0.79285800 1.37392300 P -1.98647200 -0.35775400 0.08849800 O -1.16374800 -0.68473400 1.32748700 O -1.41346000 -0.87186800 - 1.31494700 H -0.40236400 -0.79293300 - 1.37390100 C 3.69298100 -0.94179000 - 0.13186100 H 3.67020400 -2.03606600 - 0.20664100 H 4.18733000 -0.51240000 - 1.00984600	MeCl-MeBr P 2.29388500 -0.43238100 - 0.06665400 O 1.38706800 -0.41403300 - 1.29047000 O 1.57821800 -0.52977700 1.36143700 H 0.71310600 0.00310100 1.39969000 P -1.51556600 0.82152200 0.07462500 O -0.60971900 0.83793000 1.30121200 O -0.79763400 0.95446800 - 1.35142700 H 0.06993700 0.42519800 - 1.39375300 C -2.79215200 2.09970200 0.06365100 H -3.40967600 1.98474700 0.96068600 H -2.28596200 3.07336400 0.07118200	MeBr-MeBr P 1.97737200 -0.83669500 - 0.15661900 O 1.11856200 -1.16834300 - 1.37156200 O 1.45740500 -1.37538100 1.26078500 H 0.45088300 -1.28797800 1.36164400 P -1.97740300 -0.83669900 0.15666600 O -1.11869200 -1.16789800 1.37182400 O -1.45746400 -1.37591100 - 1.26055100 H -0.45107400 -1.28783900 - 1.36181300 Br -2.15122500 1.40448200 - 0.07613500 Br 2.15145800 1.40453900 0.07559000 C 3.68799500 -1.40914300 - 0.25930700

H 4.20273000 -0.63149800 0.78655000	H -3.40078800 1.99056400 - 0.84020200	H 3.66828600 -2.50348100 - 0.33870400
C -3.69297400 -0.94180800 0.13187700	Br -2.66847800 -1.12329100 - 0.00660600	H 4.14963700 -0.97109000 - 1.15052700
H -3.67019000 -2.03608100 0.20671000	C 3.52466600 -1.75130900 - 0.05736200	H 4.22403500 -1.09910300 0.64396200
H -4.18733400 -0.51237800 1.00983600	H 2.98743300 -2.70782500 - 0.06367000	C -3.68804200 -1.40909000 0.25933500
H -4.20271800 -0.63156600 - 0.78655300	H 4.14421200 -1.65870100 - 0.95575500	H -3.66835000 -2.50339500 0.33919700
Cl 2.16658500 1.71361800 0.11494400	H 4.13929900 -1.66394900 0.84492900	H -4.14981700 -0.97069500 1.15032000
Cl -2.16660500 1.71360100 - 0.11504600	Cl 3.42979500 1.32102300 0.00315100	H -4.22394900 -1.09941200 - 0.64413400