SUPPORTING INFORMATION

Wolfium Bonds in Homodimers of MX_4Y

(M= Mo, W; X= F, Cl, Br; Y= O, S, Se)

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

[1] Faculty of Chemistry, Wrocław University of Science and Technology, Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland, email: mariusz.michalczyk@pwr.edu.pl
[2] Department of Chemistry and Biochemistry, Utah State University Logan, Utah 84322-0300, United States

Figure S1. QTAIM molecular diagrams for homodimers. Bond critical point positions represented by small green balls, with density listed in au of electron density.

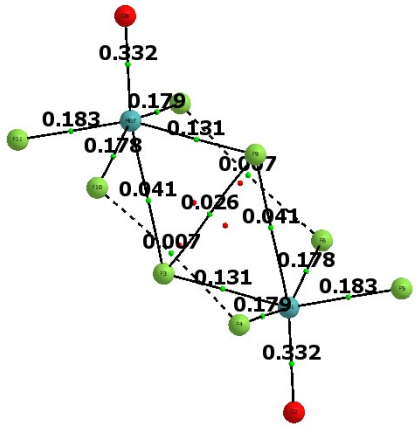
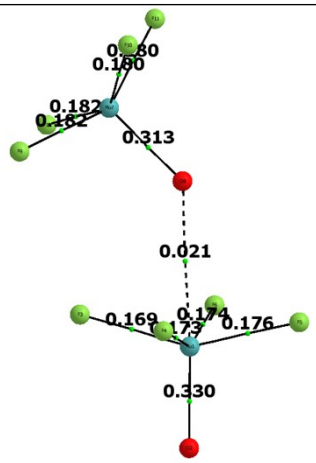
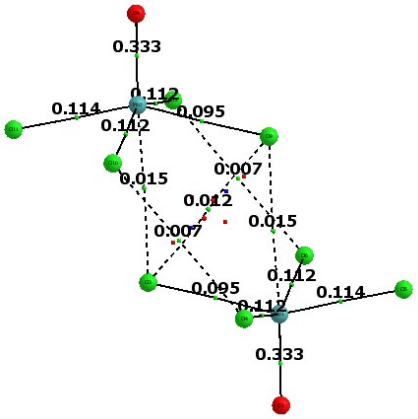
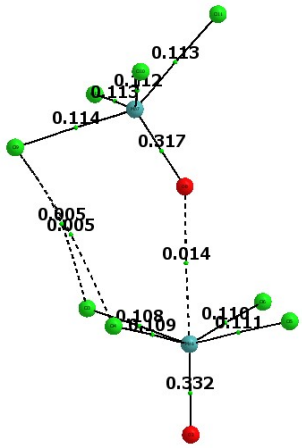
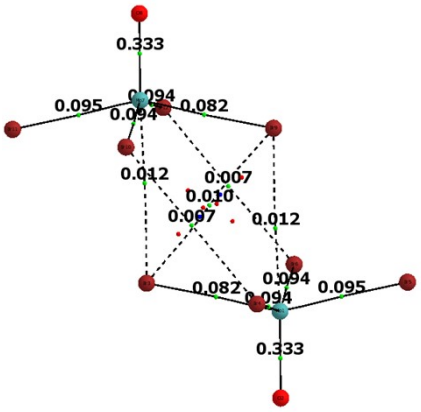
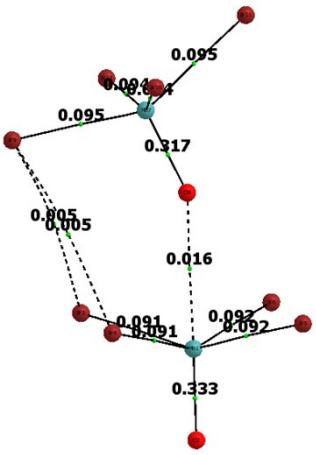
homodimer	Dual-X	Mono-Y
MoF_4O		
$MoCl_4O$		
$MoBr_4O$		

Figure S1. (continued)

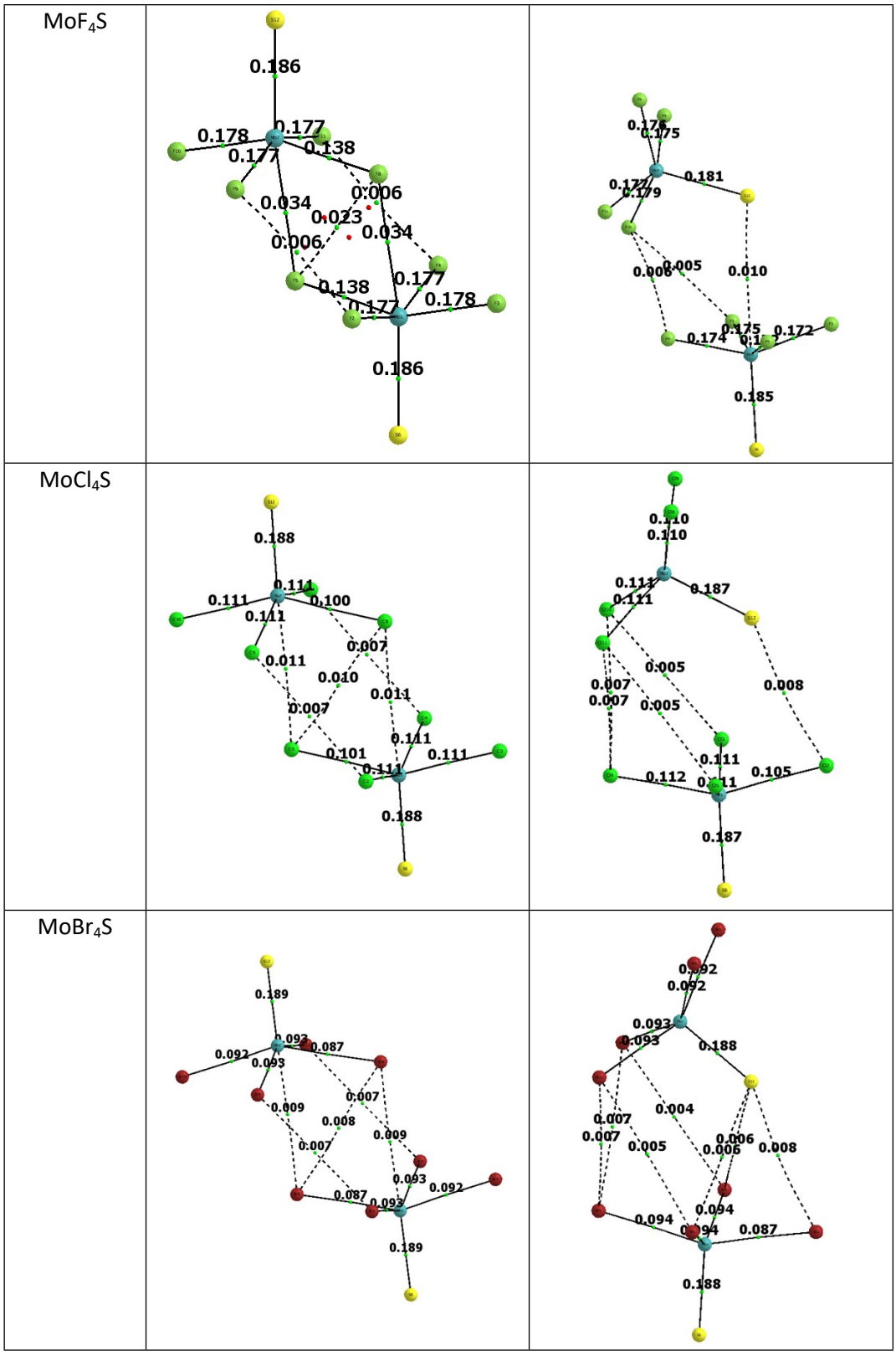


Figure S1. (continued)

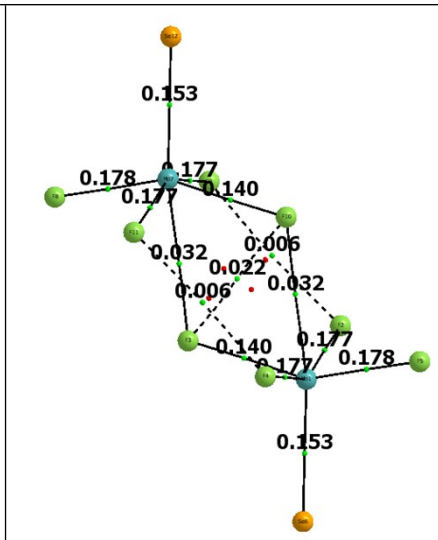
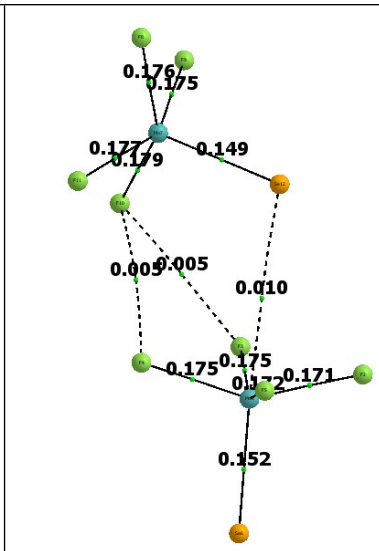
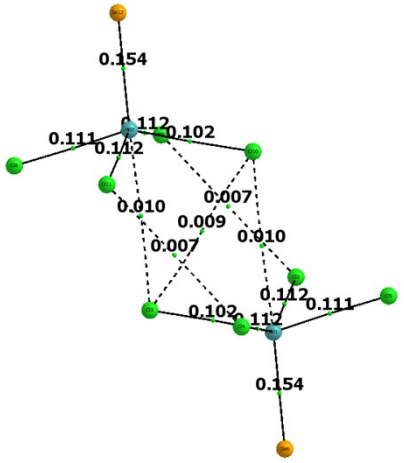
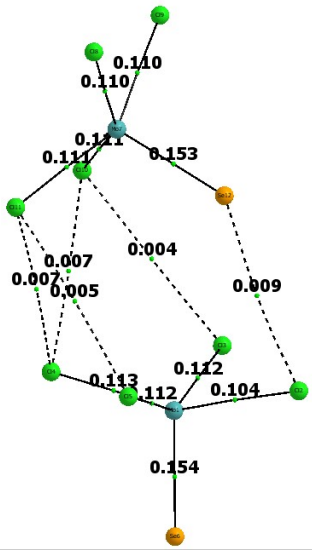
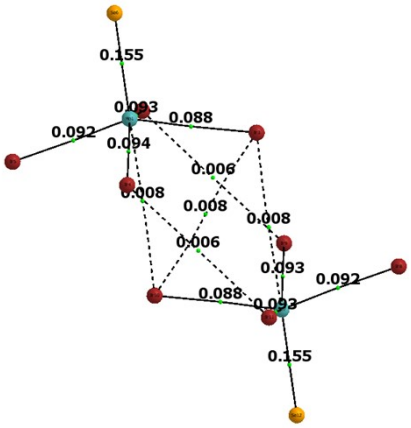
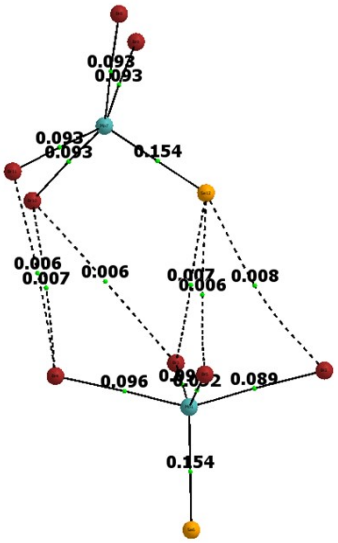
MoF_4Se		
$MoCl_4Se$		
$MoBr_4Se$		

Figure S1. (continued)

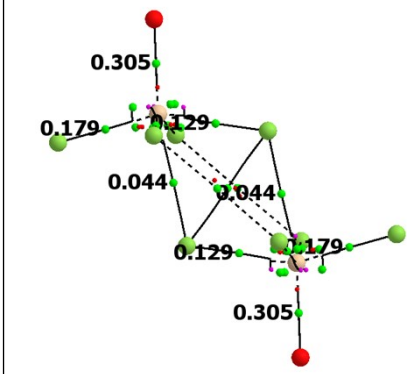
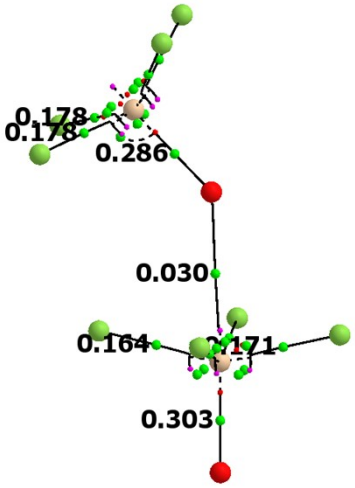
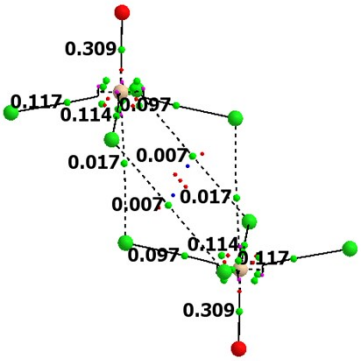
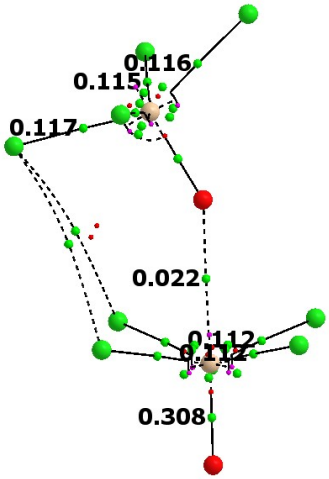
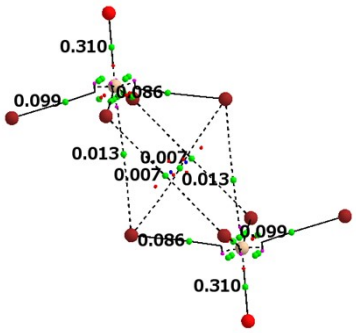
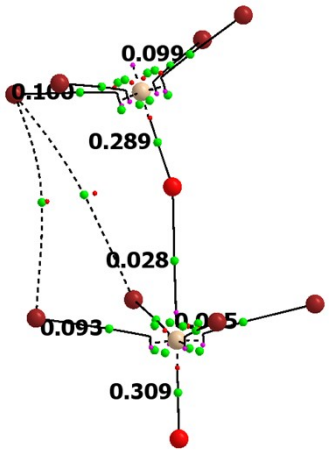
WF_4O		
WCl_4O		
WBr_4O		

Figure S1. (continued)

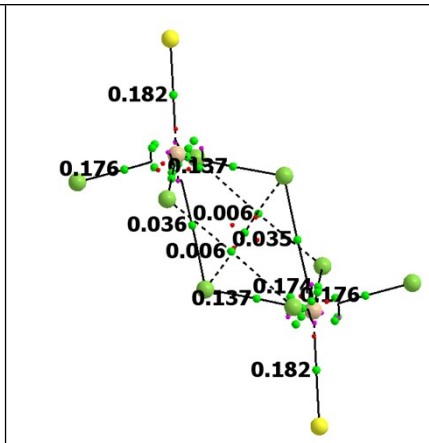
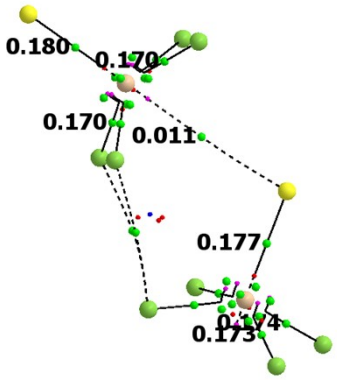
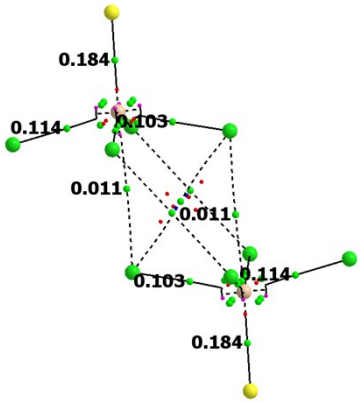
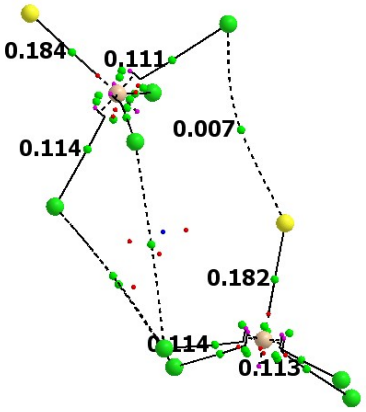
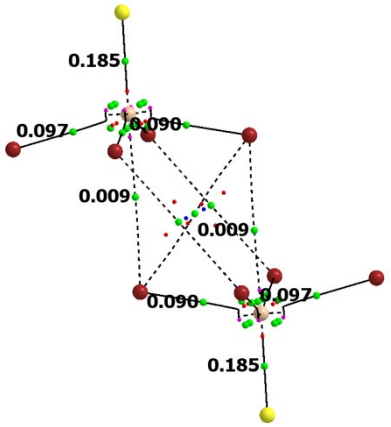
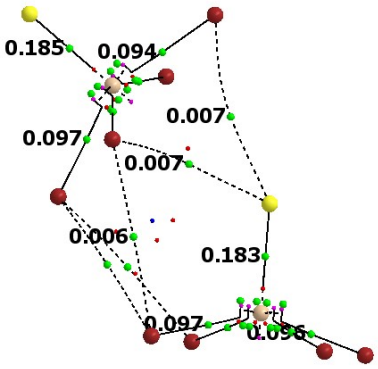
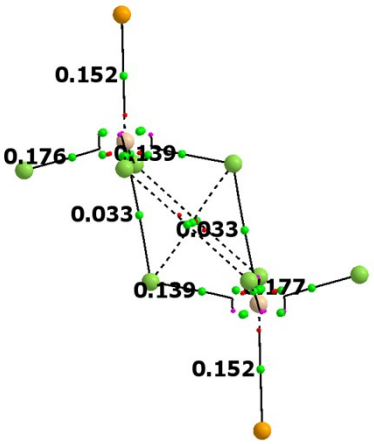
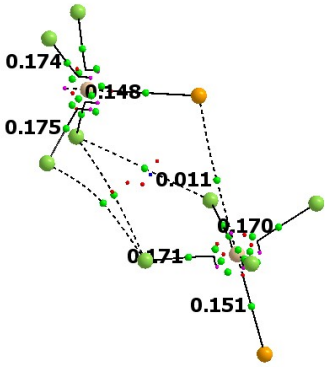
WF_4S		
WCl_4S		
WBr_4S		
WF_4Se		

Figure S1. (continued)

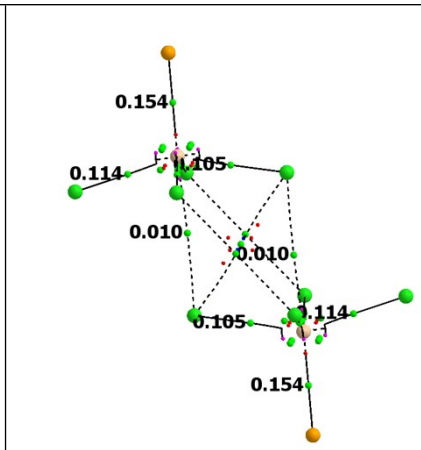
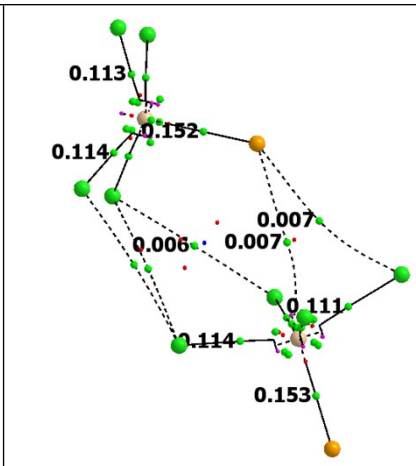
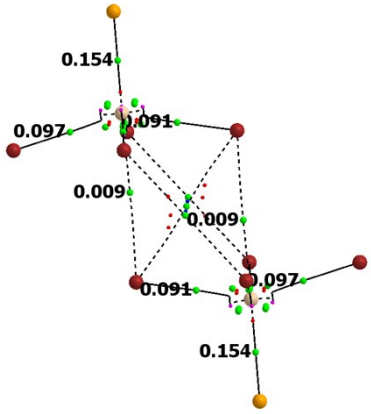
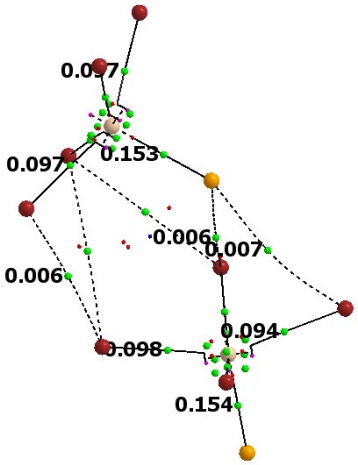
WCl_4Se		
WBr_4Se		

Figure S2. NCI molecular diagrams of four Mono-Y dimers. Blue isosurfaces represent areas of strong noncovalent contacts, while green and red correspond to weaker contacts and repulsions, respectively. RDG surface shown is 0.05 au of electron density and blue and red colors refer specifically to -0.03 and +0.03 au of electron density for $\rho * \text{sign}(\lambda_2)$.

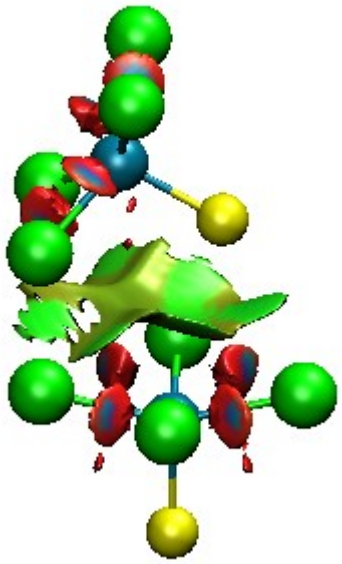
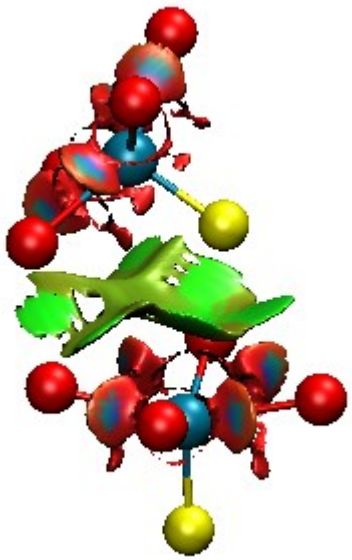
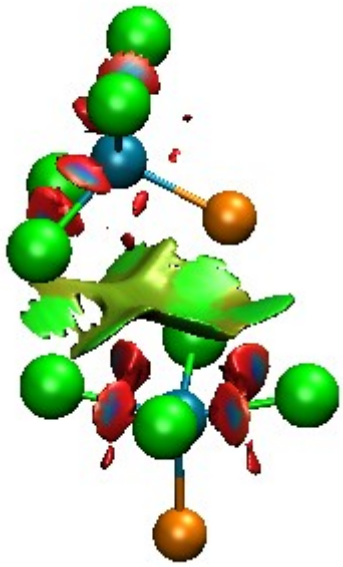
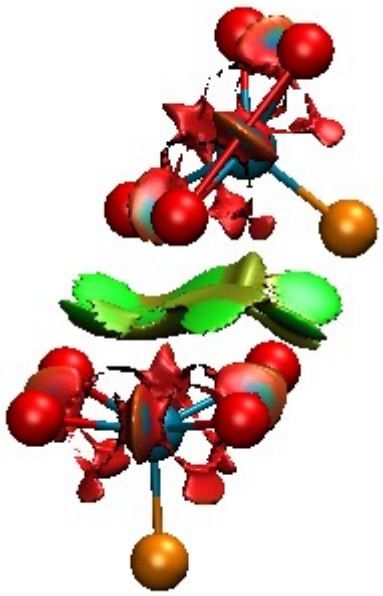
$MoCl_4S$	$MoBr_4S$
	
$MoCl_4Se$	$MoBr_4Se$
	

Figure S3. Geometry of Lin-Y and Mono-X conformers

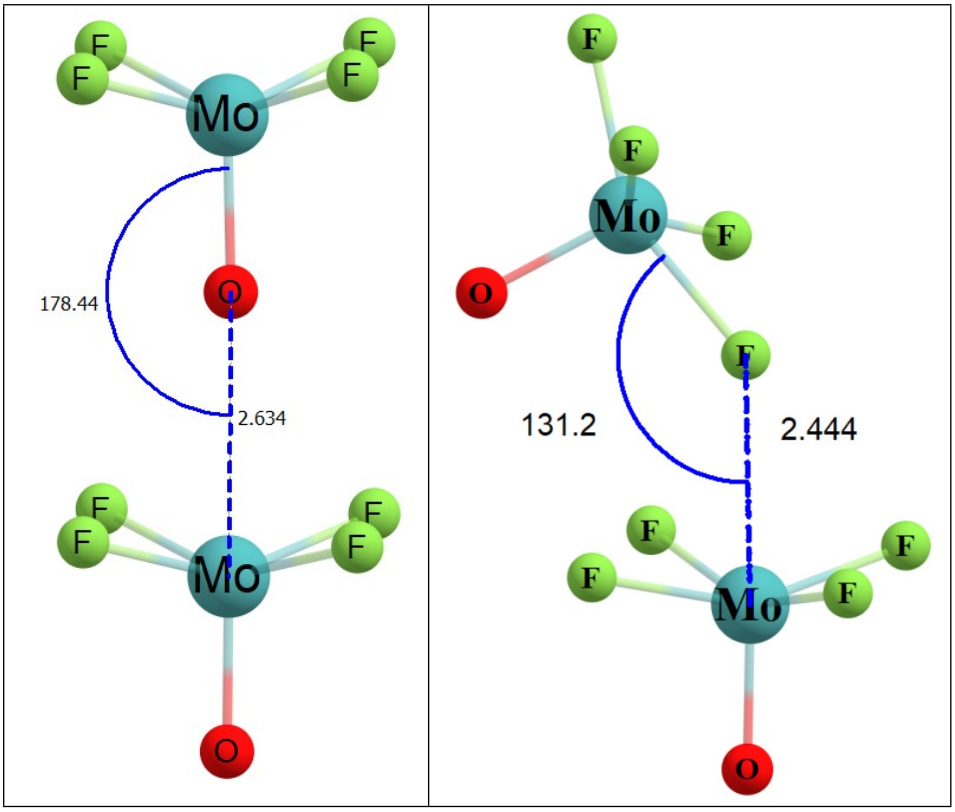


Table S1. Intermolecular distances (Å) and interaction energies (kcal/mol) for alternate homodimers.

	Lin-Y		Mono-X	
homodimer	R(M···Y)	E_{int}	R(M···X)	E_{int}
$(MoF_4O)_2$	2.634	-5.26	2.444	-11.86
$(MoCl_4O)_2$	2.775	-5.09	3.324	-6.38
$(MoBr_4O)_2$	2.664	-6.00	3.548	-6.70
$(MoF_4S)_2$	3.517	-0.46	2.484	-11.68
$(MoCl_4S)_2$	-	-	3.369	-7.75
$(MoBr_4S)_2$	-	-	3.595	-8.38
$(MoF_4Se)_2$	3.624	-0.61	2.496	-11.31
$(MoCl_4Se)_2$	-	-	3.379	-7.86
$(MoBr_4Se)_2$	-	-	3.616	-8.60
$(WF_4O)_2$	2.530	-9.30	2.450	-11.94
$(WCl_4O)_2$	2.623	-7.87	3.345	-6.34
$(WBr_4O)_2$	2.550	-8.77	3.559	-6.67
$(WF_4S)_2$	-	-	2.509	-10.67
$(WCl_4S)_2$	-	-	3.418	-6.94
$(WBr_4S)_2$	-	-	3.647	-7.54
$(WF_4Se)_2$	-	-	2.529	-10.07
$(WCl_4Se)_2$	-	-	3.440	-6.92
$(WBr_4Se)_2$	-	-	3.669	-7.65

Table S2. Relative total electron energy of four types of homodimers obtained within this study calculated at M062X/def2TZVPP level of theory. In each case the most stable is the bridged complex so the values of other conformers are referred to the most stable one. Data are given in kcal/mol.

homodimer	Dual-X	Mono-Y	Lin-Y	Mono-X
$(MoF_4O)_2$	0.00	12.10	12.37	7.71
$(MoCl_4O)_2$	0.00	4.78	5.33	5.18
$(MoBr_4O)_2$	0.00	4.05	4.56	4.03
$(MoF_4S)_2$	0.00	11.68	13.50	4.13
$(MoCl_4S)_2$	0.00	3.98	Mono-Y	1.33
$(MoBr_4S)_2$	0.00	3.32	Mono-Y	1.10
$(MoF_4Se)_2$	0.00	10.28	12.22	3.43
$(MoCl_4Se)_2$	0.00	3.13	Mono-Y	0.79
$(MoBr_4Se)_2$	0.00	2.58	Mono-Y	0.49
$(WF_4O)_2$	0.00	9.88	10.09	8.67
$(WCl_4O)_2$	0.00	3.49	3.95	4.88
$(WBr_4O)_2$	0.00	2.85	3.20	4.58
$(WF_4S)_2$	0.00	11.11	Mono-Y	5.10
$(WCl_4S)_2$	0.00	4.36	Mono-Y	2.04
$(WBr_4S)_2$	0.00	4.07	Mono-Y	1.95
$(WF_4Se)_2$	0.00	9.63	Mono-Y	5.07
$(WCl_4Se)_2$	0.00	3.58	Mono-Y	1.61
$(WBr_4Se)_2$	0.00	3.28	Mono-Y	1.45

Figure S4. Examples of neutral MX_4Y complexes drawn from the CSD database.

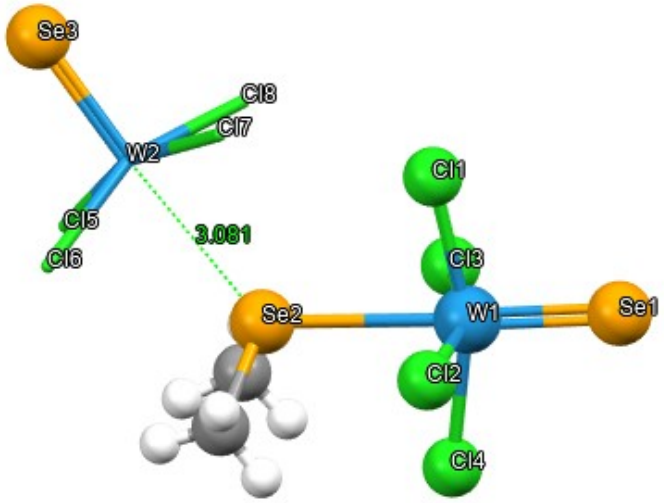
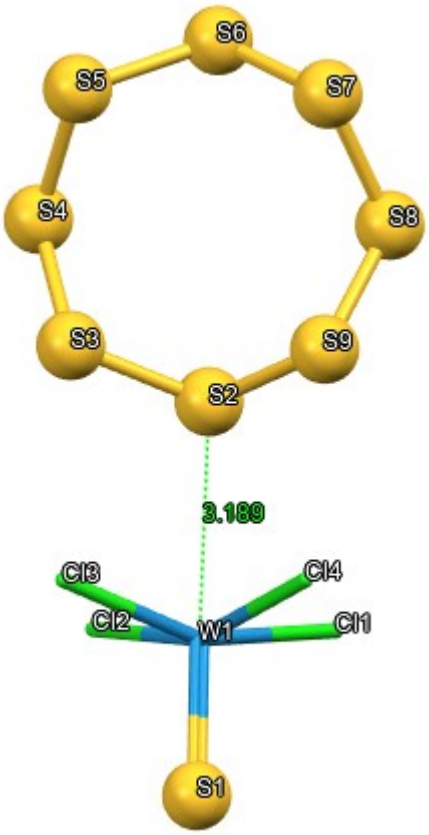
Refcode	Structure
MATCOD	
JITRUZ	

Figure S4. (continued)

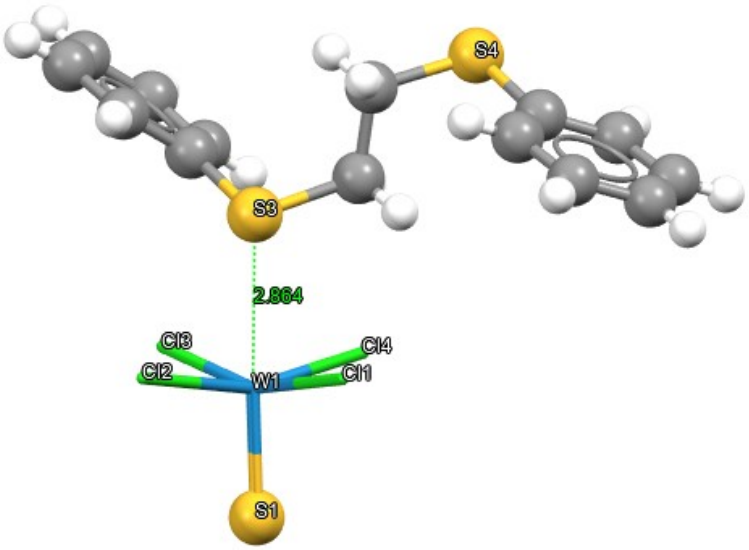
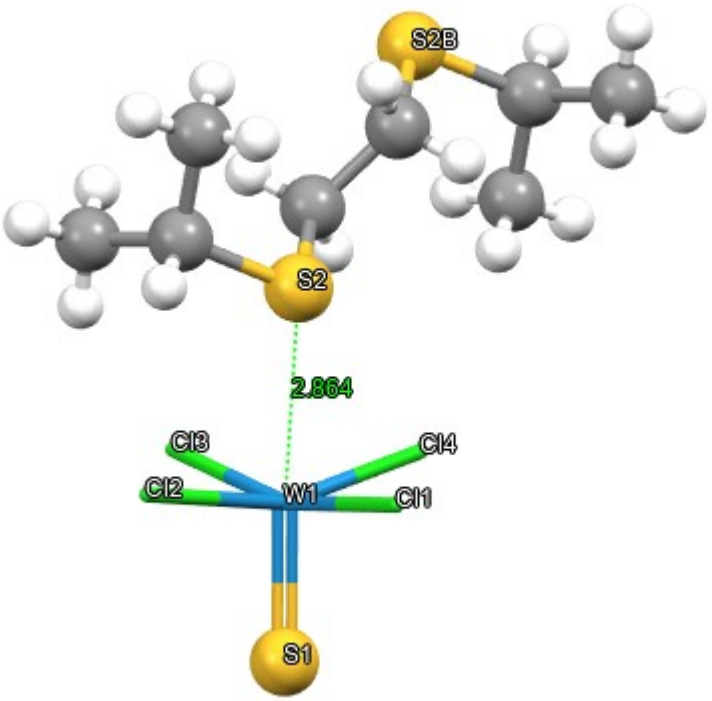
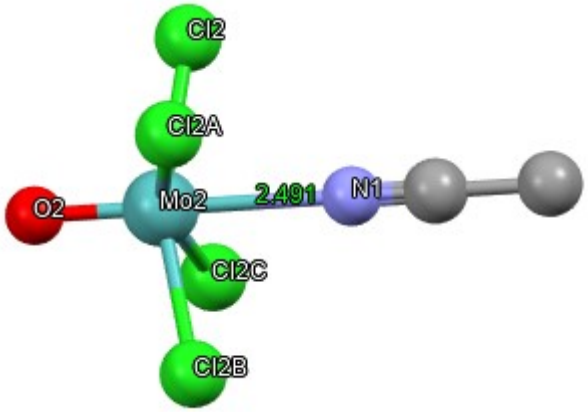
KUDFOH	
KUDGEY	
PHASOM	

Figure S5. Examples of anionic homodimers of $[MoCl_4O]^-$ drawn from the CSD database.

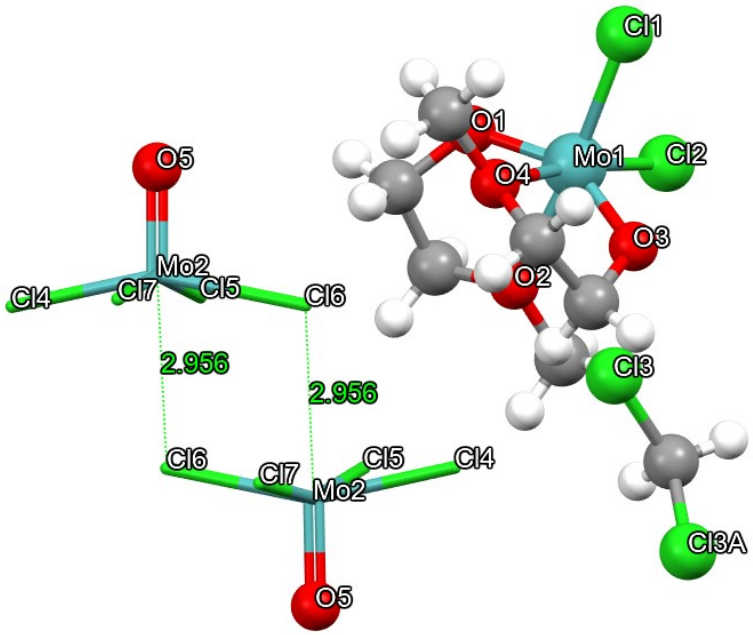
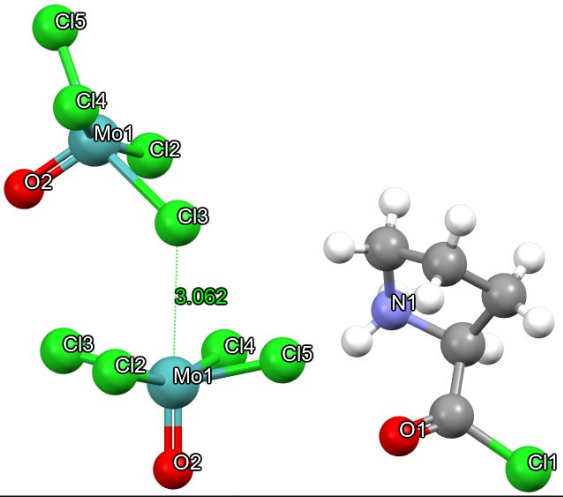
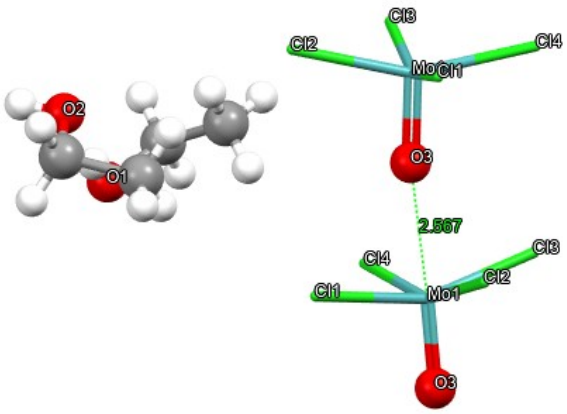
Refcode	Structure
POSWIF	
IHODAM	
NABQIQ	

Table S3. Cartesian coordinates of monomers and dimers.

monomer	coordinates			
MoF_4O	Mo	-0.39067200	1.02683800	0.38228700
	O	-0.39086200	1.02699500	2.00688600
	F	-2.15291000	1.02677700	-0.11027000
	F	-0.39057800	2.78900900	-0.11052400
	F	1.37186400	1.02676300	-0.10915600
	F	-0.39059300	-0.73566800	-0.10922200
$MoCl_4O$	Mo	-0.39077100	1.02697100	0.44108900
	O	-0.39096600	1.02723200	2.06258900
	Cl	-2.60047800	1.02661200	-0.13882300
	Cl	-0.39047300	3.23645800	-0.13964800
	Cl	1.81941000	1.02659800	-0.13752400
	Cl	-0.39047200	-1.18315600	-0.13768300
$MoBr_4O$	Mo	-0.39075500	1.02695200	0.46262200
	O	-0.39113500	1.02753200	2.08310600
	Br	-2.76744000	1.02649300	-0.14957000
	Br	-0.39040500	3.40353300	-0.14990600
	Br	1.98639700	1.02649000	-0.14829100
	Br	-0.39041100	-1.35028600	-0.14796000
MoF_4S	Mo	-0.39077300	1.02693400	0.32796500
	F	-2.15523300	1.02588500	-0.17004700
	F	-0.38972400	2.79139300	-0.17004700
	F	1.37440300	1.02583700	-0.16782300
	F	-0.38967600	-0.73824200	-0.16782300
	S	-0.39274700	1.02890800	2.37177400
$MoCl_4S$	Mo	-0.39074300	1.02693900	0.39350800
	S	-0.39250000	1.02894000	2.42740100
	Cl	-2.59931000	1.02621700	-0.20110000
	Cl	-0.39017100	3.23505300	-0.20240500
	Cl	1.81909800	1.02625300	-0.19651200
	Cl	-0.39012500	-1.18268700	-0.19689100
$MoBr_4S$	Mo	-0.39095300	1.02711300	0.41788200
	Br	-2.76460000	1.02646900	-0.21274900
	Br	-0.39030900	3.40076000	-0.21274900
	Br	1.98415200	1.02642600	-0.20860300
	Br	-0.39026600	-1.34799100	-0.20860300
	S	-0.39177500	1.02793600	2.44882100
MoF_4Se	Mo	-0.39064300	1.02680700	0.32758200
	Se	-0.39263500	1.02898600	2.51461700
	F	-2.15456700	1.02625600	-0.17081100
	F	-0.39016700	2.79026500	-0.17206800
	F	1.37438700	1.02629200	-0.16687100
	F	-0.39012500	-0.73789200	-0.16764900
$MoCl_4Se$	Mo	-0.39050700	1.02662400	0.39474600
	Se	-0.38874200	1.02459100	2.57193100
	Cl	1.81628000	1.02734500	-0.20223200
	Cl	-0.39107000	-1.17947400	-0.20402900
	Cl	-2.59860800	1.02730100	-0.19747600
	Cl	-0.39110500	3.23432800	-0.19814000
$MoBr_4Se$	Mo	-0.39093400	1.02709400	0.42051900

Table S3. (continued)

	Br	-2.76182900	1.02649300	-0.21469400
	Br	-0.39033200	3.39799000	-0.21469400
	Br	1.98141700	1.02645500	-0.21050800
	Br	-0.39029400	-1.34525600	-0.21050800
	Se	-0.39177800	1.02793900	2.59468400
WF_4O	W	-0.39066500	1.02682900	0.37908000
	O	-0.39093100	1.02712800	2.03728300
	F	-2.16840500	1.02678700	-0.11669000
	F	-0.39058700	2.80412500	-0.11820800
	F	1.38743900	1.02677300	-0.11520900
	F	-0.39060300	-0.75092800	-0.11625600
WCl_4O	W	-0.39087000	1.02697600	0.43144800
	O	-0.39118600	1.02675400	2.08427200
	Cl	-2.61266100	1.02686400	-0.14219300
	Cl	-0.39050100	3.24884200	-0.14229700
	Cl	1.83183700	1.02661500	-0.13995900
	Cl	-0.39037000	-1.19533700	-0.14127100
WBr_4O	W	-0.39084200	1.02694900	0.45074800
	O	-0.39146000	1.02708400	2.10206000
	Br	-2.77861700	1.02662100	-0.15200700
	Br	-0.39024000	3.41503800	-0.15112300
	Br	1.99779700	1.02664900	-0.14960000
	Br	-0.39038800	-1.36162600	-0.15007800
WF_4S	W	-0.39057100	1.02673100	0.33134700
	F	-2.16401100	1.02626900	-0.18044300
	F	-0.39010800	2.80017200	-0.18044300
	F	1.38364800	1.02614700	-0.17774000
	F	-0.38998600	-0.74748800	-0.17774000
	S	-0.39272300	1.02888300	2.40901800
WCl_4S	W	-0.39071200	1.02689700	0.39124500
	S	-0.39271700	1.02924800	2.45777300
	Cl	-2.60696800	1.02615400	-0.20849100
	Cl	-0.39013500	3.24282200	-0.20935900
	Cl	1.82683900	1.02616700	-0.20367200
	Cl	-0.39005600	-1.19057400	-0.20349500
WBr_4S	W	-0.39144400	1.02760400	0.41334500
	Br	-2.77217100	1.02565900	-0.21802600
	Br	-0.38949900	3.40833200	-0.21802600
	Br	1.99168800	1.02607500	-0.21489600
	Br	-0.38991500	-1.35552700	-0.21489600
	S	-0.39241000	1.02857100	2.47649800
WF_4Se	W	-0.39061100	1.02676500	0.33190800
	Se	-0.39309200	1.02967000	2.55223600
	F	-2.16223700	1.02607200	-0.18176600
	F	-0.39005400	2.79811700	-0.18255400
	F	1.38225200	1.02611600	-0.17746900
	F	-0.39000900	-0.74602700	-0.17755600
WCl_4Se	W	-0.39055500	1.02669600	0.39334900
	Se	-0.38837800	1.02412100	2.60199100
	Cl	1.82323000	1.02746000	-0.20996500
	Cl	-0.39114800	-1.18678400	-0.21076400
	Cl	-2.60566800	1.02744200	-0.20505700
	Cl	-0.39123100	3.24178000	-0.20475500

Table S3. (continued)

	W	-0.39139300	1.02755300	0.41642500
	Br	-2.76912200	1.02586600	-0.21994600
	Br	-0.38970600	3.40528300	-0.21994600
	Br	1.98866400	1.02610900	-0.21656400
	Br	-0.38994900	-1.35250300	-0.21656400
	Se	-0.39224400	1.02840500	2.62139600

Table S3. (continued)

homodimer	Lin-Y				Dual-X				Mono-Y			
MoF_4O	Mo	-0.38701600	1.02937800	0.46849300	Mo	-0.30861200	1.05659600	0.19268000	Mo	-0.34678600	1.02317800	0.52575000
	O	-0.41808700	1.01041300	2.09175300	O	-0.55357200	1.01144900	1.79377400	O	-0.16319100	0.99616000	2.13833500
	F	-2.15716700	1.03453400	-0.01437800	F	-2.12993100	1.14559800	-0.45929600	F	-2.17380400	1.06365600	0.28127000
	F	-0.37907300	2.81346600	0.04119100	F	-0.28848300	2.84993800	-0.13305500	F	-0.38206900	2.80828300	0.10476900
	F	1.40019400	1.03413900	0.05473800	F	1.49655200	0.99519800	0.03124600	F	1.36425900	1.00259100	-0.12116200
	F	-0.37873800	-0.74427700	-0.00107600	F	-0.41818400	-0.70828200	-0.25110900	F	-0.44760700	-0.74534300	0.05349900
	Mo	-0.35171400	1.05011300	-3.80340800	Mo	-2.16051300	1.22667900	-2.82288300	Mo	-2.06866600	1.25306500	-3.08467800
	O	-0.34183700	1.05664600	-2.16531600	O	-1.91656700	1.27106800	-4.42425000	O	-0.77997800	1.08728700	-2.08227500
	F	-2.10524200	1.04834100	-4.29309500	F	-0.33920400	1.13780400	-2.17062000	F	-3.12190900	2.54033800	-2.35092300
	F	-0.35442800	2.79899800	-4.30991000	F	-2.04976200	2.99160900	-2.37953100	F	-1.59007400	2.52915000	-4.29501300
	F	1.39618800	1.04832500	-4.31339000	F	-3.96549200	1.28909900	-2.66000500	F	-1.78341200	0.07288400	-4.44387900
	F	-0.35437500	-0.70250300	-4.29646900	F	-2.18021100	-0.56651500	-2.49633900	F	-3.32074000	0.06899100	-2.50508000
$MoCl_4O$	Mo	-0.40553100	1.01189500	0.55258400	Mo	-0.18560700	1.04052300	0.58961000	Mo	-0.27065000	1.01852400	0.70356200
	O	-0.60711800	0.81617600	2.14761600	O	-0.33814700	0.99444300	2.19994800	O	0.13275200	1.09915400	2.27011100
	Cl	-2.55653600	1.06696900	-0.24362700	Cl	-2.44752100	1.14697900	-0.08157200	Cl	-2.56430300	0.92403900	0.76290900
	Cl	-0.38267400	3.28611000	0.29914700	Cl	-0.14263600	3.28091400	0.18322100	Cl	-0.51589700	3.21756200	0.10096300
	Cl	1.86955000	1.06929600	0.31446000	Cl	2.05978500	0.96863000	0.26576200	Cl	1.75106400	1.07285700	-0.36112200
	Cl	-0.31263800	-1.14080600	-0.23421200	Cl	-0.30683600	-1.16656700	0.04177300	Cl	-0.31943500	-1.22749100	0.27344500
	Mo	-0.32335800	1.07794500	-3.78668500	Mo	-2.28324900	1.24285900	-3.21911900	Mo	-2.09508600	1.24267400	-3.17553300
	O	-0.08939500	1.31768400	-2.18690900	O	-2.13108600	1.28856900	-4.82952100	O	-0.99873100	0.90794400	-2.01067600
	Cl	-2.58369500	1.00628200	-4.03068900	Cl	-0.02198200	1.13512800	-2.54842700	Cl	-3.37348900	2.91530400	-2.31836800
	Cl	-0.43993000	3.17201000	-4.67646800	Cl	-2.16070800	3.45003500	-2.67286300	Cl	-1.09649200	2.85440100	-4.44061500
	Cl	1.77240000	0.97827700	-4.67470400	Cl	-4.52827000	1.31654500	-2.89470000	Cl	-1.62157000	-0.18695800	-4.88495100
	Cl	-0.37237100	-1.18426600	-4.02138000	Cl	-2.32772100	-0.99781600	-2.81350000	Cl	-3.84214200	-0.13777100	-2.69911100
$MoBr_4O$	Mo	-0.38951800	1.02750000	0.54208700	Mo	-0.12469000	1.03543500	0.73010600	Mo	-0.24643500	1.03537500	0.71717500
	O	-0.43971200	0.98110300	2.15889900	O	-0.26300300	0.99049700	2.34090200	O	0.25575600	1.12710600	2.25283700
	Br	-2.77875200	1.03725300	-0.06899700	Br	-2.54599700	1.14935000	0.03672800	Br	-2.70133000	1.00721200	0.95873300
	Br	-0.37961900	3.44512100	0.07320300	Br	-0.06700300	3.44361700	0.29966800	Br	-0.47212400	3.40462800	0.07458800
	Br	2.02922100	1.03779300	0.07842600	Br	2.28963800	0.95478500	0.36108300	Br	1.86194500	1.01753000	-0.54608500
	Br	-0.37524100	-1.36405300	-0.06245900	Br	-0.24934400	-1.33864200	0.15092400	Br	-0.38437100	-1.38791000	0.31935900
	Mo	-0.34742800	1.05457400	-3.75394300	Mo	-2.34404700	1.24779500	-3.35964600	Mo	-2.10778500	1.21954100	-3.16513100
	O	-0.31419700	1.09653100	-2.12033300	O	-2.20630300	1.29275300	-4.97048300	O	-1.12380000	0.89114800	-1.90321700
	Br	-2.73043600	1.03967400	-4.29316900	Br	0.07737900	1.13393500	-2.66790500	Br	-3.58042900	2.99528300	-2.36312100
	Br	-0.36132300	3.41040500	-4.41285300	Br	-2.21903500	3.62222600	-2.78102900	Br	-0.89791600	2.97650600	-4.36576400
	Br	2.01209500	1.04194700	-4.39823200	Br	-4.75855800	1.32896100	-2.99017300	Br	-1.42455200	-0.28957000	-4.96299400
	Br	-0.35638600	-1.33027400	-4.28349700	Br	-2.40301400	-1.16047300	-2.92956300	Br	-3.99293500	-0.29660700	-2.79576700
MoF_4S	Mo	-0.42677700	1.27182500	2.37432000	Mo	-0.43835600	1.39065600	0.31599600	Mo	-0.32810300	1.31771100	1.18427400
	F	-2.19505600	1.27808400	1.88385200	F	-2.21960000	1.37634900	-0.09222500	F	-1.92280800	0.67497700	0.53156400

Table S3. (continued)

	F	-0.43050500	3.04351800	1.89753100	F	-0.44154200	3.20417200	0.11801800	F	-1.03263100	2.98350700	0.88661300
	F	1.33413700	1.27854800	1.85849300	F	1.33632300	1.37959800	-0.12011500	F	1.30908500	2.07521000	0.85523400
	F	-0.43035000	-0.48551200	1.84516300	F	-0.44175300	-0.41762400	-0.32940200	F	0.40086000	-0.22957600	0.51136100
	S	-0.41190400	1.24114500	4.41613400	S	-0.42233100	1.11759800	2.33798800	S	-0.41082500	1.04475100	3.20674400
	Mo	-0.45478400	1.43021200	-3.18276000	Mo	-0.46092900	-0.46917400	-2.77434700	Mo	0.97637400	3.25672700	-2.52253900
	F	-2.21577900	1.46002700	-3.68467300	F	-0.45755900	1.33924200	-2.12883000	F	1.70852400	3.00190600	-4.18042400
	F	-0.45512300	3.22058300	-3.56731600	F	-2.23557600	-0.45784100	-2.33826300	F	-0.08090800	4.50397200	-3.35019700
	F	1.30755100	1.46169500	-3.67972600	F	-0.45765600	-2.28260000	-2.57592900	F	0.83629800	4.31647100	-1.04386600
	F	-0.45317800	-0.29740500	-3.79158700	F	1.32029200	-0.45444400	-2.36617300	F	2.62013300	2.78408700	-1.87640600
	S	-0.45787100	1.29743700	-1.14220200	S	-0.47697600	-0.19644300	-4.79634400	S	-0.24441600	1.63506600	-2.20524500
$MoCl_4S$					Mo	-0.43526900	1.49891100	0.76069300	Mo	-0.30917200	1.22993900	1.46209100
					Cl	-2.65572200	1.49470500	0.23525900	Cl	-2.12114200	0.29726500	0.37088000
					Cl	-0.44067400	3.74618600	0.35835700	Cl	-1.46261200	3.19517000	1.32720000
					Cl	1.77646900	1.49904100	0.19941500	Cl	1.58054900	2.49409000	1.58892500
					Cl	-0.43827000	-0.73486600	0.09438300	Cl	0.94345200	-0.29803700	0.31872900
					S	-0.41886400	1.36075600	2.78752300	S	-0.52674700	0.53339500	3.35984900
		-			Mo	-0.46391500	-0.57774400	-3.21969700	Mo	0.91524300	3.28826300	-2.72521000
					Cl	-0.46151200	1.65750100	-2.55342800	Cl	1.71821000	2.47053500	-4.70621900
					Cl	-2.67494900	-0.57772500	-2.65627900	Cl	-0.00201200	4.97153600	-3.97528800
					Cl	-0.45858700	-2.82557400	-2.81857700	Cl	1.00890700	4.80855300	-1.02213900
					Cl	1.75536600	-0.57254600	-2.69079900	Cl	2.73356800	2.30113300	-1.75589800
					S	-0.47973500	-0.43915900	-5.24647800	S	-0.64666000	2.07296600	-2.24580900
$MoBr_4S$					Mo	-0.43429900	1.55544800	0.90888400	Mo	-0.35662900	1.17734000	1.55126400
					Br	-2.81921600	1.56204300	0.34312600	Br	-2.31907000	0.20781200	0.37504400
					Br	-0.44010000	3.97118000	0.45567700	Br	-1.57689600	3.29914100	1.44786900
					Br	1.94180100	1.56734200	0.30593100	Br	1.68220300	2.50842300	1.76190400
					Br	-0.43636400	-0.83551800	0.21664100	Br	0.97565200	-0.41989300	0.25513700
					S	-0.41838400	1.43533200	2.93385400	S	-0.58291800	0.42238300	3.42269500
		-			Mo	-0.46506900	-0.63389000	-3.36652900	Mo	0.94750800	3.31919000	-2.77999400
					Br	-0.46307100	1.75644800	-2.67510400	Br	1.68551200	2.35282800	-4.91584000
					Br	-2.84113000	-0.64606300	-2.76472800	Br	-0.15323100	5.05057600	-4.13504200
					Br	-0.45886400	-3.04974300	-2.91337400	Br	1.13345500	5.02759000	-1.03005500
					Br	1.92000100	-0.64020600	-2.80253900	Br	2.95860900	2.30497600	-1.80665400
					S	-0.48096700	-0.51288500	-5.39146500	S	-0.56261200	2.11444100	-2.14921600
MoF_4Se	Mo	-0.41738900	1.03864500	1.13187500	Mo	-0.37681100	1.18364700	0.74010100	Mo	-0.33191800	1.30823900	1.20248100
	F	-2.15994000	1.02217200	0.55838000	F	-2.11625100	1.25899800	0.18648200	F	-1.92956800	0.65996600	0.55891700
	F	-0.40365000	2.79272000	0.59331700	F	-0.33921700	3.05835600	0.35542400	F	-1.03296800	2.97102000	0.88457600
	F	1.36619500	1.03756600	0.70037100	F	1.42609700	1.24561600	0.45119400	F	1.30852300	2.05406600	0.86982400
	F	-0.39039300	-0.73509100	0.66353600	F	-0.35033000	-0.58184200	0.28030600	F	0.39049200	-0.25213400	0.55210800
	Se	-0.50636700	1.08201100	3.31460600	Se	-0.53956500	1.16132000	2.91721100	Se	-0.42516200	1.04521900	3.37038100
	Mo	-0.19187000	0.88645400	-4.67015800	Mo	-0.15647000	3.45913200	-2.07864500	Mo	0.99740300	3.28932900	-2.56903100

Table S3. (continued)

	F	-1.94789700	0.86421200	-5.19221900	F	-0.18518700	5.22299400	-1.61248900	F	1.75215800	3.08666000	-4.22386200
	F	-0.18657700	2.62709900	-5.24109200	F	-1.96013800	3.39475000	-1.79210400	F	-0.04123300	4.57013500	-3.36855600
	F	1.57674700	0.86827600	-5.14518300	F	-0.19273900	1.58375900	-1.69694100	F	0.83586500	4.29504400	-1.05513800
	F	-0.18414100	-0.89610000	-5.09189200	F	1.58336900	3.38433400	-1.52649800	F	2.62882100	2.78677000	-1.91365700
	Se	-0.22010500	0.98123500	-2.48624800	Se	0.00674400	3.48788400	-4.25577300	Se	-0.32083000	1.55049300	-2.31093200
$MoCl_4Se$			-		Mo	-0.40799100	1.02740600	1.17623600	Mo	-0.30992400	1.22719900	1.47405100
					Cl	-2.57102800	1.10446100	0.45753300	Cl	-2.13567500	0.26239000	0.42689500
					Cl	-0.37564700	3.32419600	0.82295400	Cl	-1.48171800	3.17879100	1.32531500
					Cl	1.83780200	1.09386000	0.78708700	Cl	1.56853000	2.50649100	1.55945200
					Cl	-0.36046200	-1.14230300	0.46281800	Cl	0.93318400	-0.30059300	0.32413200
					Se	-0.56958100	0.87147700	3.33998100	Se	-0.50576500	0.50346700	3.51724100
					Mo	-0.12519900	3.61576500	-2.51495200	Mo	0.93882900	3.31485500	-2.76543100
					Cl	-0.17286300	5.78500700	-1.80024600	Cl	1.78268400	2.51796900	-4.73746000
					Cl	-2.37177900	3.55044300	-2.12791500	Cl	0.06871200	5.02320600	-4.01442100
					Cl	-0.15938300	1.31922100	-2.16054200	Cl	1.00310500	4.81087500	-1.04048600
					Cl	2.03770400	3.53747500	-1.79609300	Cl	2.72351300	2.29749900	-1.76679600
					Se	0.03792600	3.77193900	-4.67859300	Se	-0.75389200	2.02266000	-2.30538000
$MoBr_4Se$			-		Mo	-0.41796400	0.96069000	1.32314600	Mo	-0.43268900	1.11646200	1.57912400
					Br	-2.74419900	1.03582200	0.55819700	Br	-2.47221100	0.21350500	0.50048700
					Br	-0.37693700	3.41255400	0.94797900	Br	-1.47029000	3.31637900	1.28374100
					Br	1.99404600	1.00991100	0.89914800	Br	1.72138000	2.25529200	1.49469400
					Br	-0.37480700	-1.37037400	0.54152100	Br	0.71110800	-0.80792100	0.55663800
					Se	-0.57444500	0.79433300	3.48338200	Se	-0.69071800	0.61382200	3.67738200
					Mo	-0.11534500	3.68267400	-2.66155600	Mo	1.04343400	3.40513200	-2.83721200
					Br	-0.15912200	6.01305000	-1.87875300	Br	1.78708600	2.61631800	-5.03989200
					Br	-2.52784000	3.63279500	-2.23912100	Br	-0.34763700	5.01769700	-4.05679900
					Br	-0.15645700	1.23069400	-2.28638200	Br	1.07470700	5.05064000	-1.01715500
					Br	2.21122300	3.60733400	-1.89755100	Br	3.24172800	2.69124900	-2.01352000
					Se	0.04134900	3.84946200	-4.82174000	Se	-0.33431500	1.87623200	-2.13037600
WF_4O	Mo	-0.24643500	1.03537500	0.71717500	W	-0.29677600	1.05596800	0.19704400	W	-0.34660400	1.02575000	0.48991900
	O	0.25575600	1.12710600	2.25283700	O	-0.55449200	1.01058100	1.83019500	O	-0.13694300	0.99009000	2.13343300
	Br	-2.70133000	1.00721200	0.95873300	F	-2.12979600	1.14552600	-0.46971100	F	-2.19892700	1.08545600	0.29560700
	Br	-0.47212400	3.40462800	0.07458800	F	-0.27299600	2.86578900	-0.13247700	F	-0.37069100	2.83636900	0.10120700
	Br	1.86194500	1.01753000	-0.54608500	F	1.52421800	0.99363800	0.04864900	F	1.37950800	0.99002500	-0.16272300
	Br	-0.38437100	-1.38791000	0.31935900	F	-0.40352400	-0.72527800	-0.25164800	F	-0.47376100	-0.76433700	0.03636200
	Mo	-2.10778500	1.21954100	-3.16513100	W	-2.17236000	1.22734900	-2.82731000	W	-2.07308400	1.25133300	-3.06966400
	O	-1.12380000	0.89114800	-1.90321700	O	-1.91582300	1.27225200	-4.46070500	O	-0.78505200	1.09614200	-2.00581400
	Br	-3.58042900	2.99528300	-2.36312100	F	-0.33926800	1.13782900	-2.16041500	F	-3.16962900	2.54041700	-2.36978100
	Br	-0.89791600	2.97650600	-4.36576400	F	-2.06447000	3.00853500	-2.37862200	F	-1.56389300	2.53836000	-4.27667000
	Br	-1.42455200	-0.28957000	-4.96299400	F	-3.99315300	1.29037100	-2.67734600	F	-1.73232100	0.06215300	-4.42685700

Table S3. (continued)

	Br	-3.99293500	-0.29660700	-2.79576700	F	-2.19553700	-0.58232000	-2.49704300	F	-3.34257900	0.04848200	-2.52440600
WCl_4O	W	-0.37158300	1.04663100	0.48265700	W	-0.17935100	1.04082600	0.57596600	W	-0.26293000	1.04579800	0.63081600
	O	-0.21431200	1.21364300	2.11739300	O	-0.34309200	0.99454200	2.21677700	O	0.28539500	1.25425200	2.17365700
	Cl	-2.65762400	1.01216200	0.21844500	Cl	-2.45172100	1.14847000	-0.09370000	Cl	-2.55363400	1.04221700	0.92209800
	Cl	-0.42510500	3.24496300	-0.22188500	Cl	-0.12694800	3.29513300	0.18288200	Cl	-0.48172100	3.22996200	-0.09430900
	Cl	1.83076000	1.00114000	-0.21003200	Cl	2.07969500	0.96643500	0.28109400	Cl	1.68974200	0.95467000	-0.58006900
	Cl	-0.39258200	-1.24099300	0.23099400	Cl	-0.29330800	-1.18206200	0.04188300	Cl	-0.37896300	-1.24350600	0.46512400
	W	-0.37976400	1.02056000	-3.76006800	W	-2.28978000	1.24252900	-3.20622800	W	-2.12723800	1.20779000	-3.13727100
	O	-0.59681200	0.80645300	-2.11921500	O	-2.12663800	1.28882600	-4.84710900	O	-1.17546800	0.73663000	-1.84980700
	Cl	-2.49917200	1.09297600	-4.61404700	Cl	-0.01680200	1.13535400	-2.53675400	Cl	-3.51067900	2.81018400	-2.29320500
	Cl	-0.34411700	3.28531600	-4.03443400	Cl	-2.17559400	3.46512000	-2.67117700	Cl	-0.94705600	2.92194300	-4.08152700
	Cl	1.88587200	1.09419100	-4.02271900	Cl	-4.54881500	1.31679200	-2.91042500	Cl	-1.42633100	-0.05867000	-4.90754500
	Cl	-0.26685800	-1.09946900	-4.60795600	Cl	-2.34162400	-1.01172600	-2.81259700	Cl	-3.92509500	-0.20103000	-3.02734800
WBr_4O	W	-0.38669900	1.03156500	0.47965500	W	-0.12430600	1.03460200	0.71473200	W	-0.26679000	1.00868500	0.63243900
	O	-0.41255900	1.04394900	2.12895500	O	-0.27333500	0.98831400	2.35575500	O	0.29318700	0.78975100	2.16811400
	Br	-2.80628100	1.03028400	-0.05156100	Br	-2.55323400	1.14857200	0.02449700	Br	-2.71090100	1.19149900	1.02933700
	Br	-0.37962000	3.45643300	-0.03040400	Br	-0.05256900	3.45619400	0.30217100	Br	-0.21853100	3.47284900	0.43199200
	Br	2.04792300	1.03033700	0.02487800	Br	2.30335100	0.95289700	0.38047800	Br	1.83053600	0.93612900	-0.67258700
	Br	-0.37982100	-1.39888300	0.00625700	Br	-0.23517200	-1.35417200	0.15029800	Br	-0.67773300	-1.33188900	-0.07991000
	W	-0.35187500	1.04546500	-3.73857900	W	-2.34465600	1.24871100	-3.34476800	W	-2.11009400	1.27743100	-3.12148000
	O	-0.34889800	1.01546300	-2.07051700	O	-2.19448500	1.29568600	-4.98563100	O	-1.15136000	1.33842300	-1.75669100
	Br	-2.73372200	1.05562700	-4.31393600	Br	0.08374500	1.13433900	-2.65271600	Br	-3.83554800	2.94846300	-2.62753700
	Br	-0.35341600	3.43482200	-4.27915200	Br	-2.23371700	3.63779600	-2.77946500	Br	-1.16029000	2.92052200	-4.67261400
	Br	2.02699500	1.05558600	-4.32671600	Br	-4.77282800	1.33054500	-3.01170200	Br	-0.99969000	-0.43826300	-4.48038500
	Br	-0.35332200	-1.32307700	-4.36974700	Br	-2.41677200	-1.17324300	-2.93303700	Br	-3.80676400	-0.41336000	-2.63006500
WF_4S	-				W	-0.43819900	1.39664900	0.32932300	W	-0.33271800	1.30723000	1.17467900
					F	-2.23028900	1.38202900	-0.09208200	F	-1.94671800	0.64916600	0.55701300
					F	-0.44131200	3.21898800	0.11626700	F	-1.04670100	2.98156700	0.86165200
					F	1.34719700	1.38498700	-0.11974800	F	1.30814000	2.07558800	0.80391000
					F	-0.44189800	-0.41555800	-0.33760500	F	0.39958400	-0.25437200	0.50917900
					S	-0.42215300	1.12278700	2.38463500	S	-0.38066400	1.06048300	3.23626300
					W	-0.46108000	-0.47511300	-2.78769200	W	0.97824100	3.26316500	-2.51624400
					F	-0.45740900	1.33715800	-2.12027600	F	1.72281000	2.98963300	-4.17870500
					F	-2.24643800	-0.46345400	-2.33855100	F	-0.06484700	4.52316800	-3.36652900
					F	-0.45793300	-2.29749000	-2.57475100	F	0.83776800	4.34793100	-1.04091600
					F	1.33097300	-0.46042200	-2.36618500	F	2.63176600	2.79857900	-1.85768100
					S	-0.47712000	-0.20107300	-4.84296300	S	-0.27507900	1.62266700	-2.18550900
WCl_4S	-				W	-0.43521500	1.50785100	0.77687200	W	-0.41156600	1.16269000	1.48718800
					Cl	-2.66420800	1.50358400	0.24677000	Cl	-2.32391200	0.34188900	0.49542900
					Cl	-0.44052800	3.76087600	0.36917200	Cl	-1.36332900	3.23612500	1.24268700
					Cl	1.78513800	1.50795200	0.21115200	Cl	1.61208200	2.23238700	1.37878400

Table S3. (continued)

		Cl	-0.43814600	-0.73180100	0.10053100	Cl	0.65716100	-0.63442800	0.53196400
		S	-0.41869900	1.36894200	2.83627200	S	-0.62981300	0.68369900	3.48479000
		W	-0.46402700	-0.58643400	-3.23510900	W	1.01692000	3.35384800	-2.75330000
		Cl	-0.46164100	1.65460100	-2.56155000	Cl	1.75581100	2.67259500	-4.81696800
		Cl	-2.68403800	-0.58625200	-2.66896100	Cl	-0.28249200	4.86247000	-3.89540100
		Cl	-0.45841700	-2.83927800	-2.82615400	Cl	1.02364800	4.88415400	-1.04837500
		Cl	1.76441600	-0.58116600	-2.70397400	Cl	3.07040800	2.69702200	-1.97368200
		S	-0.48029700	-0.44938700	-5.29464900	S	-0.29333400	1.87235700	-2.13600400
WBr_4S	-	W	-0.43414200	1.56255500	0.91738800	W	-0.44320600	1.11449900	1.55711500
		Br	-2.82838300	1.56685300	0.35170200	Br	-2.47784300	0.24110100	0.44923100
		Br	-0.44008500	3.98392300	0.46760100	Br	-1.46093100	3.34180700	1.30079600
		Br	1.95111200	1.57229700	0.31470700	Br	1.73039400	2.25853500	1.51372300
		Br	-0.43637000	-0.83489100	0.22039700	Br	0.72176200	-0.80836800	0.53989300
		S	-0.41807200	1.43922300	2.97432200	S	-0.70616600	0.61425700	3.54039400
		W	-0.46518200	-0.64202700	-3.37588100	W	1.03377100	3.38377100	-2.79320300
		Br	-0.46292300	1.75809400	-2.67991900	Br	1.72732400	2.54611200	-5.00383000
		Br	-2.84976800	-0.65015600	-2.77244700	Br	-0.42011400	4.94834000	-4.01986400
		Br	-0.45877400	-3.06236600	-2.92505500	Br	1.10046200	5.08581000	-1.01853900
		Br	1.92836200	-0.64437400	-2.80958200	Br	3.26717500	2.70608700	-2.01162700
		S	-0.48143600	-0.51964300	-5.43285800	S	-0.24104400	1.93285400	-2.05697600
WF_4Se	-	W	-0.37794500	1.17729600	0.75675400	W	-0.33412800	1.29471900	1.18887600
		F	-2.12595200	1.25469700	0.18747900	F	-1.95520200	0.61994300	0.60859200
		F	-0.33857100	3.05680600	0.34858800	F	-1.06166400	2.95954100	0.86545700
		F	1.43566900	1.24134400	0.45246900	F	1.29559700	2.06295900	0.78071100
		F	-0.35025500	-0.59341700	0.27685600	F	0.39183000	-0.27313300	0.53264300
		Se	-0.54230100	1.14869000	2.96592100	Se	-0.34716100	1.06286300	3.39633300
		W	-0.15545900	3.46572400	-2.09536600	W	0.99508100	3.29621000	-2.55687500
		F	-0.18501800	5.23494100	-1.61121500	F	1.79895600	3.05370700	-4.19561300
		F	-1.96986500	3.39940600	-1.79294700	F	0.01300500	4.60002000	-3.41180100
		F	-0.19341500	1.58587300	-1.68905900	F	0.81098900	4.34025200	-1.05745700
		F	1.59289400	3.38889300	-1.52672300	F	2.61263200	2.78667300	-1.84729800
		Se	0.00971800	3.49869400	-4.30449000	Se	-0.38835100	1.56105400	-2.30645500
WCl_4Se	-	W	-0.41053000	1.01572300	1.19381000	W	-0.41748000	1.14768100	1.51380000
		Cl	-2.58226700	1.09451800	0.47273800	Cl	-2.35452000	0.31820100	0.57597500
		Cl	-0.37858400	3.31972200	0.83429100	Cl	-1.35471100	3.21925400	1.22504100
		Cl	1.84390200	1.08581000	0.79975900	Cl	1.61280800	2.19057400	1.34042200
		Cl	-0.36093100	-1.15599200	0.46843400	Cl	0.61314000	-0.68571300	0.58798100
		Se	-0.57292700	0.85215100	3.38844300	Se	-0.61970500	0.69756100	3.66570600
		W	-0.12290700	3.62749000	-2.53264400	W	1.04090100	3.39158700	-2.80961200
		Cl	-0.17087700	5.79960900	-1.80815200	Cl	1.84198200	2.78370200	-4.87210800
		Cl	-2.37734600	3.55910100	-2.13837000	Cl	-0.23468400	4.92872100	-3.93760800

Table S3. (continued)

		Cl	-0.15632700	1.32365500	-2.17170800	Cl	0.98697300	4.86355900	-1.05641000
		Cl	2.04861300	3.54742800	-1.81096100	Cl	3.07936600	2.73212400	-1.99704300
		Se	0.03968200	3.78973200	-4.72737200	Se	-0.36248700	1.77755600	-2.23903100
WBr_4Se	-	W	-0.42200100	0.95496000	1.33230900	W	-0.43664200	1.07304800	1.58279200
		Br	-2.75551500	1.03814100	0.56450400	Br	-2.50595300	0.20463800	0.53403000
		Br	-0.37686300	3.41660400	0.95156000	Br	-1.44598100	3.30200000	1.32982100
		Br	1.99862300	1.00575900	0.90938300	Br	1.74076000	2.19739000	1.46456300
		Br	-0.38168200	-1.38189900	0.55518600	Br	0.68198600	-0.86673100	0.54771600
		Se	-0.58238000	0.79079900	3.52340800	Se	-0.66441600	0.55998200	3.71412100
		W	-0.11130900	3.68831300	-2.67080900	W	1.04536000	3.44608400	-2.84912300
		Br	-0.15237300	6.02408500	-1.89121300	Br	1.79653900	2.71171100	-5.07620100
		Br	-2.53238100	3.63678200	-2.24973900	Br	-0.37570200	5.06478700	-4.04075700
		Br	-0.15638400	1.22662100	-2.29057800	Br	1.06436200	5.06568200	-0.99941700
		Br	2.22257100	3.60488400	-1.90396400	Br	3.26287400	2.74469500	-2.04703300
		Se	0.04919600	3.85389800	-4.86177900	Se	-0.33160300	1.86151800	-2.16339900