molecules

MDPI

Supplementary Materials

IR and NMR Spectral Changes Induced by Halogen, Chalcogen, Pnicogen, and Tetrel Bonds in a Model Protein Environment

Mariusz Michalczyk [1], Wiktor Zierkiewicz [1,*], Rafał Wysokiński [1] and Steve Scheiner [2,*]

[1] Faculty of Chemistry, Wrocław University of Science and Technology, Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland
[2] Department of Chemistry and Biochemistry, Utah State University, Logan, UT 84322-0300, USA
* Correspondence: wiktor.zierkiewicz@pwr.edu.pl (W.Z.); steve.scheiner@usu.edu (S.S.)

Table S1. NMR chemical shielding (ppm) of isolated monomers at the MP2/aug-cc-pVDZ level.

Monomer	Atoms	
HB	X	H
HF	428.0	29.6
HCl	995.0	30.9
HBr	2729.0	31.3
HI	460.4	31.7
XB	X	F
ClF	-430.6	635.7
BrF	-568.7	766.1
IF	311.73	928.7
YB	Y	F
SHF	-90.2	654.3
SeHF	317.4	695.2
TeHF	330.0	752.9
ZB	Z	F
PH_2F	328.2	526.9
AsH_2F	1409.5	535.6
SbH_2F	348.4	539.0
TB	T	F
SiH_3F	463.5	442.3
GeH_3F	1683.0	471.7
SnH_3F	307.2	487.9

Table S2. NMR chemical shielding (ppm) of the isolated NMA molecule at the MP2/aug-cc-pVDZ level.

	O	C	N
NMA	-2.1	43.3	176.5

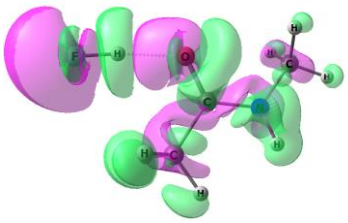
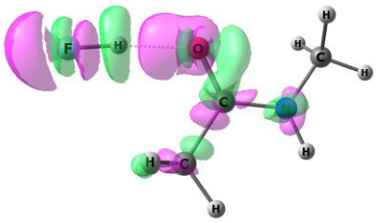
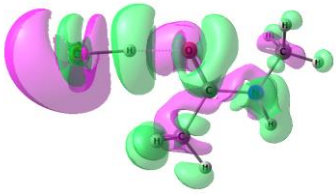
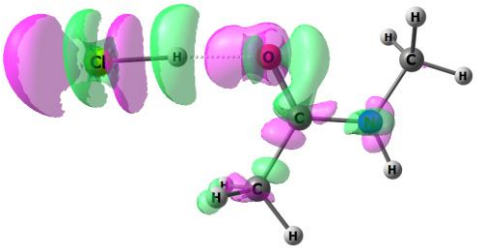
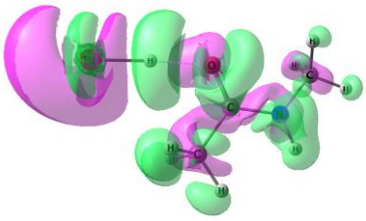
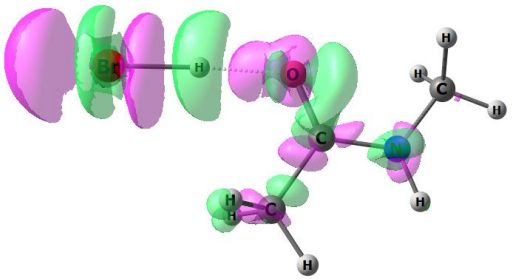
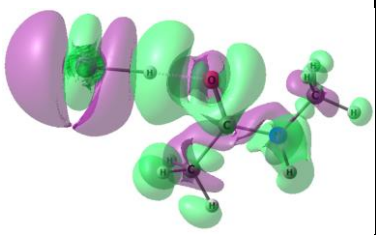
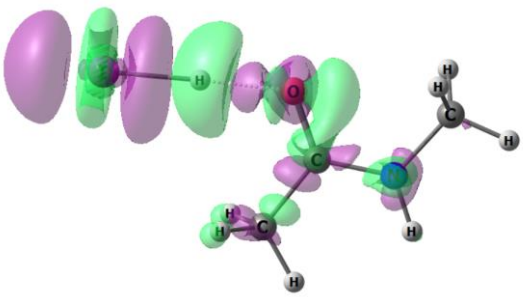
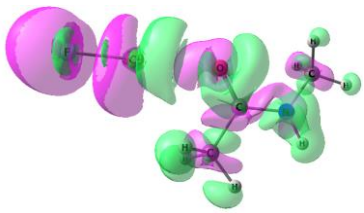
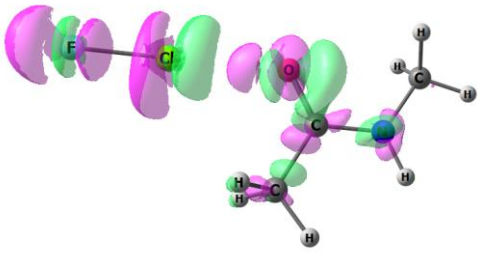
Table S3. NMR chemical shielding (ppm) for complexes at the MP2/aug-cc-pVDZ level.

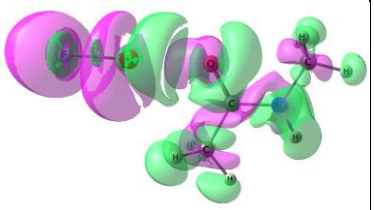
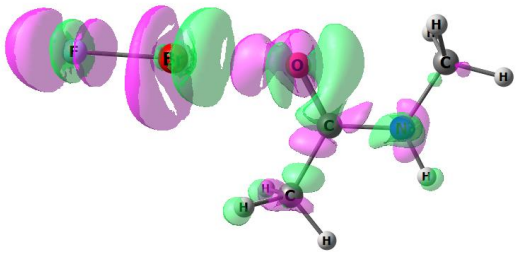
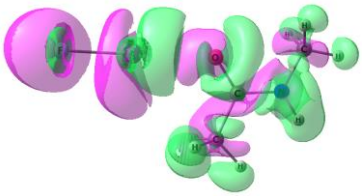
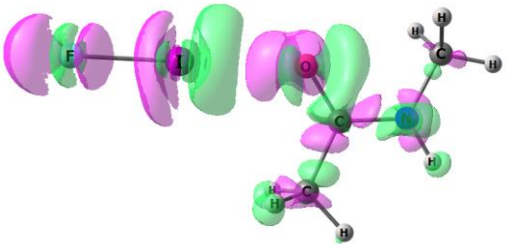
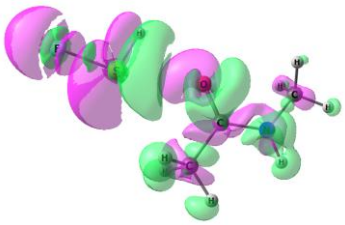
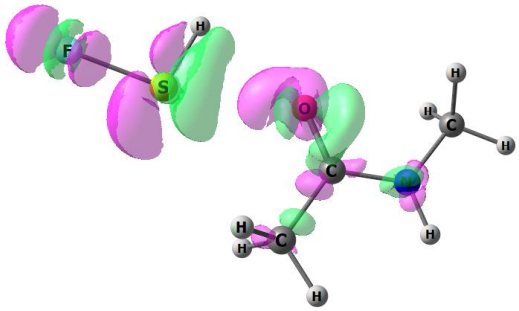
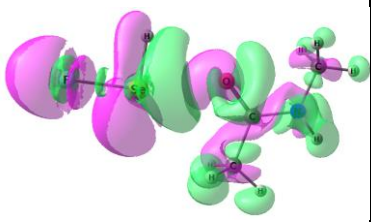
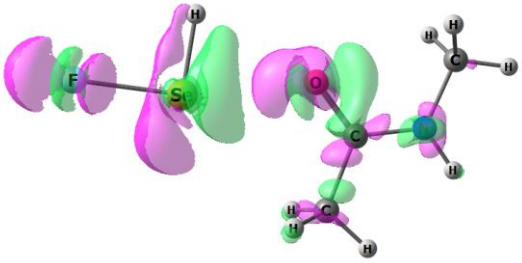
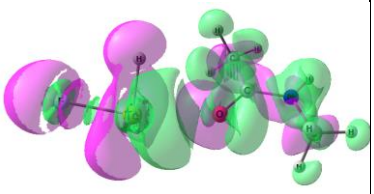
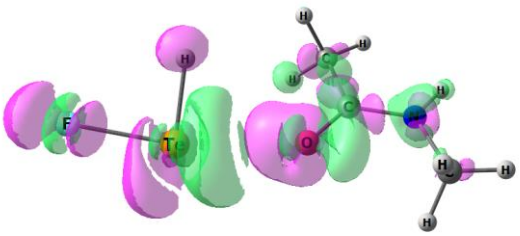
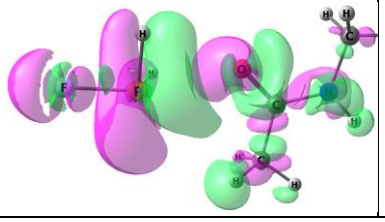
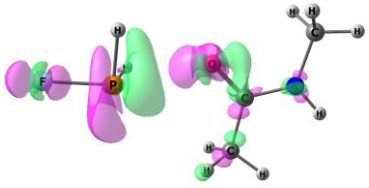
System	Atoms				
HB	H	X	O	C	N
FH···NMA	22.7	408.5	32.3	37.0	171.4
ClH···NMA	21.4	994.0	17.9	37.3	171.1
BrH···NMA	20.7	2764.8	13.3	37.1	170.9
IH···NMA	20.4	466.4	5.0	37.2	170.9
XB	X	F			
FCl···NMA	-191.3	496.5	26.3	37.9	171.1
FBr···NMA	360.5	557.3	44.4	36.2	168.8
FI···NMA	358.7	646.4	63.2	35.5	166.6
YB	Y	F			
HFS···NMA	51.0	542.3	26.0	39.3	171.9
HFSe···NMA	838.6	543.3	36.7	38.4	170.0
HFTe···NMA	355.9	564.2	50.4	35.6	168.0
ZB	Z	F			
H_2FP···NMA	368.2	464.7	19.9	39.3	172.2
H_2FAs···NMA	1517.1	464.5	25.4	38.8	171.0
H_2FSb···NMA	351.4	461.2	35.2	36.9	169.2
TB	T	F			
H_3FSi···NMA	480.8	399.8	14.9	39.3	172.0
H_3FGe···NMA	1725.5	424.4	17.7	39.0	171.3
H_3FSn···NMA	306.5	434.9	26.3	37.5	169.0

[a] MP2/aug-cc-pVDZ level.

Table S4. AIM descriptors of complexes studied. Bond critical point (BCP) properties: electron density ρ, Laplacian of the electron density $\nabla^2\rho$, ellipticity ε, and total electron energy H, were obtained at the MP2/aug-cc-pVDZ level. Data are given in atomic units.

	Interaction	ρ	$\nabla^2\rho$	ε	H
HB					
FH···NMA	H···O	0.052	0.173	0.010	-0.005
ClH···NMA	H···O	0.054	0.143	0.013	-0.006
BrH···NMA	H···O	0.057	0.142	0.014	-0.007
IH···NMA	H···O	0.058	0.136	0.014	-0.008
XB					
FCl···NMA	Cl···O	0.043	0.146	0.019	-0.001
FBr···NMA	Br···O	0.049	0.144	0.018	-0.004
FI···NMA	I···O	0.046	0.132	0.015	-0.006
YB					
HFS···NMA	S···O	0.032	0.099	0.180	-0.001
HFSe···NMA	Se···O	0.039	0.108	0.260	-0.004
HFTe···NMA	Te···O	0.039	0.111	0.234	-0.004
ZB					
H_2FP···NMA	P···O	0.025	0.064	0.019	-0.002
H_2FAs···NMA	As···O	0.029	0.077	0.035	-0.003
H_2FSb···NMA	Sb···O	0.030	0.090	0.058	-0.002
TB					
H_3FSi···NMA	Si···O	0.022	0.052	0.417	-0.003
H_3FGe···NMA	Ge···O	0.025	0.081	0.018	-0.002
H_3FSn···NMA	Sn···O	0.032	0.106	0.009	-0.002

	0.0005	0.0015
HB		
FH···NMA		
ClH···NMA		
BrH···NMA		
IH···NMA		
XB		
FCl···NMA		

FBr···NMA		
FI···NMA		
YB		
HFS···NMA		
HFSe···NMA		
HFTe···NMA		
ZB		
H_2FP···NMA		

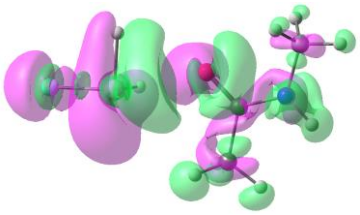
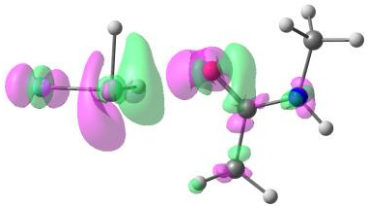
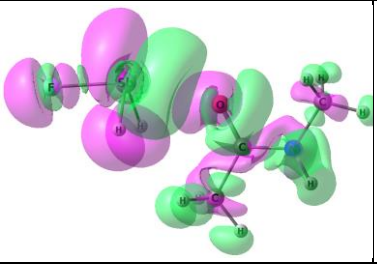
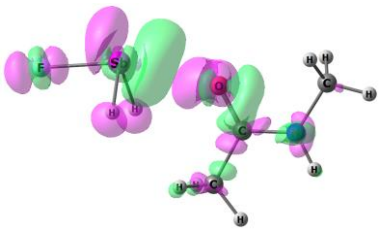
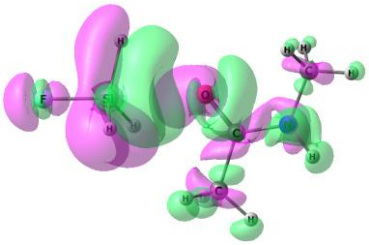
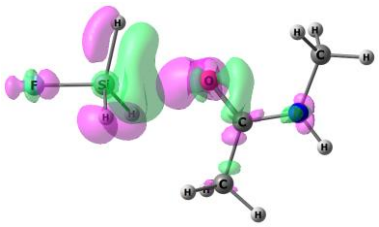
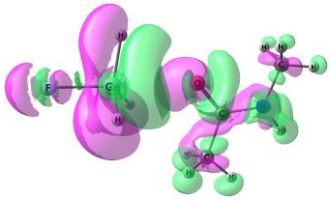
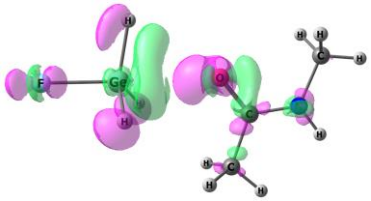
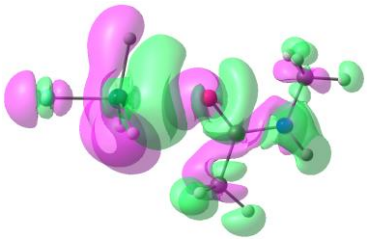
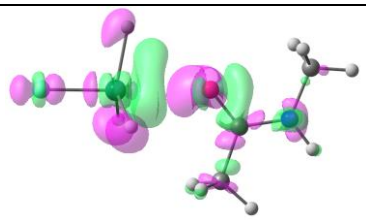
$H_2FAs\cdots NMA$		
$H_2FSb\cdots NMA$		
TB		
$H_3FSi\cdots NMA$		
$H_3FGe\cdots NMA$		
$H_3FSn\cdots NMA$		

Figure S1. Electron density shifts calculated at the MP2/aug-cc-pVDZ level. Purple indicates gain and loss is shown in green. Contours of $\Delta\rho = \pm 0.0005$ au on left and ± 0.0015 au. on right.

Table S5. Coordinates of complexes optimized at the MP2/aug-cc-pVDZ level.

System	Coordinates
HB	
FH···NMA	C -1.52710000 1.23369400 0.00493700 C -0.77809500 -0.08012800 -0.01091300 H -1.05591600 -0.65589100 0.88361600 H -1.10035600 -0.65985200 -0.88780300 H 0.31236200 0.05618900 -0.03857600 H 0.21740300 2.30287700 -0.04095800 C -1.43734700 3.68125600 -0.00259900 H -2.04848500 3.79576600 0.90417600

	H	-0.65899500	4.45440600	-0.02376800
	H	-2.09316600	3.79196400	-0.87808900
	N	-0.79094800	2.37168500	-0.01602600
	O	-2.77526200	1.29509400	0.03606900
	H	-3.51846700	-0.13316800	0.05785100
	F	-3.86570500	-1.02530600	0.06854300
ClH···NMA	C	-1.51083800	1.25814100	0.00508000
	C	-0.77120800	-0.06133900	-0.00876800
	H	-1.05430300	-0.63715600	0.88419000
	H	-1.09150900	-0.63930900	-0.88768500
	H	0.32015700	0.06912200	-0.03191200
	H	0.24348500	2.31128700	-0.03709400
	C	-1.39862400	3.70508000	-0.00349300
	H	-2.01100300	3.82550800	0.90165900
	H	-0.61269800	4.47054100	-0.02287700
	H	-2.05091000	3.82135200	-0.88088700
	N	-0.76448300	2.38930800	-0.01461400
	O	-2.75932400	1.33161500	0.03323900
	H	-3.54617200	-0.10138400	0.05277400
	Cl	-4.11264800	-1.31417800	0.06684700
BrH···NMA	C	-1.51111900	1.26612200	0.00551500
	C	-0.78315600	-0.05960900	-0.00864900
	H	-1.07072700	-0.63385200	0.88388000
	H	-1.10836500	-0.63553800	-0.88708900
	H	0.30909900	0.06313600	-0.03200800
	H	0.25169800	2.30301300	-0.03789300
	C	-1.37783200	3.71190900	-0.00340400
	H	-1.98790800	3.83876200	0.90240700
	H	-0.58500900	4.47014300	-0.02451100
	H	-2.02999500	3.83295400	-0.88022400
	N	-0.75558000	2.39038300	-0.01381500
	O	-2.75981200	1.35282100	0.03394100
	H	-3.53917300	-0.06671100	0.05198700
	Br	-4.17219900	-1.40494600	0.06632400
IH···NMA	C	-1.50115800	1.27814300	0.00449400
	C	-0.76443800	-0.04269300	-0.01127700
	H	-1.04364100	-0.61823400	0.88313800
	H	-1.08804700	-0.62193300	-0.88817500
	H	0.32680300	0.08822900	-0.03891900
	H	0.25543200	2.32526800	-0.04206800
	C	-1.38239500	3.72469200	-0.00405700
	H	-1.99174100	3.84688600	0.90290800
	H	-0.59408200	4.48760800	-0.02572200

	H -2.03672100 3.84274800 -0.87969100
	N -0.75240800 2.40679600 -0.01688600
	O -2.75061300 1.35800800 0.03540600
	H -3.52323700 -0.07253600 0.05763300
	I -4.27383000 -1.57439500 0.07967700
XB	
FCl···NMA	C -1.42373200 1.34473500 0.00272600
	C -0.72565900 0.00373800 -0.00910600
	H -1.02669300 -0.56102900 0.88476600
	H -1.06166800 -0.56359200 -0.88878400
	H 0.36909800 0.10245100 -0.03083500
	H 0.36501600 2.34059600 -0.03469700
	C -1.23063800 3.78738200 -0.00513900
	H -1.84086100 3.92840700 0.89860100
	H -0.42012900 4.52683100 -0.02289500
	H -1.87685300 3.92500300 -0.88404400
	N -0.63986100 2.45181500 -0.01453100
	O -2.66865700 1.46495400 0.02732500
	Cl -3.97735600 -0.45673500 0.05585500
	F -4.96208500 -1.86597100 0.07721900
FBr···NMA	C -1.39669700 1.34409400 0.00204000
	C -0.66974000 0.02148300 -0.01047100
	H -0.95899400 -0.55133800 0.88223900
	H -0.99350500 -0.55355700 -0.88980000
	H 0.42191200 0.14847000 -0.03188400
	H 0.35958200 2.38694700 -0.03333300
	C -1.27629700 3.79013100 -0.00324300
	H -1.89042000 3.91154000 0.90048700
	H -0.48624200 4.55114700 -0.01950700
	H -1.92505900 3.90938800 -0.88273100
	N -0.64818800 2.47080300 -0.01385400
	O -2.64794400 1.44036800 0.02622900
	Br -3.97000300 -0.47099700 0.05397400
	F -5.03848100 -1.96989300 0.07631400
FI···NMA	C -1.96787200 0.46003500 0.00011700
	C -1.55283800 1.90949000 -0.00000200
	H -0.92895600 2.09937900 0.88528000
	H -0.92883900 2.09921700 -0.88523500
	H -2.41669200 2.58919600 -0.00010900
	H -3.94872500 0.94911200 -0.00068200
	C -3.76732900 -1.19943200 -0.00025400
	H -3.40153400 -1.72731300 0.89192200
	H -4.86426900 -1.18717000 -0.00078500

	H -3.40062900 -1.72738400 -0.89201800 N -3.28947300 0.18196600 -0.00006200 O -1.14507800 -0.48988900 0.00045800 I 1.25731800 -0.15603600 0.00005000 F 3.24077500 0.08884900 -0.00038100
YB	
HFS···NMA	C -1.25643500 1.26896400 0.05047900 C -0.43313000 0.00401800 0.14894400 H -0.69258800 -0.51235000 1.08479800 H -0.70524900 -0.65839200 -0.68589100 H 0.64863800 0.19882600 0.12514800 H 0.43162500 2.42739700 -0.05769300 C -1.29426900 3.71118700 -0.15119600 H -1.92645200 3.86481600 0.73543900 H -0.55831900 4.52194500 -0.22370000 H -1.93961400 3.71784800 -1.04162400 N -0.57927900 2.44252000 -0.05157700 O -2.50372500 1.25952100 0.06047300 F -4.82341600 -2.14491100 0.35841900 H -4.60032100 0.08621400 0.17255100 S -3.67388900 -0.88725600 0.24623500
HFSe···NMA	C -1.22975800 1.26691600 0.07539300 C -0.38315700 0.02963300 0.26023700 H -0.68914400 -0.46991500 1.19156100 H -0.58289700 -0.66076400 -0.57283500 H 0.69196400 0.25466000 0.30062600 H 0.42126900 2.47541500 0.04461000 C -1.33593800 3.69899000 -0.19378700 H -2.02861500 3.85126200 0.64646500 H -0.62287700 4.53157700 -0.24020900 H -1.92138600 3.66080800 -1.12373300 N -0.58805000 2.45736500 -0.01489600 O -2.47763000 1.22294500 0.00497000 F -4.85425300 -2.24738600 0.23678000 H -4.67510000 0.11885700 -0.00831900 Se -3.63085000 -0.89001800 0.16394200
HFTe···NMA	C -2.01848800 0.47549200 -0.01127900 C -1.64278700 1.93598100 0.04604000 H -0.87475900 2.07298700 0.82078900 H -1.19513900 2.22607600 -0.91654600 H -2.50790800 2.58198500 0.25282300 H -4.01105000 0.91514500 0.08928300 C -3.78155600 -1.22353400 -0.04772300

	H -3.37560000 -1.79703500 0.79777700
	H -4.87797500 -1.23822100 -0.01263500
	H -3.43304400 -1.68764900 -0.98137700
	N -3.33471600 0.16600400 0.02309800
	O -1.17158000 -0.44547500 -0.10031200
	F 3.23157700 0.22357800 -0.14923700
	H 0.95614600 0.71686400 -1.26573700
	Te 1.30014900 -0.20246600 0.06302600
ZB	
$H_2FP\cdots NMA$	C -1.30590400 1.35954100 0.00819500
	C -0.58705000 0.02792300 -0.03268700
	H -0.90259400 -0.56858200 0.83505900
	H -0.89791700 -0.51341600 -0.93853500
	H 0.50728800 0.13560300 -0.03252900
	H 0.47389200 2.37936200 -0.05826000
	C -1.13758800 3.80479000 0.01495200
	H -1.71344400 3.94083800 0.94207500
	H -0.33845700 4.55527600 -0.03548100
	H -1.82025200 3.93465500 -0.83728500
	N -0.53157200 2.47747500 -0.01928000
	O -2.54750600 1.45171500 0.05887100
	H -4.23411300 -0.32172100 -0.81846400
	H -4.76267700 0.61150300 0.96113900
	P -4.06016800 -0.56440200 0.57513800
	F -5.38130600 -1.61789200 0.73258700
$H_2FAs\cdots NMA$	C -1.31024800 1.37273600 0.04297800
	C -0.61578600 0.03205600 -0.05422400
	H -0.83713500 -0.54525100 0.85551400
	H -1.03055600 -0.52024700 -0.91045100
	H 0.47294300 0.12512100 -0.17541200
	H 0.46829700 2.37273800 -0.15267200
	C -1.11834800 3.81480100 0.05088600
	H -1.61539600 3.95165600 1.02230100
	H -0.31818300 4.55714500 -0.06188200
	H -1.86635400 3.95350900 -0.74290100
	N -0.53036200 2.48121300 -0.03735700
	O -2.54498200 1.48050000 0.18827900
	H -3.98429000 -0.50298900 -0.83550000
	H -4.94870300 0.71077200 0.73564900
	As -4.04155300 -0.50241000 0.68404700
	F -5.41871100 -1.68868200 0.74623900
$H_2FSb\cdots NMA$	C -2.08759400 0.48724500 0.00009800
	C -1.74004700 1.95747600 -0.00013000

	H -1.12394900 2.17602100 0.88419400 H -1.13055000 2.17728800 -0.88874900 H -2.63143100 2.60078700 0.00351600 H -4.09168500 0.90062000 0.00075300 C -3.82729900 -1.23715200 0.00003900 H -3.44317200 -1.75253200 0.89207300 H -4.92406300 -1.26795100 -0.00110100 H -3.44130300 -1.75260200 -0.89113200 N -3.40267100 0.16039500 0.00028000 O -1.22155800 -0.41570000 -0.00017200 H 0.93060200 0.84169700 1.22889500 H 0.93068200 0.84345000 -1.22755000 Sb 1.35921000 -0.26316400 -0.00010900 F 3.23621600 0.40133400 0.00044500
TB	
$H_3FSi\cdots NMA$	C -1.41766800 1.27934800 0.00365900 C -0.65563700 -0.02854900 0.00182200 H -0.93930100 -0.60450700 0.89468100 H -0.95405100 -0.61060000 -0.88228200 H 0.43428000 0.11481300 -0.00783900 H 0.32793300 2.35662400 -0.02623900 C -1.33201200 3.72801800 -0.01400000 H -1.95585500 3.84488100 0.88399800 H -0.55665200 4.50444100 -0.02797000 H -1.97689300 3.83380700 -0.89842500 N -0.68093800 2.42137200 -0.01340400 O -2.66292800 1.33231100 0.01965300 H -3.48371700 -0.83506000 1.27997600 H -3.49951500 -0.84905700 -1.20566100 H -5.11672500 0.59023000 0.03904700 F -5.36978400 -1.89060600 0.05491200 Si -4.26874200 -0.61920500 0.04086300
$H_3FGe\cdots NMA$	C -1.40959300 1.28969400 0.00406100 C -0.65628800 -0.02294300 0.00280300 H -0.94422200 -0.59688700 0.89570100 H -0.95834100 -0.60326900 -0.88131000 H 0.43451500 0.11282400 -0.00648000 H 0.34004200 2.35773000 -0.02602800 C -1.31391500 3.73710300 -0.01447600 H -1.93685800 3.85670600 0.88370700 H -0.53507900 4.50991500 -0.02902000 H -1.95832100 3.84476800 -0.89893700 N -0.66858600 2.42729900 -0.01335100

	O	-2.65540700	1.34894300	0.01999000
	H	-3.48004800	-0.86037700	1.32682200
	H	-3.49468200	-0.87449600	-1.25277600
	H	-5.17774200	0.61252500	0.03813800
	F	-5.43239400	-1.96938200	0.05393800
	Ge	-4.26128900	-0.60189300	0.04000500
$H_3FSn\cdots NMA$	C	-2.06187600	0.46094400	0.00154700
	C	-1.73388800	1.93616600	0.00009000
	H	-1.12730500	2.16431100	0.88891800
	H	-1.12700200	2.16253000	-0.88900600
	H	-2.63227400	2.56933000	-0.00075800
	H	-4.07074000	0.84320300	-0.00689400
	C	-3.77342600	-1.29074600	-0.00238400
	H	-3.38315000	-1.79850100	0.89119800
	H	-4.86947000	-1.33800800	-0.00557100
	H	-3.37784800	-1.80081400	-0.89232400
	N	-3.37029200	0.11364300	-0.00289000
	O	-1.17983100	-0.42648600	0.00670100
	H	0.98640700	0.69153200	1.44521400
	H	0.97837200	0.69704900	-1.43920800
	H	1.19987500	-1.82380000	-0.00322900
	F	3.29921400	0.05325400	-0.00482100
	Sn	1.32352100	-0.13735800	0.00052300