

Evaluation of Steric Properties of Lewis Acids

Ludwig Zapf,^[a,b] Melanie Riethmann,^[a,b] Steffen A. Föhrenbacher,^[a]

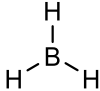
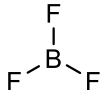
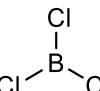
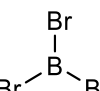
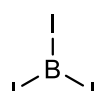
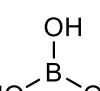
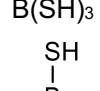
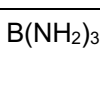
Maik Finze,^[a,b]* and Udo Radius^[a]*

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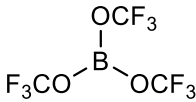
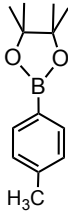
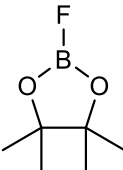
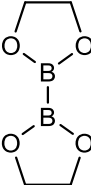
1. %V_{Bur} and FIA of selected Lewis Acids

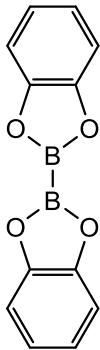
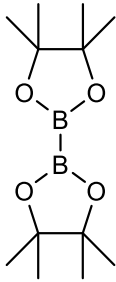
Table S1. %V_{Bur}¹ of selected Lewis acids *LA* obtained from geometry optimized corresponding anionic fluoride adducts [F–*LA*][−] (def2-SVP; BP86; *R* = 3.5 Å) together with the cartesian coordinates of the optimized structures and the FIAs reported either by Krossing *et al.* or Greb *et al.*² Values for %V_{Bur} have been obtained from the SambVca 2.1 web application: <https://www.molnac.unisa.it/OMtools/sambvca2.1/index.html>.

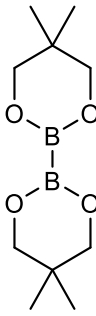
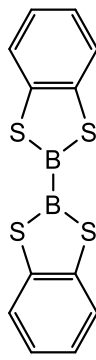
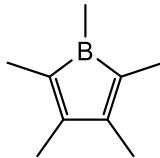
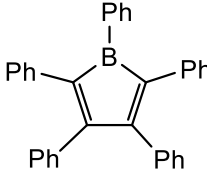
<i>LA</i>	Anion	%V _{Bur}	<i>d</i> (<i>LA</i> –F) [Å]	Coordinates	FIA [kJ/mol] Greb ^{2a}	FIA [kJ/mol] Krossing
BH_3 	[H ₃ BF] [−]	27.3	1.448	B -0.00000 0.00000 -1.44797 H -0.59668 1.03349 -1.90964 H -0.59670 -1.03349 -1.90962 H 1.19337 0.00000 -1.90962 F 0.00000 0.00000 0.00000	279	
BF_3 	[BF ₄] [−]	33.3	1.418	B 0.00000 0.00000 -1.41804 F 1.33693 0.00000 -1.89066 F -0.66821 -1.15792 -1.89088 F 0.00000 0.00000 0.00000 F -0.66869 1.15774 -1.89077	346	338 ^{2b} 346 ^{2c}
BCl_3 	[Cl ₃ BF] [−]	40.9	1.379	B 0.00000 0.00000 -1.37899 F 0.00000 0.00000 0.00000 Cl 1.78785 0.00000 -2.02265 Cl -0.89393 1.54832 -2.02265 Cl -0.89393 -1.54832 -2.02265	404	405 ^{2b} 384 ^{2c}
BBr_3 	[Br ₃ BF] [−]	43.0	1.369	B -0.00000 0.00000 -1.36883 F 0.00000 0.00000 0.00000 Br -0.97568 -1.68995 -2.07103 Br -0.97574 1.68997 -2.07098 Br 1.95143 0.00000 -2.07098	428	433 ^{2b} 425 ^{2c}
BI_3 	[I ₃ BF] [−]	45.5	1.357	B 0.00000 -0.00000 -1.35678 F 0.00000 0.00000 0.00000 I 2.18164 -0.00000 -2.13653 I -1.09095 1.88928 -2.13653 I -1.09073 -1.88934 -2.13665	446	448 ^{2b}
B(OH)_3 	[(OH) ₃ BF] [−]	35.6	1.450	B -0.00000 -0.00000 -1.44963 F 0.00000 0.00000 0.00000 O -0.64733 1.27513 -1.89413 H -1.41425 1.36176 -1.29224 O 1.35811 -0.00000 -2.02553 H 1.55658 0.95658 -2.09025 O -0.71615 -1.21994 -1.86606 H -0.42399 -1.32162 -2.79419	190	204 ^{2c} 208 ^{2c}
B(SH)_3 	[(SH) ₃ BF] [−]	42.4	1.402	B 0.00000 0.00000 -1.40220 F 0.00000 0.00000 0.00000 S -0.85251 1.68737 -1.96250 H -1.05193 1.33169 -3.26756 S 1.80259 0.00000 -2.16353 H 2.15934 -1.27059 -1.77437 S -0.88307 -1.59127 -2.12662 H -2.05791 -1.46797 -1.42206	309	
$\text{B(NH}_2)_3$ 	[(NH ₂) ₃ BF] [−]	37.9	1.464	B 0.00000 0.00000 -1.46406 F 0.00000 0.00000 0.00000 N 1.47458 0.00000 -1.95269 H 1.83448 -0.94317 -1.71756 H 1.43862 -0.00424 -2.98827 N -0.77737 -1.29879 -1.88557 H -1.67433 -1.30442 -1.36121 H -1.07370 -1.15451 -2.86916 N -0.68240 1.27900 -2.03674 H -1.61107 1.35398 -1.58150 H -0.15232 2.08801 -1.66214	120	

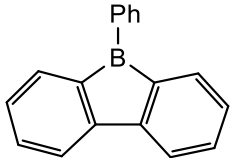
$\begin{array}{c} \text{B}(\text{CH}_3)_3 \\ \\ \text{CH}_3 \\ \\ \text{H}_3\text{C}-\text{B}-\text{CH}_3 \end{array}$	$[(\text{CH}_3)_3\text{BF}]^-$	40.7	1.474	B 0.00000 0.00000 -1.47431 F 0.00000 0.00000 0.00000 C -0.78769 1.36428 -1.98790 H -1.84527 1.39893 -1.61694 H -0.28891 2.29751 -1.61694 H -0.83640 1.44865 -3.10445 C 1.57529 0.00000 -1.98782 H 1.67283 0.00019 -3.10434 H 2.13403 0.89845 -1.61656 H 2.13378 -0.89873 -1.61686 C -0.78762 -1.36426 -1.98782 H -0.83654 -1.44864 -3.10434 H -0.28852 -2.29728 -1.61685 H -1.84507 -1.39893 -1.61656	248	
$\begin{array}{c} \text{B}(\text{NC})_3 \\ \\ \text{NC} \\ \\ \text{CN}-\text{B}-\text{NC} \end{array}$	$[(\text{CN})_3\text{BF}]^-$	38.4	1.395	B 0.00000 -0.00000 -1.39461 N -0.72151 1.24972 -1.92755 N 1.44302 -0.00000 -1.92751 N -0.72143 -1.24967 -1.92781 C 2.56195 -0.00014 -2.31699 C -1.28069 -2.21864 -2.31771 C -1.28086 2.21882 -2.31703 F 0.00000 0.00000 0.00000		
$\begin{array}{c} \text{B}(\text{CN})_3 \\ \\ \text{CN} \\ \\ \text{NC}-\text{B}-\text{CN} \end{array}$	$[(\text{NC})_3\text{BF}]^-$	38.9	1.419	B 0.00000 -0.00000 -1.41873 F 0.00000 0.00000 0.00000 C -0.75898 1.31459 -1.98401 C 1.51796 -0.00000 -1.98401 C -0.75898 -1.31459 -1.98401 N -1.31292 -2.27404 -2.37353 N 2.62583 0.00000 -2.37353 N -1.31292 2.27404 -2.37353		540 ^{2c}
$\begin{array}{c} \text{B}(\text{C}\equiv\text{CH})_3 \\ \\ \text{CCH} \\ \\ \text{HCC}-\text{B}-\text{CCH} \end{array}$	$[(\text{HC}\equiv\text{C})_3\text{BF}]^-$	39.3	1.443	B -0.00000 -0.00000 -1.44258 F 0.00000 0.00000 0.00000 C -0.75948 1.31545 -1.98890 C 1.51897 -0.00000 -1.98888 C -0.75947 -1.31547 -1.98888 C -1.34097 2.32259 -2.39725 H -1.85143 3.20670 -2.75561 C 2.68194 0.00003 -2.39717 H 3.70285 0.00005 -2.75548 C -1.34097 -2.32263 -2.39718 H -1.85144 -3.20675 -2.75549	334	
$\begin{array}{c} \text{B}(\text{CF}_3)_3 \\ \\ \text{CF}_3 \\ \\ \text{F}_3\text{C}-\text{B}-\text{CF}_3 \end{array}$	$[(\text{CF}_3)_3\text{BF}]^-$	50.8	1.429	B -0.00000 -0.00000 -1.42917 C 1.56626 -0.00000 -1.94525 C -0.78284 -1.35648 -1.94600 C -0.78362 1.35614 -1.94525 F -2.08150 1.42584 -1.49691 F -0.86399 1.49114 -3.31121 F -0.19428 2.51597 -1.50047 F 2.27564 1.09056 -1.50046 F 2.27595 -1.08890 -1.49691 F 1.72337 -0.00204 -3.31121 F 0.00000 0.00000 0.00000 F -0.19392 -2.51605 -1.50004 F -2.08149 -1.42672 -1.50005 F -0.86094 -1.49181 -3.31211		552 ^{2b} 556 ^{2c}
$\begin{array}{c} \text{B}(\text{C}_2\text{F}_3)_3 \\ \\ \text{C}_2\text{F}_3 \\ \\ \text{F}_3\text{C}_2-\text{B}-\text{C}_2\text{F}_3 \end{array}$	$[(\text{C}_2\text{F}_3)_3\text{BF}]^-$	53.0	1.434	B 0.00000 0.00000 -1.43348 C -0.69533 1.37467 -1.98007 C 1.54517 0.00000 -1.99561 C -0.75136 -1.33533 -1.99839 C -1.44298 -2.27877 -1.32929 C 2.66781 -0.39865 -1.36545 C -1.87929 1.58500 -2.58873 F 3.90990 -0.36313 -1.89417 F 2.71662 -0.89500 -0.12454 F 1.74931 0.44711 -3.27932 F 0.00000 0.00000 0.00000 F 0.01378 2.52948 -1.73465 F -2.35908 2.79082 -2.95524 F -2.75619 0.63021 -2.92213 F -0.63450 -1.57483 -3.34876 F -1.70424 -2.26211 -0.01787 F -1.98334 -3.38237 -1.88996		
$\begin{array}{c} \text{B}(\text{CF}_3)\text{F}_2 \\ \\ \text{CF}_3 \\ \\ \text{F}-\text{B}-\text{F} \end{array}$	$[(\text{CF}_3)\text{BF}_3]^-$	39.2	1.429	B 0.00000 -0.00000 -1.41506 F -0.64548 -1.16060 -1.90345 F -0.64571 1.16040 -1.90384 F 0.00000 0.00000 0.00000 C 1.57127 -0.00000 -1.94788 F 2.30346 -1.09391 -1.53168 F 2.30469 1.09184 -1.52847 F 1.69637 0.00189 -3.32282		
$\text{B}(\text{CF}_3)_2\text{F}$	$[(\text{CF}_3)_2\text{BF}_2]^-$	45.1	1.418	B -0.00000 -0.00000 -1.41821 F -0.64585 1.15858 -1.92008 F 0.00000 0.00000 0.00000 C 1.56820 0.00000 -1.94575 F 2.30539 -1.08513 -1.52753 F 2.26941 1.09976 -1.50088		

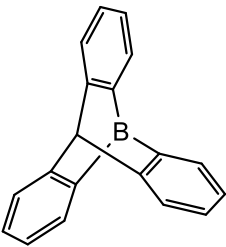
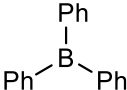
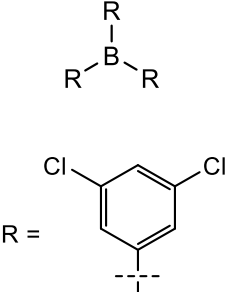
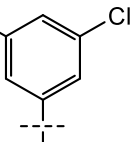
$\begin{array}{c} \text{CF}_3 \\ \\ \text{F}-\text{B}-\text{CF}_3 \end{array}$				F 1.70466 0.02148 -3.31556 C -0.82456 -1.33419 -1.94534 F -0.30438 -2.53097 -1.50663 F -2.13590 -1.33924 -1.52159 F -0.89284 -1.45230 -3.31550		
$\text{B}(\text{C}_2\text{F}_5)_2\text{F}$ $\begin{array}{c} \text{C}_2\text{F}_5 \\ \\ \text{F}-\text{B}-\text{C}_2\text{F}_5 \end{array}$	$[(\text{C}_2\text{F}_5)_2\text{BF}_2]^-$	49.9	1.413	B 0.00000 -0.00000 -1.41276 F 0.00000 0.00000 0.00000 F -0.61553 -1.16558 -1.92099 C 1.60374 -0.00000 -1.88167 F 2.19358 -1.15998 -1.38990 F 2.30498 1.05644 -1.31217 C -0.92448 1.28653 -1.94330 F -1.07804 1.27186 -3.32468 F -2.20325 1.14221 -1.41479 C -0.53698 2.74383 -1.60122 C 1.99936 0.01983 -3.37651 F 0.61041 3.11661 -2.20911 F -1.49955 3.62346 -2.00623 F -0.37887 2.92212 -0.27126 F 1.41124 -0.98305 -4.06490 F 3.34725 -0.12804 -3.53703 F 1.66284 1.18473 -3.97210		
$\text{B}(\text{C}_2\text{F}_5)\text{F}_2$ $\begin{array}{c} \text{C}_2\text{F}_5 \\ \\ \text{F}-\text{B}-\text{F} \end{array}$	$[(\text{C}_2\text{F}_5)\text{BF}_3]^-$	39.7	1.412	B 0.00000 0.00000 -1.41063 F -0.63830 -1.15976 -1.90484 F -0.63964 1.15868 -1.90483 F 0.00000 0.00000 0.00000 C 1.59316 -0.00000 -1.91897 F 2.29039 -1.09726 -1.41839 F 2.27608 1.12519 -1.46289 C 1.86508 -0.02972 -3.43780 F 1.36216 -1.14275 -4.01899 F 1.32711 1.03991 -4.06756 F 3.20492 -0.01472 -3.72046		
$\text{B}(\text{CN})_2(\text{CF}_3)$ $\begin{array}{c} \text{CF}_3 \\ \\ \text{NC}-\text{B}-\text{CN} \end{array}$	$[(\text{NC})_2(\text{CF}_3)\text{BF}]^-$	42.9	1.422	B 0.00000 0.00000 -1.42211 F 0.00000 0.00000 0.00000 C 1.55636 -0.00000 -1.96920 F 2.26755 -1.09270 -1.54142 F 2.26812 1.09156 -1.53955 F 1.66168 0.00110 -3.33765 C -0.75362 -1.31423 -1.98398 C -0.75369 1.31401 -1.98453 N -1.30768 -2.27695 -2.36529 N -1.30768 2.27649 -2.36653		
$\text{B}(\text{CN})(\text{CF}_3)_2$ $\begin{array}{c} \text{CF}_3 \\ \\ \text{NC}-\text{B}-\text{CF}_3 \end{array}$	$[(\text{NC})(\text{CF}_3)_2\text{BF}]^-$	46.9	1.426	B -0.00000 -0.00000 -1.42567 F 0.00000 0.00000 0.00000 C -0.75861 -1.36417 -1.95461 F -2.06136 -1.46007 -1.53133 F -0.14573 -2.50620 -1.49707 F -0.80548 -1.49468 -3.32095 C -0.75964 1.36390 -1.95390 F -2.05654 1.46736 -1.51514 F -0.13704 2.50662 -1.51112 F -0.82307 1.48598 -3.32043 C 1.51320 -0.00000 -1.98474 N 2.62616 -0.00049 -2.35974		
$\text{B}(\text{CN})(\text{C}_2\text{F}_5)_2$ $\begin{array}{c} \text{C}_2\text{F}_5 \\ \\ \text{NC}-\text{B}-\text{C}_2\text{F}_5 \end{array}$	$[(\text{C}_2\text{F}_5)_2(\text{NC})\text{BF}]^-$	51.8	1.421	B 0.00000 -0.00000 -1.42070 F 0.00000 0.00000 0.00000 C 1.57234 -0.00000 -1.96221 F 2.20784 1.11846 -1.43989 F 1.64398 0.11904 -3.34228 C -0.94036 -1.29487 -1.88573 F -0.48446 -2.46251 -1.29117 F -2.22143 -1.09089 -1.38992 C -1.15738 -1.66148 -3.37548 C 2.52237 -1.17358 -1.60773 F -0.01525 -2.08068 -3.96056 F -2.06257 -2.67058 -3.50298 F -1.62730 -0.61246 -4.08249 F 2.56124 -1.40113 -0.27810 F 3.79724 -0.90398 -2.00550 F 2.15558 -2.32033 -2.21765 C -0.66056 1.36497 -1.97287 N -1.14042 2.37600 -2.32751		
$\text{B}(\text{CN})_2(\text{C}_2\text{F}_5)$ $\begin{array}{c} \text{C}_2\text{F}_5 \\ \\ \text{NC}-\text{B}-\text{CN} \end{array}$	$[(\text{NC})_2(\text{C}_2\text{F}_5)\text{BF}]^-$	43.9	1.421	B -0.00000 0.00000 -1.42071 F 0.00000 0.00000 0.00000 C -0.80145 1.37741 -1.90731 F -0.16900 2.49275 -1.38106 F -2.08601 1.37544 -1.38689 C -0.97807 1.68847 -3.41277 F 0.21341 1.81512 -4.03566 F -1.67396 0.71644 -4.04102 F -1.65585 2.85389 -3.60087 C -0.75024 -1.31931 -1.97191 C 1.51813 0.00000 -1.97045 N -1.28630 -2.30074 -2.33006 N 2.63700 -0.01950 -2.32628		

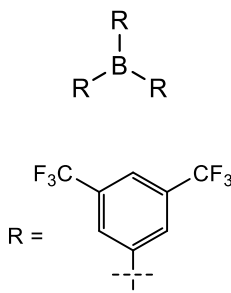
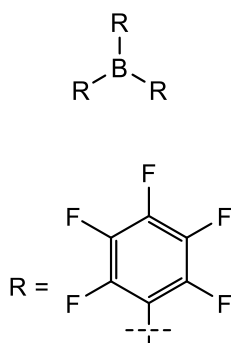
$\text{B}(\text{OCF}_3)_3$ 	$[(\text{OCF}_3)_3\text{BF}]^-$	46.5	1.383	B -0.00000 0.00000 -1.38280 O -0.75413 -1.20738 -1.81920 O 1.39426 0.00000 -1.92504 O -0.68951 1.19834 -1.93589 C -1.37352 -1.38247 -2.96027 C -0.18181 2.40046 -2.05738 C 2.23153 -1.00541 -1.87523 F 0.00000 0.00000 0.00000 F 0.64148 2.55514 -3.14130 F 0.54530 2.82402 -0.97575 F -1.18548 3.31779 -2.22365 F 1.95010 -2.01479 -2.76286 F 2.32585 -1.61351 -0.65057 F 3.49491 -0.58146 -2.18714 F -0.70575 -0.91631 -4.05796 F -1.58809 -2.71701 -3.17914 F -2.61700 -0.79986 -3.00765		
$p\text{Tol-Bpin}$ 	$[p\text{Tol-BpinF}]^-$	46.3	1.436	F 0.00000 0.00000 0.00000 B 0.00000 0.00000 -1.43678 C 4.28567 -0.04827 -2.91407 C 3.82126 -0.98539 -1.96426 C 2.49380 -0.95426 -1.50373 C 1.55423 0.00000 -1.96394 C 2.03699 0.93370 -2.90931 C 3.36600 0.91802 -3.37286 H 4.52126 -1.75072 -1.57586 H 2.17182 -1.69460 -0.74884 H 1.33590 1.70388 -3.27804 H 3.70216 1.67529 -4.10793 C 5.70592 -0.10016 -3.44104 H 6.42073 -0.46118 -2.66630 H 5.80517 -0.79028 -4.31489 H 6.05443 0.90141 -3.78207 O -0.74557 1.16106 -1.99504 O -0.76905 -1.19449 -1.90773 C -2.05032 0.73323 -2.33027 C -1.81180 -0.78039 -2.76293 C -2.60844 1.64339 -3.43931 C -2.96653 0.84289 -1.08427 C -3.02727 -1.70544 -2.56210 C -1.33559 -0.89174 -4.23414 H -3.60410 1.29442 -3.80054 H -2.72864 2.67894 -3.04606 H -1.91343 1.69444 -4.30385 H -2.90636 1.88540 -0.69848 H -4.03441 0.61009 -1.30861 H -2.60483 0.16880 -0.27963 H -3.90849 -1.37250 -3.15969 H -2.76484 -2.73989 -2.88262 H -3.31646 -1.75298 -1.49132 H -0.96476 -1.92737 -4.40371 H -2.14185 -0.67813 -4.97481 H -0.48639 -0.19833 -4.41498		
FBpin 	$[\text{FpinBF}]^-$	39.4	1.418	B -0.00000 0.00000 -1.41765 O -0.61411 1.26290 -1.91838 O 1.38053 0.00000 -1.98022 C 1.65408 1.27990 -2.49825 C 0.20950 1.79109 -2.93039 C 0.04823 3.32220 -2.97088 H 0.74920 3.79769 -3.69688 H -0.99204 3.58038 -3.27699 H 0.21715 3.76442 -1.96626 C -0.21608 1.20115 -4.30075 H -1.30576 1.38530 -4.43594 H 0.32986 1.65135 -5.16383 H -0.05802 0.10170 -4.30154 C 2.26085 2.16849 -1.38054 H 3.13837 1.63547 -0.94992 H 2.59666 3.16849 -1.74516 H 1.51822 2.30676 -0.56615 C 2.66998 1.15650 -3.64915 H 2.85101 2.13441 -4.15456 H 3.64396 0.78952 -3.25013 H 2.32334 0.42024 -4.40492 F -0.69730 -1.14932 -1.86830 F 0.00000 0.00000 0.00000		
B_2eg_2 	$[\text{B}_2\text{eg}_2\text{F}]^-$	40.5	1.432	B 0.00000 0.00000 -1.43179 O -0.68686 -1.26023 -1.91644 O -0.84660 1.11096 -1.97022 C -2.07184 0.56220 -2.35888 H -2.82816 0.54451 -1.51783 H -2.53138 1.15276 -3.19669 C -1.72363 -0.88612 -2.77203 H -2.60129 -1.58317 -2.68072 H -1.40775 -0.90153 -3.85802 B 1.60883 0.00000 -2.13025 O 1.90270 0.41730 -3.44416 O 2.76518 -0.56311 -1.55529 C 3.23209 0.04755 -3.78880		241 ³

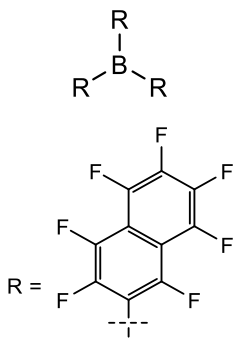
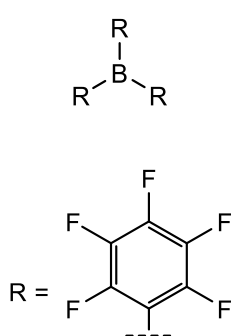
				H 3.78781 0.93335 -4.18272 H 3.21310 -0.72064 -4.60207 C 3.84849 -0.50903 -2.47600 H 4.29024 -1.52670 -2.60817 H 4.65636 0.15350 -2.07485 F 0.00000 0.00000 0.00000		
B₂cat₂ 	[B₂cat₂F]⁻	40.3	1.416	B 1.60887 0.00000 -2.08588 B 0.00000 0.00000 -1.41558 O 2.60987 0.99345 -1.85692 O 2.15374 -0.95198 -2.99813 O -0.76967 1.21891 -1.92577 O -0.83067 -1.16835 -1.92595 C 3.69948 0.64997 -2.60248 C 4.93243 1.29669 -2.72251 C 3.42042 -0.54458 -3.30165 C 5.89152 0.70465 -3.57558 H 5.13728 2.22852 -2.17175 C 4.36279 -1.13586 -4.14701 C 5.61241 -0.48740 -4.27384 H 6.87682 1.18665 -3.69626 H 4.13064 -2.06730 -4.68748 H 6.38229 -0.92374 -4.93307 C -1.94234 -0.66080 -2.48273 C -3.03535 -1.34803 -3.02625 C -1.90518 0.76767 -2.48643 C -4.09996 -0.59386 -3.58550 H -3.05390 -2.45100 -3.01521 C -2.95868 1.50930 -3.03571 C -4.06256 0.80997 -3.59036 H -4.96633 -1.12197 -4.02266 H -2.91853 2.61175 -3.03010 H -4.89965 1.38078 -4.03080 F 0.00000 0.00000 0.00000		341³
B₂pin₂ 	[B₂pin₂F]⁻	45.1	1.437	B -0.00000 0.00000 -1.43683 O -0.72925 -1.23436 -1.91292 O -0.81748 1.12750 -1.97908 C -2.10049 0.63594 -2.30771 C -1.78733 -0.85491 -2.76530 B 1.62610 0.00000 -2.09265 O 1.96159 0.39127 -3.40689 O 2.78506 -0.48574 -1.45781 C 3.29010 -0.07124 -3.72183 C 3.93653 -0.23216 -2.28677 C 4.92198 -1.39944 -2.13944 H 5.80293 -1.27791 -2.81122 H 5.29093 -1.44349 -1.09046 H 4.43499 -2.37116 -2.36187 C 4.59305 1.06566 -1.77241 H 4.81474 0.94550 -0.68935 H 5.54262 1.30273 -2.30453 H 3.89807 1.92612 -1.87763 C 3.97134 0.95618 -4.63586 H 5.02574 0.67045 -4.85617 H 3.42112 1.01622 -5.60121 H 3.96359 1.96990 -4.18488 C 3.14446 -1.41255 -4.46901 H 2.49388 -1.25686 -5.35718 H 4.12412 -1.81502 -4.81419 H 2.65043 -2.17021 -3.82394 C -2.95650 -1.84239 -2.58661 H -3.85087 -1.54419 -3.18360 H -2.64159 -2.85763 -2.92185 H -3.24862 -1.92142 -1.51833 C -1.30036 -0.91070 -4.23645 H -0.88997 -1.92797 -4.42918 H -2.11133 -0.71268 -4.97691 H -0.47714 -0.18024 -4.38786 C -3.01454 0.67649 -1.05494 H -3.00136 1.71312 -0.64871 H -4.07277 0.39769 -1.27641 H -2.61328 0.00545 -0.26669 C -2.71315 1.53257 -3.39986 H -3.68729 1.13412 -3.77024 H -2.89321 2.55203 -2.98710 H -2.01913 1.64052 -4.25992 F 0.00000 0.00000 0.00000		287³
B₂neop₂	[B₂neop₂F]⁻	47.5	1.463	B 0.00000 -0.00000 -1.46278 O -0.70834 1.22781 -1.93268 O -0.71520 -1.22374 -1.93037 C -2.07423 1.24958 -1.66594 H -2.28732 1.29212 -0.55911 H -2.52314 2.17949 -2.11316 C -2.08053 -1.23683 -1.66060 H -2.53527 -2.16648 -2.10241 H -2.29193 -1.27215 -0.55328 C -2.82253 0.00697 -2.23665 C -2.73485 0.00303 -3.77184 H -3.23231 -0.89926 -4.20272 H -3.22539 0.90695 -4.20735		238³

				H -1.66963 -0.00218 -4.08444 C -4.28732 0.01186 -1.78159 H -4.82911 0.91269 -2.15936 H -4.83349 -0.88841 -2.15438 H -4.36441 0.01515 -0.66875 B 1.65198 -0.00000 -2.04610 O 2.39150 1.19220 -2.11296 O 2.32340 -1.19591 -2.34843 C 3.76532 1.21377 -2.43450 H 4.22993 2.09222 -1.91982 H 3.89915 1.37821 -3.53607 C 3.69550 -1.22959 -2.67753 H 4.10786 -2.21704 -2.34995 H 3.82436 -1.17985 -3.79062 C 4.50371 -0.08230 -2.03080 C 4.52072 -0.23531 -0.49627 H 3.49165 -0.24543 -0.07733 H 5.02029 -1.18662 -0.19974 H 5.07484 0.60737 -0.02159 C 5.93851 -0.06895 -2.58044 H 6.52613 0.77520 -2.14957 H 6.47433 -1.01383 -2.32825 H 5.95129 0.04148 -3.68962 F 0.00000 0.00000 0.00000		
B₂Scat₂ 	[B₂Scat₂F]⁻	44.7	1.412	B 1.56496 -0.00000 -2.13740 B 0.00000 0.00000 -1.41183 C 4.16331 0.50585 -2.77839 C 5.49851 0.96032 -2.81103 C 3.67182 -0.32512 -3.82393 C 6.33985 0.59172 -3.87254 H 5.87304 1.60527 -1.99839 C 4.52735 -0.68911 -4.88575 C 5.85432 -0.23235 -4.90887 H 7.38339 0.95005 -3.89317 H 4.14369 -1.33255 -5.69534 H 6.51703 -0.52029 -5.74300 C -2.54123 -0.56691 -2.54555 C -3.75838 -1.18799 -2.90176 C -2.45864 0.86057 -2.55102 C -4.87828 -0.42175 -3.27384 H -3.81876 -2.28986 -2.88855 C -3.59272 1.61679 -2.91960 C -4.79531 0.98328 -3.28335 H -5.81890 -0.92723 -3.55564 H -3.52315 2.71820 -2.91948 H -5.66996 1.59243 -3.57234 F 0.00000 0.00000 0.00000 S 3.01906 0.89966 -1.48532 S 1.98372 -0.84846 -3.70005 S -0.91774 1.60193 -2.11550 S -1.08851 -1.47753 -2.13174		
BC₄(CH₃)₅ 	[(CH₃)₅C₄BF]⁻	44.3	1.461	C -0.83670 -1.25632 -2.11713 C -1.75942 -0.75357 -2.99505 C -1.75806 0.75110 -2.99778 C -0.83542 1.25577 -2.12077 B -0.00000 -0.00000 -1.46100 C -0.56737 2.70679 -1.84325 H -0.68389 2.93149 -0.75309 H 0.49378 2.97549 -2.07951 H -1.21950 3.42633 -2.40085 C -2.69513 1.52117 -3.90380 H -2.57736 2.62192 -3.78385 H -2.52838 1.29088 -4.98634 H -3.77100 1.28398 -3.70725 C -2.69843 -1.52556 -3.89717 H -3.77309 -1.27802 -3.70755 H -2.52538 -1.30772 -4.98136 H -2.58945 -2.62597 -3.76573 C -0.57105 -2.70634 -1.83242 H -0.67833 -2.92258 -0.73962 H -1.23071 -3.42731 -2.37916 H 0.48704 -2.98035 -2.07633 C 1.56902 -0.00000 -1.99551 H 1.65122 -0.00101 -3.10949 H 2.12303 0.89924 -1.62242 H 2.12445 -0.89759 -1.62054 F 0.00000 0.00000 0.00000		
BC₄(C₆H₅)₅ 	[(C₆H₅)₅C₄BF]⁻	53.5	1.434	C -0.76784 1.26661 -2.14858 C -1.52580 0.75781 -3.19237 C -1.55480 -0.73598 -3.17669 C -0.79468 -1.25719 -2.14200 B -0.00000 0.00000 -1.43350 C -0.64771 -2.67130 -1.77509 C 0.52466 -3.10732 -1.09220 C -1.65404 -3.65598 -1.99705 C 0.69356 -4.44012 -0.69215 H 1.31774 -2.37327 -0.88713 C -1.48899 -4.98685 -1.58677 H -2.59605 -3.36221 -2.48387		

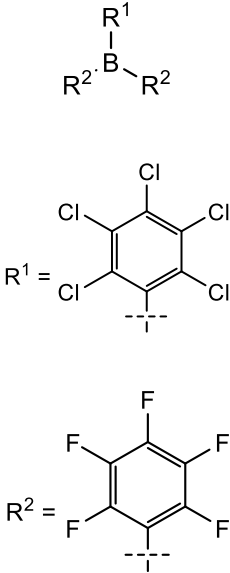
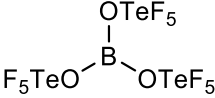
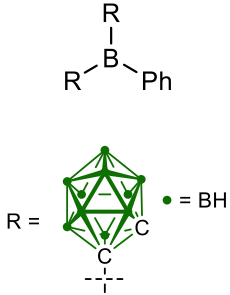
				C -0.30986 -5.39595 -0.93681 H 1.62323 -4.73588 -0.17415 H -2.29775 -5.71560 -1.77504 H -0.17948 -6.44427 -0.61576 C -2.23789 -1.52191 -4.25275 C -1.47896 -2.12822 -5.28136 C -3.64094 -1.70670 -4.27829 C -2.09419 -2.88251 -6.29446 H -0.38342 -2.00550 -5.27078 C -4.26086 -2.46327 -5.28702 H -4.25113 -1.27063 -3.46963 C -3.48956 -3.05304 -6.30378 H -1.47556 -3.34511 -7.08318 H -5.35681 -2.59708 -5.27597 H -3.97428 -3.64699 -7.09789 C -2.13136 1.56029 -4.29797 C -1.29419 2.34498 -5.12964 C -3.52235 1.58905 -4.56001 C -1.82055 3.11927 -6.17544 H -0.20890 2.33926 -4.93651 C -4.05357 2.36493 -5.60434 H -4.20285 1.01308 -3.91390 C -3.20531 3.13276 -6.42073 H -1.14119 3.71950 -6.80559 H -5.14379 2.37106 -5.77922 H -3.62163 3.74057 -7.24277 C -0.63019 2.67917 -1.77835 C 0.55255 3.14494 -1.13537 C -1.67612 3.63120 -1.95526 C 0.69369 4.48056 -0.73285 H 1.37494 2.43383 -0.96558 C -1.53825 4.96375 -1.54166 H -2.62547 3.30437 -2.40772 C -0.34805 5.40526 -0.93350 H 1.63198 4.80323 -0.24745 H -2.37599 5.66798 -1.69256 H -0.23883 6.45502 -0.60935 C 1.56817 -0.00000 -1.98462 C 2.63184 0.01179 -1.04875 C 1.93144 -0.00690 -3.35307 C 3.98135 0.01563 -1.45244 H 2.38014 0.01764 0.02619 C 3.27343 -0.00329 -3.77018 H 1.13184 -0.01467 -4.11676 C 4.31146 0.00821 -2.81857 H 4.78355 0.02460 -0.69158 H 3.51514 -0.00919 -4.84871 H 5.36781 0.01142 -3.14129 F 0.00000 0.00000 0.00000		
Benzoborole 	[BenzoboroleF] ⁻	47.3	1.448	C -0.93416 -3.89711 -3.44195 C -1.94314 -3.35616 -2.62167 C -1.73273 -2.12877 -1.95674 C -0.51947 -1.43173 -2.08608 C 0.49449 -1.99949 -2.91447 C 0.28952 -3.21764 -3.59364 H -1.10179 -4.85507 -3.96700 H -2.90158 -3.89502 -2.50470 H -2.53813 -1.70989 -1.32470 H 1.07864 -3.64659 -4.23826 C 1.52273 0.00000 -2.08782 C 2.59144 0.90371 -1.96175 C 3.81552 0.68335 -2.62950 C 3.97875 -0.44996 -3.44955 C 2.92304 -1.36948 -3.59801 C 1.70952 -1.14723 -2.91601 H 2.47313 1.80418 -1.33030 H 4.64869 1.40128 -2.51517 H 4.93514 -0.61836 -3.97726 H 3.05623 -2.25769 -4.24267 B -0.00000 0.00000 -1.44775 C -0.88879 1.27110 -1.98846 C -1.49574 2.16431 -1.07245 C -1.09611 1.54579 -3.36366 C -2.26362 3.26629 -1.49599 H -1.35273 1.97647 0.00627 C -1.85966 2.64112 -3.80297 H -0.64172 0.87525 -4.11626 C -2.45109 3.51249 -2.86763 H -2.72143 3.94121 -0.74839 H -1.99720 2.82012 -4.88560 H -3.05259 4.37532 -3.20696 F 0.00000 0.00000 0.00000		
B(tript)	[(tript)BF] ⁻	47.3	1.429	B 0.00000 -0.00000 -1.42861 C 1.48203 -0.00000 -2.13500 C -0.74137 -1.28378 -2.13347 C -0.74098 1.28384 -2.13386 C 2.74915 0.00067 -1.52430 C 1.42382 -0.00016 -3.55417 C -0.71366 -1.23454 -3.55259 C -1.37381 -2.38085 -1.52122		

				C -1.37261 2.38158 -1.52183 C -0.71347 1.23402 -3.55303 H 2.81478 0.00088 -0.42074 C 3.92918 0.00125 -2.29842 C 2.59073 0.00041 -4.33353 C -0.00162 -0.00044 -4.12295 C -1.29755 -2.24593 -4.33054 C -1.96411 -3.40370 -2.29378 H -1.40531 -2.43670 -0.41755 H -1.40378 2.43796 -0.41818 C -1.96240 3.40459 -2.29469 C -1.29708 2.24553 -4.33117 H 4.91773 0.00188 -1.80261 C 3.85278 0.00116 -3.70266 H 2.52295 0.00039 -5.43765 H -0.00216 -0.00054 -5.23409 H -1.26491 -2.18803 -5.43475 C -1.92738 -3.33864 -3.69808 H -2.45734 -4.25965 -1.79667 H -2.45486 4.26109 -1.79779 C -1.92610 3.33895 -3.69901 H -1.26487 2.18730 -5.43540 H 4.77518 0.00175 -4.31112 H -2.38887 -4.13815 -4.30543 H -2.38716 4.13850 -4.30660 F 0.00000 0.00000 0.00000		
BPh₃ 	[Ph ₃ BF] ⁻	53.1	1.459	B 0.00000 0.00000 -1.45854 F 0.00000 0.00000 0.00000 C -0.78517 -1.35858 -1.96863 C -1.69025 -2.01191 -1.09502 C -0.63661 -1.93292 -3.25488 C -2.41432 -3.15446 -1.48011 H -1.81535 -1.60345 -0.07700 C -1.35729 -3.07328 -3.65850 H 0.08597 -1.48639 -3.96245 C -2.25558 -3.69221 -2.77096 H -3.11016 -3.63422 -0.76648 H -1.20901 -3.48912 -4.67238 H -2.82157 -4.58976 -3.07968 C 1.56940 0.00000 -1.96788 C 2.58750 -0.45456 -1.09266 C 1.99332 0.41507 -3.25411 C 3.93957 -0.50852 -1.47607 H 2.29562 -0.76645 -0.07467 C 3.34186 0.36315 -3.65597 H 1.24555 0.81561 -3.96296 C 4.32679 -0.10267 -2.76681 H 4.70264 -0.86937 -0.76113 H 3.62841 0.69917 -4.66980 H 5.38754 -0.14232 -3.07415 C -0.78450 1.35891 -1.96907 C -0.90173 2.46845 -1.09478 C -1.35357 1.51759 -3.25648 C -1.53051 3.66601 -1.48019 H -0.48749 2.37234 -0.07596 C -1.98205 2.71112 -3.66044 H -1.32535 0.66922 -3.96474 C -2.07290 3.79759 -2.77214 H -1.60122 4.50772 -0.76596 H -2.41429 2.79065 -4.67519 H -2.56829 4.73585 -3.08119	320	342 ⁴
B(C₆H₃Cl₂)₃  R = 	[(C ₆ H ₃ Cl ₂) ₃ BF] ⁻	53.4	1.449	B 0.00000 -0.00000 -1.44862 F 0.00000 0.00000 0.00000 C -0.78379 -1.35881 -1.96175 C -1.68134 -1.99751 -1.07273 C -0.62747 -1.92042 -3.25037 C -2.39453 -3.13554 -1.47284 H -1.80903 -1.59629 -0.05564 C -1.35726 -3.05806 -3.62970 H 0.08816 -1.48654 -3.96758 C -2.25554 -3.69076 -2.75602 H -2.81900 -4.58380 -3.05996 C 1.56902 -0.00000 -1.96076 C 2.56872 -0.46439 -1.07258 C 1.97996 0.42187 -3.24661 C 3.91141 -0.51348 -1.47073 C 3.33071 0.35847 -3.62393 H 1.24819 0.82951 -3.96289 C 4.32556 -0.10932 -2.75107 H 5.38115 -0.15078 -3.05338 C -0.78526 1.35802 -1.96198 C -0.88837 2.45557 -1.07386 C -1.35246 1.50204 -3.24957 C -1.51896 3.64146 -1.47377 H -0.47504 2.36681 -0.05751 C -1.97470 2.70198 -3.62862 H -1.33558 0.66479 -3.96616 C -2.07238 3.79703 -2.75581 H -2.56555 4.73080 -3.05951 CL -1.14164 -3.73616 -5.24860		

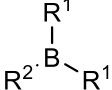
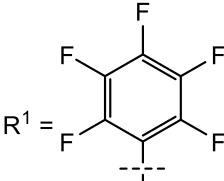
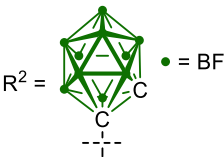
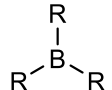
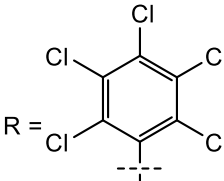
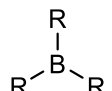
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BAr^F 	[Ar ^F ₃ BF] ⁻	53.7	1.450	B 0.00000 0.00000 -1.45036 F 0.00000 0.00000 0.00000 C -0.78346 -1.35594 -1.96016 C -1.65160 -2.02101 -1.06291 C -0.66480 -1.91121 -3.25273 C -2.37356 -3.16915 -1.43817 H -1.75178 -1.62241 -0.04074 C -1.39459 -3.05246 -3.64575 H 0.03391 -1.46210 -3.97918 C -2.25656 -3.68985 -2.73949 H -2.82367 -4.58241 -3.04012 C 1.56649 0.00000 -1.95843 C 2.57635 -0.40853 -1.05737 C 1.98814 0.37161 -3.25427 C 3.93197 -0.46527 -1.43321 C 3.34191 0.31698 -3.64373 H 1.24747 0.73109 -3.98844 C 4.32520 -0.10596 -2.73408 H 5.38260 -0.14886 -3.03249 C -0.78181 1.35725 -1.95923 C -0.92969 2.43882 -1.06161 C -1.31465 1.53398 -3.25583 C -1.55397 3.64280 -1.44165 H -0.54999 2.32045 -0.03392 C -1.93906 2.73445 -3.64918 H -1.25977 0.70958 -3.98667 C -2.05980 3.80166 -2.74289 H -2.54640 4.74042 -3.04453 C -1.28175 -3.55814 -5.06270 C -3.23053 -3.88925 -0.42664 C 3.75029 0.78138 -5.01993 C -1.63114 4.78696 -0.46084 C -2.54828 2.85843 -5.02382 F -2.04036 -2.82612 -5.92676 F -1.69324 -4.85010 -5.18894 F -0.00697 -3.49975 -5.52841 F -3.77553 -3.04600 0.48636 F -4.26046 -4.56504 -1.00989 F -2.51917 -4.81521 0.27874 F 3.97672 2.12537 -5.06127 F 2.79975 0.52242 -5.95426 F 4.90025 0.18753 -5.44487 F -0.46245 5.48591 -0.39642 F -2.59889 5.68824 -0.78836 F -1.89477 4.36416 0.80260 F -2.53480 4.14294 -5.47837 F -3.85267 2.46144 -5.04329 F -1.90081 2.10287 -5.94682 C 4.96358 -0.96891 -0.45400 F 6.21456 -0.50807 -0.73666 F 5.04894 -2.32988 -0.45494 F 4.68531 -0.60254 0.82326 H 2.28204 -0.67775 -0.03031	471 ^{2b} 482 ^{2c}	
B(OC₆F₅)₃ 	[(OC ₆ F ₅) ₃ BF] ⁻	54.9	1.385	B -0.00000 0.00000 -1.38498 F 0.00000 0.00000 0.00000 O 1.41004 0.00000 -1.90543 O -0.63265 -1.21328 -1.97101 O -0.77939 1.15867 -1.86513 C 2.47512 0.51896 -1.30940 C 3.71807 -0.15932 -1.45254 C 2.50042 1.72378 -0.55544 C 4.91045 0.33155 -0.90034 C 3.69148 2.21137 0.01257 C 4.90206 1.51988 -0.15066 C -0.03700 -2.40610 -1.92363 C 0.76518 -2.87091 -2.99786 C -0.19396 -3.27925 -0.81650 C 1.33905 -4.15291 -2.99138 C 0.37812 -4.56343 -0.80250 C 1.16809 -4.99574 -1.88025 C -1.02997 1.34967 -3.15961 C -2.24439 0.90640 -3.74612 C -0.12435 2.03772 -4.00846 C -2.55234 1.16294 -5.09265 C -0.42529 2.29705 -5.35667 C -1.63405 1.84353 -5.90970 F 3.75804 -1.30778 -2.14977 F 6.06369 -0.34446 -1.06681 F 6.04136 1.99491 0.39143 F 3.67475 3.36040 0.71497 F 1.38686 2.44805 -0.38544 F -0.94596 -2.90465 0.22789 F 0.19353 -5.37685 0.25548 F 1.72445 -6.22258 -1.86574	419	

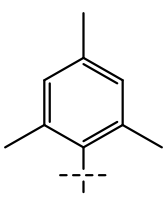
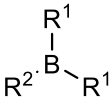
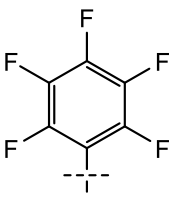
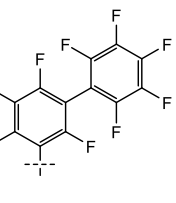
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B(C₁₀F₇)₃ 	[(C₁₀F₇)₃BF]⁻	58.8	1.423	B 0.00000 -0.00000 -1.42246 C -0.84212 -1.37394 -1.85305 C -0.35422 -2.61690 -1.45399 C -2.11345 -1.41328 -2.47238 C -1.02185 -3.86588 -1.64468 C -2.83426 -2.58610 -2.69931 C -0.49075 -5.12796 -1.23182 C -2.32030 -3.84678 -2.29689 C -1.19154 -6.30901 -1.44513 C -3.01103 -5.08057 -2.49883 C -2.46028 -6.28500 -2.08225 C 1.59221 0.00000 -1.94283 C 2.48663 0.89465 -1.35690 C 2.15246 -0.81836 -2.95368 C 3.87970 0.99047 -1.67380 C 3.49474 -0.78708 -3.32647 C 4.78018 1.90478 -1.04326 C 4.40423 0.10826 -2.70200 C 6.12426 1.95148 -1.39587 C 5.79028 0.18389 -3.03672 C 6.63223 1.08620 -2.39967 C -0.66441 1.40542 -2.01947 C -1.24714 2.40333 -1.24170 C -0.60045 1.69571 -3.40463 C -1.72988 3.65357 -1.75568 C -1.05078 2.87490 -3.98662 C -2.31284 4.67338 -0.94050 C -1.62484 3.89868 -3.18393 C -2.76674 5.86776 -1.49026 C -2.10012 5.13620 -3.71271 C -2.66064 6.10087 -2.88526 F 0.85124 -2.66411 -0.84761 F -2.71339 -0.27516 -2.87921 F -4.03812 -2.50067 -3.30078 F 0.70149 -5.22083 -0.62413 F -4.21467 -5.11169 -3.09752 F -3.11394 -7.44262 -2.27420 F -0.68468 -7.49033 -1.05355 F 0.00000 0.00000 0.00000 F 1.37855 -1.69373 -3.62546 F 3.91876 -1.61994 -4.29877 F 6.32159 -0.61473 -3.97909 F 7.93541 1.15318 -2.71880 F 6.96333 2.81219 -0.79486 F 4.36704 2.74785 -0.08495 F 2.02347 1.75318 -0.42625 F -0.08940 0.76752 -4.24250 F -1.39226 2.21464 0.08246 F -2.44430 4.52470 0.38660 F -3.31151 6.81871 -0.71201 F -3.10604 7.26402 -3.38883 F -2.02007 5.40546 -5.02803 F -0.94116 3.03155 -5.32171	469 ^{2b} 483 ^{2c}		
B(C₆F₅)₃ 	[(C₆F₅)₃BF]⁻	58.9	1.425	B -0.00000 -0.00000 -1.42506 F 0.00000 0.00000 0.00000 C 1.59352 -0.00000 -1.93791 C 2.48934 -0.89839 -1.32778 C 2.15644 0.79966 -2.94566 C 3.85611 -0.97995 -1.65399 C 3.51572 0.75389 -3.30879 C 4.37227 -0.14590 -2.65744 C -0.83701 1.37321 -1.86540 C -0.33264 2.62407 -1.46164 C -2.09202 1.42187 -2.49210 C -0.99858 3.84307 -1.67158 C -2.79960 2.61837 -2.72738 C -2.24841 3.83789 -2.31176 C -0.67651 -1.40705 -2.00794 C -1.30787 -2.36920 -1.19949 C -0.59450 -1.74290 -3.37027 C -1.80661 -3.58877 -1.70193 C -1.07828 -2.94233 -3.91807 C -1.68784 -3.87902 -3.06847 F 0.86416 2.70613 -0.84205 F -0.46078 5.01241 -1.27019 F -2.90930 4.99218 -2.52256 F -4.00349 2.60289 -3.33455 F -2.71806 0.29813 -2.91099 F -1.48901 -2.17564 0.12088 F -2.40249 -4.48032 -0.88372 F -2.16072 -5.03952 -3.56300 F -0.97038 -3.20480 -5.23628 F -0.04325 -0.87085 -4.24713	448 444 ^{2b} 452 ^{2c}		

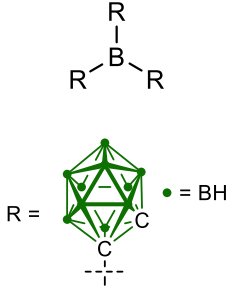
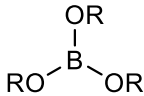
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$B(C_5F_4N)_3$ R =	$[(C_5F_4N)_3BF]^-$	59.4	1.427	B 0.00000 -0.00000 -1.42705 F 0.00000 0.00000 0.00000 C -0.79853 -1.37354 -1.91805 C -2.01237 -1.72452 -1.29702 C -0.36903 -2.29013 -2.89135 C -2.68048 -2.91396 -1.63653 C -1.10718 -3.45658 -3.16394 C 1.58802 -0.00000 -1.92061 C 2.50959 -0.85545 -1.28693 C 2.15775 0.82258 -2.90621 C 3.87360 -0.82693 -1.62567 C 3.53808 0.78052 -3.17660 C -0.79536 1.37109 -1.92931 C -0.56320 2.59470 -1.27256 C -1.74461 1.44861 -2.96166 C -1.27019 3.75460 -1.63614 C -2.40189 2.65747 -3.25385 N -2.23382 -3.76075 -2.54723 N 4.37455 -0.02319 -2.54717 N -2.17123 3.78186 -2.60200 F -0.66060 -4.31929 -4.09914 F 0.75688 -2.08181 -3.61005 F -2.58110 -0.92040 -0.37831 F -3.83920 -3.22421 -1.02034 F 1.40496 1.67400 -3.63851 F 2.10829 -1.74326 -0.35727 F 4.73156 -1.65582 -0.99692 F 4.05236 1.59222 -4.12269 F -2.04981 0.37211 -3.72078 F -3.31433 2.69259 -4.24619 F 0.35854 2.69886 -0.29648 F -1.02821 4.91036 -0.98480		
$B(C_2B_{10}H_{11})Ph_2$ R =	$[Ph_2(C_2B_{10}H_{11})BF]^-$	60.6	1.455	B -0.00000 0.00000 -1.45525 C 1.66987 -0.00000 -1.85905 B 2.60918 1.18774 -1.01557 B 2.51510 1.19264 -2.78171 B 2.46465 -1.54581 -1.90493 B 2.41374 -0.49099 -3.32820 C 2.65618 -0.46639 -0.60625 B 4.09306 1.43578 -1.97627 B 4.13455 0.37500 -0.54568 H 2.03612 1.95982 -0.28275 B 3.97310 0.38499 -3.42546 H 1.87756 2.06624 -3.32485 B 4.04441 -1.31866 -1.09988 B 3.93892 -1.32292 -2.88002 H 1.79645 -2.54057 -1.74777 H 1.70784 -0.80282 -4.26343 H 2.10369 -0.72127 0.30796 H 4.64719 2.52092 -1.97905 B 4.98179 -0.12425 -2.03793 H 4.61114 0.63268 0.54271 H 4.44637 0.70839 -4.50175 H 4.45806 -2.21426 -0.38944 H 4.38150 -2.24531 -3.54165 H 6.19927 -0.17802 -2.08126 C -0.77566 -1.36110 -1.95316 C -1.01583 -1.70904 -3.30512 C -1.29613 -2.24988 -0.97984 C -1.71686 -2.87297 -3.66834 H -0.64761 -1.05304 -4.11128 C -2.00265 -3.41597 -1.32646 H -1.13988 -2.00750 0.08490 C -2.21587 -3.73760 -2.67800 H -1.87650 -3.10617 -4.73652 H -2.39122 -4.08058 -0.53319 H -2.76808 -4.65228 -2.95828 C -0.75873 1.35418 -1.97886 C -1.39428 2.19500 -1.03278 C -0.88159 1.73629 -3.33752 C -2.11278 3.34347 -1.41260 H -1.31826 1.92962 0.03521 C -1.59601 2.88119 -3.73316 H -0.39639 1.12991 -4.12146 C -2.21934 3.69406 -2.76953 H -2.59398 3.97210 -0.64112 H -1.66295 3.14376 -4.80432 H -2.78128 4.59468 -3.07499 F 0.00000 0.00000 0.00000		
$B(C_6Cl_5)(C_6F_5)_2$ 	$[(C_6Cl_5)(C_6F_5)_2BF]^-$	63.2	1.430	B -0.00000 0.00000 -1.42968 F 0.00000 0.00000 0.00000 C 1.61864 0.00000 -1.82968 C 2.45085 -0.96028 -1.22422 C 2.28863 0.95005 -2.61639		

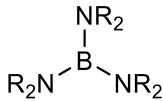
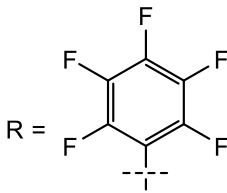
				C 3.84922 -0.98196 -1.36641 C 3.68584 0.97088 -2.78855 C 4.47240 -0.00346 -2.15684 C -0.79170 1.37424 -1.93672 C -0.53436 2.59372 -1.28200 C -1.76021 1.44293 -2.95022 C -1.20052 3.79479 -1.58190 C -2.45367 2.62122 -3.28852 C -2.17254 3.80657 -2.59474 C -0.81156 -1.38952 -1.92470 C -1.96273 -1.80807 -1.20891 C -0.43031 -2.24247 -2.98650 C -2.61009 -3.04650 -1.43655 C -1.04842 -3.49043 -3.24476 C -2.13363 -3.90613 -2.44733 CL -0.49926 -4.52391 -4.53884 CL -3.99971 -3.52781 -0.49787 CL -2.89501 -5.44818 -2.72719 CL 0.81601 -1.76157 -4.12782 CL -2.71253 -0.75506 -0.02479 F 1.91790 -1.94891 -0.47671 F 4.59701 -1.93031 -0.76750 F 5.81066 -0.00193 -2.30858 F 4.27691 1.91029 -3.55456 F 1.60993 1.90635 -3.29110 F 0.41613 2.67193 -0.32872 F -0.91150 4.93538 -0.92346 F -2.82194 4.94594 -2.90094 F -3.38086 2.62407 -4.26723 F -2.08624 0.35202 -3.68051		
$B(OTeF_5)_3$ 	$[(OTeF_5)_3BF]^-$	66.3	1.372	B 0.00000 0.00000 0.00000 B 0.00000 -0.00000 -1.37204 O 1.36491 0.00000 -1.98211 TE 2.77688 -1.22004 -1.48794 F 1.68869 -2.46390 -0.49705 F 3.21747 -0.29584 0.14363 F 4.02722 -0.11339 -2.44278 F 2.53847 -2.28097 -3.07751 F 4.26421 -2.37734 -1.08701 O -0.67560 -1.18396 -1.98673 TE -2.44698 -1.81094 -1.54753 F -3.24968 -0.90669 -3.04665 F -2.95435 -0.35038 -0.39692 F -1.86689 -2.81965 -0.01231 F -2.13650 -3.34771 -2.66213 F -4.19852 -2.54104 -1.21200 O -0.68761 1.17900 -1.98275 TE -0.26823 3.02356 -1.59581 F 1.36178 2.71135 -0.61513 F -1.25974 3.06067 0.05575 F -1.85520 3.54994 -2.54693 F 0.74707 3.22896 -3.21903 F 0.05140 4.90211 -1.30631		550 ^{2b}
$B(C_2B_{10}H_{11})_2Ph$ 	$[Ph(C_2B_{10}H_{11})_2BF]^-$	66.5	1.440	B 0.00000 0.00000 -1.43945 C 1.65081 -0.00000 -1.88784 B 2.73770 -0.76150 -0.75623 B 2.71443 1.00168 -0.95535 B 2.19526 -0.16940 -3.51758 B 2.39868 1.36716 -2.66034 C 2.50559 -1.35605 -2.33282 B 4.27639 0.12927 -0.84983 B 4.09300 -1.41208 -1.72565 H 2.26794 -1.36791 0.17512 B 4.06791 1.45003 -2.04007 H 2.23388 1.68291 -0.07692 B 3.75751 -1.04895 -3.44073 B 3.73968 0.72041 -3.64493 H 1.37989 -0.40225 -4.37807 H 1.70851 2.30911 -2.96913 H 1.91524 -2.27574 -2.41872 H 4.99020 0.21752 0.13281 B 4.91642 -0.04688 -2.52383 H 4.54663 -2.49448 -1.41199 H 4.63227 2.52345 -1.92221 H 3.98344 -1.88176 -4.29552 H 4.05927 1.23899 -4.69928 H 6.11029 -0.09165 -2.76430 C -0.92942 -1.40160 -1.84276 B -0.37841 -2.95162 -1.27812 B -0.66078 -2.65134 -3.00414 B -2.62970 -1.18881 -1.51844 B -2.05013 -1.56385 -3.14984 C -1.63059 -2.11415 -0.50022 B -1.20934 -4.18442 -2.25950 B -1.80289 -3.80491 -0.62175 H 0.69403 -3.01919 -0.72680 B -2.26248 -3.31866 -3.42584 H 0.27395 -2.55310 -3.76667		

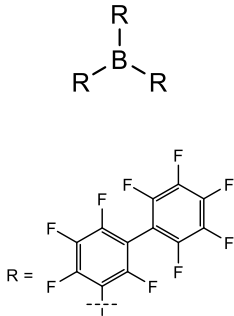
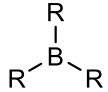
				B -3.20053 -2.70932 -0.77005 B -3.49244 -2.40114 -2.49996 H -3.00632 -0.10588 -1.13967 H -2.08316 -0.70488 -3.99985 H -1.34649 -1.62888 0.44235 H -0.65859 -5.24145 -2.50751 B -2.97344 -4.03180 -1.94924 H -1.65099 -4.47159 0.38213 H -2.48124 -3.75142 -4.54323 H -4.00809 -2.62898 0.13374 H -4.60731 -2.16141 -2.92582 H -3.72133 -4.99329 -1.96601 C -0.72545 1.36348 -1.97000 C -1.19898 2.29556 -1.01606 C -0.91746 1.69968 -3.33161 C -1.83698 3.49121 -1.39313 H -1.05862 2.07108 0.05438 C -1.55694 2.88858 -3.72321 H -0.54499 1.02329 -4.11834 C -2.02345 3.79276 -2.75270 H -2.19122 4.19380 -0.61767 H -1.68654 3.11363 -4.79646 H -2.52484 4.72880 -3.05574 F 0.00000 0.00000 0.00000		
$B(OTf)_3$ $R =$	$[(OTf)_3BF]^-$	66.7	1.365	B -0.00000 0.00000 -1.36530 F 0.00000 0.00000 0.00000 O -0.69061 -1.18764 -1.97184 O -0.69701 1.20114 -1.94872 S -2.12465 -1.75347 -1.54221 S -0.27504 2.72258 -1.70225 O -1.48762 3.53183 -1.51663 O -2.74951 -2.35705 -2.72812 O -2.87110 -0.84846 -0.65461 C -1.59092 -3.22728 -0.47153 C 0.32870 3.14756 -3.45003 O 0.89117 2.87055 -0.81596 F -0.83737 -4.07912 -1.17840 F -0.91982 -2.82864 0.61142 F -2.71031 -3.87062 -0.07469 F 1.39562 2.41911 -3.79213 F 0.67114 4.45223 -3.46686 F -0.64718 2.95021 -4.34970 O 1.38076 0.00000 -1.96408 S 2.55735 -1.00673 -1.56658 O 3.41902 -1.19129 -2.74301 O 2.09752 -2.15100 -0.76273 C 3.56575 0.09535 -0.39450 F 4.65572 -0.60486 -0.01294 F 3.97076 1.20650 -1.02282 F 2.86671 0.42588 0.69321	565	
$B(C_6Cl_5)_2(C_6F_5)$ $R^1 =$ $R^2 =$	$[(C_6Cl_5)_2(C_6F_5)BF]^-$	66.8	1.429	B -0.00000 -0.00000 -1.42847 F 0.00000 0.00000 0.00000 C -0.76913 -1.40877 -1.87006 C -1.93294 -1.79436 -1.17698 C -0.31044 -2.33915 -2.81636 C -2.59637 -3.01551 -1.38874 C -0.94027 -3.57327 -3.06445 C -2.09170 -3.91526 -2.34058 C 1.60193 -0.00000 -1.94388 C 2.56035 -0.77036 -1.23585 C 2.12027 0.73766 -3.03369 C 3.94910 -0.71910 -1.50731 C 3.50112 0.81564 -3.33716 C 4.42597 0.09747 -2.55301 C -0.83417 1.41611 -1.81457 C -0.47960 2.60259 -1.11921 C -1.97157 1.53452 -2.64856 C -1.24453 3.79183 -1.16837 C -2.77119 2.70258 -2.71335 C -2.41447 3.83500 -1.95422 CL -4.19045 2.77409 -3.72602 CL -0.76632 5.21355 -0.27815 CL 4.08289 1.78124 -4.66837 CL 2.06246 -1.91251 -0.00265 CL 5.08793 -1.66126 -0.58034 CL 1.04795 1.57725 -4.13999 CL 6.13254 0.19593 -2.88970 CL -3.39124 5.27662 -2.00526 CL -2.42288 0.25036 -3.75792 CL 1.00011 2.67771 -0.18317 F -2.50331 -0.96455 -0.28076 F -3.71396 -3.32882 -0.70321 F -2.71024 -5.09094 -2.56051 F -0.45243 -4.42868 -3.98507 F 0.77861 -2.08371 -3.57590		
$B(C_2B_{10}F_{11})(C_6F_5)_2$	$[(C_2B_{10}F_{11})(C_6F_5)_2BF]^-$	69.9	1.403	B -0.00000 -0.00000 -1.40260 C -0.81581 -1.58182 -1.74674 B -1.90503 -2.09918 -0.41777 B -0.37414 -2.94900 -0.75555		

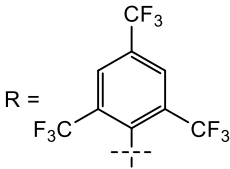
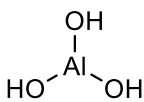
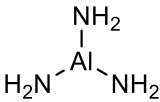
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$B(C_6Cl_5)_3$  	$[(C_6Cl_5)_3BF]^-$	70.2	1.428	B 0.00000 0.00000 -1.42747 F 0.00000 0.00000 0.00000 C 1.63199 0.00000 -1.85057 C 2.52249 -0.82884 -1.11755 C 2.25478 0.85435 -2.79180 C 3.93080 -0.74774 -1.23269 C 3.65933 0.96893 -2.93073 C 4.50533 0.17524 -2.13033 C -0.81735 1.41238 -1.85202 C -0.55114 2.59773 -1.11640 C -1.86562 1.52299 -2.79682 C -1.33019 3.77384 -1.23087 C -2.67131 2.67908 -2.93582 C -2.41436 3.80754 -2.13156 C -0.81625 -1.41294 -1.85174 C -1.97943 -1.77036 -1.11937 C -0.38821 -2.37804 -2.79464 C -2.61414 -3.02998 -1.23691 C -0.99177 -3.65115 -2.93583 C -2.10261 -3.98764 -2.13633 CL 4.36826 2.07303 -4.08042 CL 4.97657 -1.77736 -0.28987 CL -0.39028 -4.81551 -4.08730 CL -4.02896 -3.42170 -0.29487 CL -3.97808 2.73848 -4.08999 CL 0.83801 2.69877 -0.05328 CL -0.97008 5.19349 -0.28349 CL -2.18530 0.23315 -3.94097 CL 1.30108 1.78525 -3.93134 CL 6.23635 0.31406 -2.26744 CL 1.91119 -2.08266 -0.05712 CL -3.40588 5.23331 -2.26801 CL -2.84922 -5.55519 -2.27696 CL 0.89470 -2.01585 -3.93391 CL -2.75888 -0.61573 -0.05653		
$B[C_6H_2(CH_3)_3]_3$ 	$\{[(CH_3)_3C_6H_2]_3BF\}^-$	71.0	1.474	B -0.00000 0.00000 -1.47406 F 0.00000 0.00000 0.00000 C 1.63288 0.00000 -1.88102 C 2.51454 -0.85545 -1.13514 C 2.25230 0.80847 -2.88669 C 3.90621 -0.85938 -1.37265 C 3.65153 0.78000 -3.09289 C 4.50830 -0.03731 -2.34031 H 4.54356 -1.54327 -0.77943 H 4.08438 1.42098 -3.88477 C -0.81824 1.41341 -1.88036 C -0.52319 2.60344 -1.13094		

R = 				C -1.82748 1.54524 -2.88698 C -1.22127 3.80832 -1.36403 C -2.50776 2.76885 -3.08905 C -2.23458 3.91768 -2.33126 H -0.95207 4.70128 -0.76737 H -3.27873 2.82289 -3.88154 C -0.81561 -1.41442 -1.88214 C -1.99481 -1.75365 -1.13431 C -0.42623 -2.35266 -2.89084 C -2.69185 -2.95840 -1.37130 C -1.14847 -3.55123 -3.09696 C -2.28153 -3.88853 -2.34117 H -3.60054 -3.17136 -0.77570 H -0.81089 -4.24434 -3.89133 C -2.58569 -0.83938 -0.07247 H -1.97957 -0.85105 0.85732 H -2.60400 0.21964 -0.40632 H -3.62692 -1.15025 0.17493 C 0.75469 -2.13201 -3.82346 H 0.77555 -1.10610 -4.24738 H 1.73089 -2.26461 -3.30757 H 0.71856 -2.85100 -4.67368 C -3.01780 -5.19566 -2.54868 H -2.66268 -5.98958 -1.84729 H -4.11275 -5.08340 -2.37679 H -2.87387 -5.58858 -3.58061 C -2.22587 0.41341 -3.82127 H -1.34724 -0.11464 -4.24780 H -2.82634 -0.36810 -3.30611 H -2.83259 0.80479 -4.66966 C 0.56641 2.65852 -0.07162 H 0.25575 2.13885 0.85868 H 1.49245 2.14581 -0.40769 H 0.81729 3.71580 0.17573 C -3.00220 5.20744 -2.53392 H -3.85992 5.29760 -1.82357 H -2.35699 6.10094 -2.37114 H -3.42545 5.27595 -3.56158 C 2.01607 -1.82533 -0.07528 H 1.72369 -1.29550 0.85518 H 1.10729 -2.36860 -0.41041 H 2.80448 -2.57339 0.17133 C 1.47253 1.72569 -3.81586 H 2.11449 2.05766 -4.66370 H 0.57396 1.23318 -4.24337 H 1.09883 2.63498 -3.29610 C 6.00840 -0.02607 -2.54872 H 6.52532 0.64302 -1.81840 H 6.45023 -1.04076 -2.42019 H 6.27823 0.33595 -3.56650		
B(C₆F₅)₂(C₁₂F₉)  R¹ =  R² = 	[(C₆F₅)₂(C₁₂F₉)BF]⁻	71.5	1.436	B 0.00000 0.00000 -1.43571 C -0.88510 1.33807 -1.87598 C -0.40583 2.48109 -2.53507 C -2.22468 1.42147 -1.45079 C -1.19231 3.62472 -2.78075 C -3.04857 2.53806 -1.67032 C -2.52343 3.65323 -2.34295 C 1.56342 0.00000 -1.99524 C 2.71490 0.05560 -1.15987 C 1.80450 -0.16471 -3.36885 C 4.00750 -0.05829 -1.71488 C 3.08486 -0.27693 -3.93217 C 4.20596 -0.23285 -3.09046 C -0.68546 -1.44010 -1.93948 C -0.28128 -2.63418 -1.31257 C -1.63799 -1.60358 -2.95936 C -0.80067 -3.90147 -1.63652 C -2.18491 -2.84944 -3.32123 C -1.76104 -4.00834 -2.65410 C 2.65874 0.24891 0.32151 C 2.23983 1.46224 0.89793 C 3.07264 -0.77077 1.19778 C 2.20218 1.64920 2.28876 C 3.05137 -0.60738 2.59304 C 2.61468 0.60991 3.13928 F 0.66225 -2.61877 -0.34782 F -2.09668 -0.54553 -3.66322 F -3.10438 -2.94499 -4.30216 F -2.26976 -5.20976 -2.98617 F -0.38005 -5.01049 -0.99689 F 0.00000 0.00000 0.00000 F 5.10475 0.00352 -0.92715 F 5.44671 -0.33910 -3.60174 F 3.25197 -0.43176 -5.25782 F 0.76864 -0.20699 -4.23848 F 1.85113 2.48008 0.11865 F 3.49832 -1.94611 0.71102 F 3.44948 -1.60072 3.40621 F 2.59372 0.78131 4.47107 F 1.79035 2.81529 2.81357		

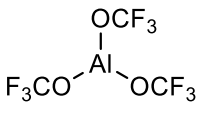
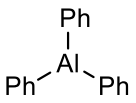
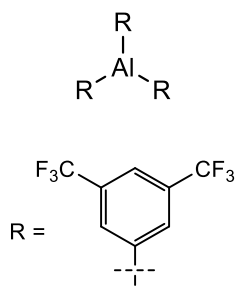
				F 0.86866 2.55895 -2.97914 F -0.67772 4.69334 -3.42094 F -3.29081 4.73686 -2.56419 F -4.32847 2.55579 -1.24871 F -2.79722 0.38443 -0.80285		
$B(C_2B_{10}H_{11})_3$ 	$[(C_2B_{10}H_{11})_3BF]^-$	71.9	1.420	B -0.00000 0.00000 -1.41977 C -0.84707 1.47797 -1.83700 B -0.07206 3.06583 -1.95057 B -1.11137 2.66837 -0.58026 B -2.20280 1.42633 -2.93139 B -2.43804 1.65966 -1.17752 C -0.81792 2.32962 -3.28469 B -1.23463 4.26935 -1.37472 B -1.00324 4.02543 -3.12368 H 1.11405 3.19449 -1.93121 B -2.71783 3.39752 -0.89678 H -0.61715 2.47185 0.50610 B -2.32806 3.01110 -3.72642 B -3.39737 2.60790 -2.35487 H -2.38482 0.44300 -3.58757 H -2.86423 0.77602 -0.47755 H -0.15382 1.91618 -4.05650 H -0.82854 5.27250 -0.81795 B -2.65280 4.23719 -2.47418 H -0.37594 4.73588 -3.88268 H -3.42286 3.76698 0.02483 H -2.62488 3.01862 -4.90361 H -4.58403 2.39517 -2.51785 H -3.29978 5.23630 -2.73203 C -0.89299 -1.47591 -1.83252 B -0.09813 -2.79598 -2.65815 B -1.55332 -2.07664 -3.33020 B -1.83715 -2.09814 -0.47245 B -2.63941 -1.67170 -1.98756 C -0.37884 -2.81370 -0.97278 B -1.33601 -3.86034 -3.33221 B -0.52682 -4.29907 -1.80289 H 0.99542 -2.64026 -3.11075 B -2.92400 -3.16006 -2.92039 H -1.44691 -1.38870 -4.32136 B -1.60984 -3.87354 -0.45804 B -3.09271 -3.16992 -1.13796 H -1.86838 -1.45968 0.54844 H -3.37474 -0.72610 -2.01297 H 0.48358 -2.63453 -0.31924 H -1.10477 -4.46211 -4.36433 B -2.28618 -4.53787 -1.97181 H 0.34974 -5.12551 -1.65097 H -3.88576 -3.24755 -3.66196 H -1.47944 -4.41294 0.62218 H -4.16300 -3.25855 -0.56581 H -2.76764 -5.65603 -2.00636 C 1.72135 0.00000 -1.78878 B 2.55870 1.32705 -1.00819 B 2.55297 1.14364 -2.78429 B 2.69902 -1.45618 -1.60783 B 2.62038 -0.58037 -3.15294 C 2.72475 -0.24954 -0.42969 B 4.05122 1.62361 -1.93945 B 4.12569 0.72285 -0.40592 H 1.92762 2.08687 -0.32515 B 4.10309 0.41894 -3.26979 H 1.91471 1.87399 -3.49883 B 4.20968 -1.01096 -0.77664 B 4.18589 -1.21494 -2.54698 H 2.21158 -2.51476 -1.32691 H 2.00832 -1.02098 -4.09819 H 2.16851 -0.45663 0.49376 H 4.49456 2.75193 -2.03973 B 5.08259 0.15725 -1.80286 H 4.50714 1.14430 0.66670 H 4.58645 0.67508 -4.35733 H 4.64480 -1.79973 0.03757 H 4.72743 -2.16289 -3.08362 H 6.29877 0.21007 -1.79230 F 0.00000 0.00000 0.00000		
$B[OC(CF_3)_3]_3$ 	$\{[OC(CF_3)_3]_3BF\}^-$	71.9	1.390	B 0.00000 -0.00000 -1.39032 F 0.00000 0.00000 0.00000 O -0.68207 -1.18729 -1.96703 O -0.67798 1.19908 -1.95237 O 1.38240 -0.00000 -1.94180 C -1.93719 -1.71659 -1.94415 C 2.37219 -0.93158 -2.01522 C -0.50916 2.54686 -1.83662 C 0.96742 3.03316 -1.54816 C -1.45237 3.12976 -0.70318 C -0.96539 3.14020 -3.23201 C -2.26591 -2.13346 -3.43483 C -1.93217 -3.01560 -1.03542 C -3.08863 -0.76340 -1.43204	423	

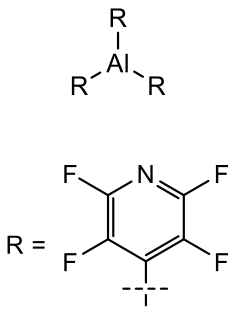
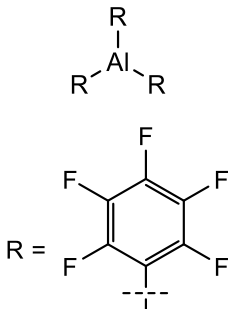
$R = \begin{array}{c} \text{CF}_3 \\ \\ \text{F}_3\text{C}-\text{C}-\text{CF}_3 \\ \\ - \end{array}$				C 2.61798 -1.73876 -0.68152 C 2.12720 -1.96216 -3.20360 C 3.68167 -0.10502 -2.34873 F -2.66421 2.55657 -0.74997 F -1.63741 4.47178 -0.82653 F -0.93817 2.90643 0.52344 F -0.65623 4.45360 -3.37632 F -2.30352 3.02608 -3.38179 F -0.38458 2.47273 -4.23950 F 1.76000 2.83622 -2.61956 F 0.99674 4.36726 -1.27166 F 1.50256 2.40353 -0.49595 F -2.75483 -0.16346 -0.28308 F -3.38584 0.18219 -2.34252 F -4.23338 -1.46529 -1.19993 F -1.99831 -1.12429 -4.27550 F -3.56597 -2.48370 -3.60975 F -1.51356 -3.19163 -3.80962 F -0.81717 -3.73200 -1.23430 F -2.98922 -3.83147 -1.28973 F -1.98078 -2.68810 0.27394 F 3.29882 -2.46169 -3.68886 F 1.49676 -1.35517 -4.21801 F 1.38917 -3.01990 -2.81852 F 3.52941 -2.73268 -0.87080 F 3.10130 -0.93005 0.28588 F 1.49802 -2.30868 -0.22083 F 3.80369 0.94866 -1.52684 F 3.62870 0.36435 -3.61428 F 4.81746 -0.83729 -2.23372		
$\text{B}[\text{N}(\text{C}_6\text{F}_5)_2]_3$   $R = \text{C}_6\text{F}_5$	$\{[\text{N}(\text{C}_6\text{F}_5)_2]_3\text{BF}\}^-$	80.4	1.410	B -0.00000 0.00000 -1.40995 F 0.00000 0.00000 0.00000 N -0.83128 -1.20733 -2.00151 N -0.76594 1.35602 -1.78682 N 1.52533 0.00000 -1.85968 C -2.22222 -1.25227 -1.70530 C -2.76355 -1.38639 -0.40194 C -3.15578 -1.22263 -2.77279 C -4.15315 -1.36424 -0.18084 C -4.54320 -1.22718 -2.56775 C -5.04739 -1.30382 -1.26003 C -0.39408 -2.36308 -2.68288 C -0.63855 -3.66053 -2.15326 C 0.25399 -2.32827 -3.94332 C -0.26340 -4.83565 -2.82406 C 0.67297 -3.49379 -4.60727 C 0.40143 -4.75701 -4.05814 C -0.82870 2.42481 -0.85496 C -1.43481 2.33972 0.42701 C -0.32731 3.70325 -1.21394 C -1.41074 3.41854 1.32953 C -0.32995 4.80043 -0.33809 C -0.88099 4.66007 0.94485 C -1.56544 1.56519 -2.93332 C -2.95677 1.82562 -2.79495 C -1.07440 1.56481 -4.26279 C -3.80732 2.04242 -3.88870 C -1.92011 1.75300 -5.37141 C -3.28521 2.01762 -5.19128 C 2.33862 -1.14117 -2.03595 C 3.36916 -1.12614 -3.01573 C 2.25334 -2.32462 -1.25573 C 4.21507 -2.22256 -3.24503 C 3.06311 -3.44696 -1.50445 C 4.07157 -3.39098 -2.47899 C 2.28429 1.09935 -1.34929 C 2.60027 2.24810 -2.11429 C 2.81267 1.05704 -0.03070 C 3.31025 3.33253 -1.56336 C 3.53426 2.12544 0.52589 C 3.78869 3.27003 -0.24676 F -1.98605 -1.56304 0.66167 F -4.63462 -1.47846 1.06787 F -6.37179 -1.30725 -1.04442 F -5.38581 -1.14919 -3.61178 F -2.71266 -1.15280 -4.04023 F -1.40664 1.74184 -6.61268 F -4.08653 2.21843 -6.24949 F -5.12039 2.25241 -3.69397 F -3.51848 1.81695 -1.57261 F 0.21888 1.38615 -4.51565 F 3.54469 -0.03938 -3.78039 F 5.16561 -2.15914 -4.19285 F 4.87088 -4.44811 -2.69507 F 2.91897 -4.55653 -0.76039 F 1.35437 -2.43223 -0.27179 F -1.23821 -3.79843 -0.96183 F 0.50125 -1.16084 -4.54290 F 1.29129 -3.40473 -5.79599 F 0.77572 -5.87390 -4.70143	368	

				F -0.51644 -6.03678 -2.27847 F 2.25206 2.34957 -3.39283 F 3.57957 4.41129 -2.31618 F 4.48300 4.29423 0.27170 F 4.00374 2.05185 1.78313 F 2.64449 -0.03027 0.72872 F 0.20379 3.88884 -2.43389 F -2.08463 1.24643 0.82722 F -1.98006 3.29306 2.54027 F -0.89045 5.69694 1.79771 F 0.18711 5.97990 -0.72211		
B(C₁₂F₉)₃ 	[(C ₁₂ F ₉) ₃ BF] ⁻	82.9	1.444	B -0.00000 0.00000 -1.44437 C -0.79617 1.38455 -1.90932 C -0.57779 1.94127 -3.17916 C -1.72505 2.08305 -1.07189 C -1.23331 3.08355 -3.66615 C -2.40282 3.21985 -1.56531 C -2.16534 3.73249 -2.84814 C 1.60195 -0.00000 -1.91545 C 2.55341 0.84170 -1.26933 C 2.12116 -0.83415 -2.92018 C 3.91415 0.82023 -1.63037 C 3.47950 -0.86765 -3.28713 C 4.39247 -0.02884 -2.63743 C -0.80337 -1.39461 -1.91461 C -0.42581 -2.55860 -1.21518 C -1.85479 -1.56709 -2.86350 C -1.04990 -3.80846 -1.36958 C -2.48396 -2.81905 -3.02596 C -2.10141 -3.94350 -2.28439 C 2.21415 1.81000 -0.17928 C 1.97927 3.16509 -0.47112 C 2.26453 1.43712 1.17638 C 1.77704 4.12049 0.53869 C 2.04984 2.37033 2.20450 C 1.81659 3.71826 1.88297 F 0.60827 -2.53961 -0.34853 F -3.48196 -2.97113 -3.92652 F -2.71705 -5.12751 -2.45280 F -0.64241 -4.87559 -0.66071 F 0.00000 0.00000 0.00000 F 4.80384 1.62724 -1.01032 F 5.69497 -0.04226 -2.97203 F 3.90908 -1.69470 -4.25592 F 1.32867 -1.67540 -3.61887 F 1.95458 3.58191 -1.74821 F 2.53916 0.17449 1.51913 F 2.09334 1.99217 3.49234 F 1.62654 4.61676 2.85887 F 1.55263 5.40661 0.23088 F 0.28459 1.35899 -4.04707 F -0.99207 3.54558 -4.90472 F -2.82232 4.81733 -3.28839 F -3.30882 3.86847 -0.80369 C -2.35193 -0.52326 -3.82151 C -1.77105 -0.40320 -5.10016 C -3.49805 0.25470 -3.56725 C -2.24922 0.51087 -6.05478 C -3.99523 1.17665 -4.50371 C -3.37019 1.30084 -5.75528 C -2.00867 1.75671 0.36447 C -2.59894 0.55676 0.80766 C -1.72619 2.71685 1.35821 C -2.85290 0.30588 2.16664 C -1.97329 2.49574 2.72254 C -2.54596 1.28071 3.12908 F -2.92896 -0.40368 -0.05877 F -3.40612 -0.85482 2.54998 F -2.79672 1.05226 4.42630 F -1.67575 3.43727 3.63154 F -1.18404 3.90134 1.01880 F -4.15225 0.14049 -2.40411 F -5.07141 1.92655 -4.21832 F -3.84102 2.17208 -6.65761 F -1.65975 0.61601 -7.25480 F -0.73452 -1.17508 -5.44445	447 ^{2b} 431 ^{2c}	
B[C₆H₂(CF₃)₃]₃ 	{[C ₆ H ₂ (CF ₃) ₃ BF] ⁻	85.9	1.441	B -0.00000 -0.00000 -1.44059 F 0.00000 0.00000 0.00000 C -0.82981 1.43996 -1.80361 C -0.57434 2.59358 -0.98043 C -1.89379 1.62474 -2.74690 C -1.32851 3.77720 -1.07977 C -2.64542 2.81347 -2.83366 C -2.37548 3.89539 -1.99703 H -1.08615 4.62822 -0.42946 H -3.45388 2.89265 -3.57127 C -0.83094 -1.43990 -1.80046 C -1.95559 -1.79419 -0.97547 C -0.45672 -2.45782 -2.73939 C -2.59738 -3.04384 -1.06394		

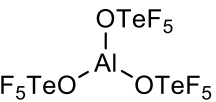
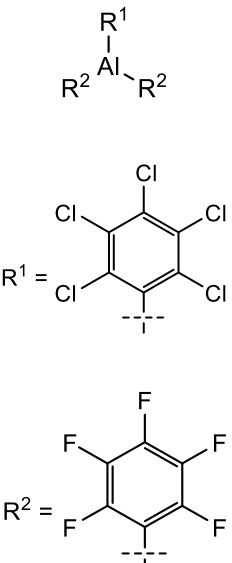
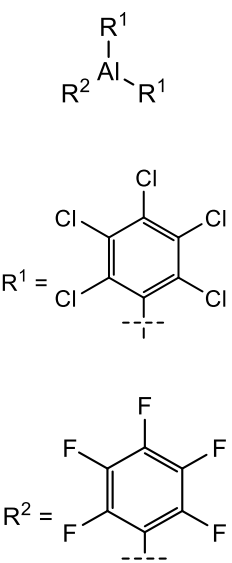
				C -1.10476 -3.70599 -2.81678 C -2.17293 -4.01383 -1.97409 H -3.45337 -3.25935 -0.41125 H -0.76810 -4.44786 -3.55226 C 1.66241 -0.00000 -1.80187 C 2.53272 -0.79555 -0.97681 C 2.35550 0.83129 -2.74362 C 3.93587 -0.72742 -1.06829 C 3.76025 0.89302 -2.82383 C 4.56237 0.12288 -1.98141 H 4.55127 -1.36027 -0.41579 H 4.23321 1.55360 -3.56185 C 2.09842 -1.76446 0.13572 C 1.69436 1.81614 -3.70733 C 6.06374 0.23778 -2.02321 C 0.72776 -2.38018 -3.70205 C -2.57881 -0.93109 0.13431 C -2.82367 -5.37186 -2.00999 C 0.47848 2.69964 0.13570 C -2.42085 0.55721 -3.70505 C -3.20302 5.15309 -2.04530 F 6.51684 0.60555 -3.25118 F 6.53104 1.16973 -1.14521 F 6.67687 -0.93226 -1.70222 F 2.00227 -1.14506 1.33465 F 3.05247 -2.74211 0.30787 F 0.95636 -2.43874 -0.08678 F -2.71132 -5.96408 -3.22848 F -4.14888 -5.31338 -1.71207 F -2.26585 -6.23086 -1.11073 F -3.90296 -1.26759 0.30476 F -2.59056 0.39474 -0.09071 F -1.99649 -1.15557 1.33473 F 0.56833 -3.23500 -4.75968 F 0.94430 -1.17207 -4.25074 F 1.88634 -2.76889 -3.09607 F -3.33862 -0.24726 -3.09589 F -3.08010 1.11920 -4.76541 F -1.48420 -0.23858 -4.25014 F -3.93063 5.25137 -3.18830 F -4.08850 5.22207 -1.01174 F -2.43384 6.27231 -1.96177 F 1.63422 2.04874 -0.08688 F -0.01240 2.30299 1.33217 F 0.84742 4.01427 0.31298 F 1.44836 3.01372 -3.10274 F 2.51416 2.10698 -4.76471 F 0.54128 1.39591 -4.25638		
AlH_3 	$[\text{H}_3\text{AlF}]^-$	24.8	1.738	AL 0.00000 -0.00000 -1.73789 H -0.78517 1.35996 -2.29156 H -0.78519 -1.35997 -2.29154 H 1.57036 -0.00000 -2.29154 F 0.00000 0.00000 0.00000	384	
AlF_3 	$[\text{AlF}_4]^-$	29.6	1.711	AL 0.00000 0.00000 -1.71068 F 0.00000 0.00000 0.00000 F 1.61284 0.00000 -2.28090 F -0.80642 -1.39676 -2.28090 F -0.80642 1.39676 -2.28090	484	467 ^{2b} 482 ^{2c}
$\text{Al}(\text{OH})_3$ 	$[(\text{OH})_3\text{AlF}]^-$	31.1	1.732	AL 0.00000 0.00000 -1.73165 F 0.00000 0.00000 0.00000 O 1.73005 0.00000 -2.20673 H 2.26201 0.36536 -1.47300 O -0.71574 -1.46232 -2.47122 H 0.02461 -2.05963 -2.69735 O -0.96127 1.40508 -2.26572 H -1.44667 1.14817 -3.07374	377	
$\text{Al}(\text{NH}_2)_3$ 	$[(\text{NH}_2)_3\text{AlF}]^-$	32.2	1.752	AL 0.00000 0.00000 -1.75170 F 0.00000 0.00000 0.00000 N 1.77456 0.00000 -2.37706 H 2.48393 0.23255 -1.66394 H 2.03921 -0.92498 -2.75122 N -0.88644 -1.53514 -2.38136 H -1.01882 -2.27777 -1.67648 H -1.82899 -1.30597 -2.73444 N -0.88742 1.53640 -2.37781 H -1.45318 2.02618 -1.66644 H -0.21613 2.23381 -2.73657	316	
$\text{Al}(\text{CN})_3$	$[(\text{NC})_3\text{AlF}]^-$	33.4	1.702	F 0.00000 0.00000 0.00000 C -0.93288 1.61633 -2.39666 C 1.86623 -0.00000 -2.39663 C -0.93323 -1.61607 -2.39668 N -1.48551 -2.57244 -2.80113 N 2.97074 0.00018 -2.80077		

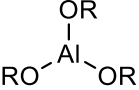
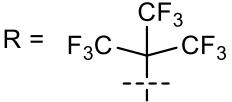
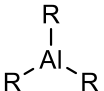
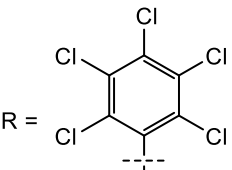
$\begin{array}{c} \text{CN} \\ \\ \text{NC}-\text{Al}-\text{CN} \end{array}$				N -1.48485 2.57303 -2.80082 AL -0.00000 -0.00000 -1.70221		
$\text{Al}(\text{C}\equiv\text{CH})_3$ $\begin{array}{c} \text{CCH} \\ \\ \text{HCC}-\text{Al}-\text{CCH} \end{array}$	$[(\text{HC}\equiv\text{C})_3\text{AlF}]^-$	33.5	1.718	AL -0.00000 -0.00000 -1.71754 F 0.00000 0.00000 0.00000 C 1.87082 0.00000 -2.37959 C -0.93546 -1.62015 -2.37960 C -0.93545 1.62015 -2.37960 C -1.51868 2.63041 -2.78993 H -2.02940 3.51510 -3.15096 C 3.03727 0.00000 -2.79012 H 4.05873 0.00001 -3.15135 C -1.51868 -2.63041 -2.78993 H -2.02940 -3.51510 -3.15096	448	
$\text{Al}(\text{CH}_3)_3$ $\begin{array}{c} \text{CH}_3 \\ \\ \text{H}_3\text{C}-\text{Al}-\text{CH}_3 \end{array}$	$[(\text{CH}_3)_3\text{AlF}]^-$	34.1	1.747	AL -0.00000 -0.00000 -1.74668 F 0.00000 0.00000 0.00000 C 1.93161 -0.00000 -2.39536 H 2.50005 -0.89701 -2.04138 H 2.00529 0.00000 -3.51263 H 2.50005 0.89700 -2.04138 C -0.96598 -1.67280 -2.39510 H -2.02722 -1.71568 -2.04161 H -1.00221 -1.73750 -3.51233 H -0.47402 -2.61348 -2.03995 C -0.96598 1.67281 -2.39510 H -1.00222 1.73751 -3.51232 H -2.02722 1.71568 -2.04160 H -0.47402 2.61348 -2.03995	369	
AlCl_3 $\begin{array}{c} \text{Cl} \\ \\ \text{Cl}-\text{Al}-\text{Cl} \end{array}$	$[\text{Cl}_3\text{AlF}]^-$	34.5	1.702	AL 0.00000 0.00000 -1.70213 F 0.00000 0.00000 0.00000 CL 2.06148 0.00000 -2.42115 CL -1.03074 -1.78529 -2.42115 CL -1.03074 1.78529 -2.42115	505	502 ^{2c}
$\text{Al}(\text{SH})_3$ $\begin{array}{c} \text{SH} \\ \\ \text{HS}-\text{Al}-\text{SH} \end{array}$	$[(\text{SH})_3\text{AlF}]^-$	35.4	1.715	AL -0.00000 0.00000 -1.71487 F 0.00000 0.00000 0.00000 S -1.07905 1.92598 -2.32952 H -1.15180 1.55870 -3.64737 S 2.09369 0.00000 -2.63330 H 2.28697 -1.33590 -2.38806 S -0.98385 -1.92708 -2.47869 H -2.02838 -1.86140 -1.59184	445	
AlBr_3 $\begin{array}{c} \text{Br} \\ \\ \text{Br}-\text{Al}-\text{Br} \end{array}$	$[\text{Br}_3\text{AlF}]^-$	35.6	1.701	AL 0.00000 0.00000 -1.70063 F 0.00000 0.00000 0.00000 BR -1.10763 -1.91955 -2.48406 BR -1.10918 1.91901 -2.48330 BR 2.21650 0.00000 -2.48330	513	494 ^{2b} 505 ^{2c}
AlI_3 $\begin{array}{c} \text{I} \\ \\ \text{I}-\text{Al}-\text{I} \end{array}$	$[\text{I}_3\text{AlF}]^-$	37.2	1.699	AL -0.00000 -0.00000 -1.69927 F 0.00000 0.00000 0.00000 I 2.44076 -0.00000 -2.55198 I -1.22292 2.11229 -2.55198 I -1.21863 -2.11366 -2.55447	512	499 ^{2b}
$\text{Al}(\text{C}_2\text{F}_3)_3$ $\begin{array}{c} \text{C}_2\text{F}_3 \\ \\ \text{F}_3\text{C}_2-\text{Al}-\text{C}_2\text{F}_3 \end{array}$	$[(\text{C}_2\text{F}_3)_3\text{AlF}]^-$	40.1	1.717	C -0.97329 -1.62727 -2.42343 C -0.98362 1.62361 -2.41716 C 1.88676 -0.00000 -2.42738 C 3.06934 0.02474 -1.77940 C -0.45717 2.81744 -2.76398 C -0.43981 -2.83409 -2.70903 F -1.13734 3.89127 -3.20868 F 0.85045 3.10258 -2.70584 F -2.35963 1.56789 -2.53933 F 0.00000 0.00000 0.00000 F -2.33830 -1.56049 -2.62942 F -1.10221 -3.91341 -3.16704 F 0.85944 -3.12810 -2.56465 F 2.00961 -0.02916 -3.80810 F 3.19347 0.05603 -0.44736 F 4.28894 0.02266 -2.35089 AL -0.00000 -0.00000 -1.71727		
$\text{Al}(\text{CF}_3)_3$ $\begin{array}{c} \text{CF}_3 \\ \\ \text{F}_3\text{C}-\text{Al}-\text{CF}_3 \end{array}$	$[(\text{CF}_3)_3\text{AlF}]^-$	40.5	1.711	AL 0.00000 0.00000 -1.71131 F 0.00000 0.00000 0.00000 C -0.96543 -1.67530 -2.39273 C -0.96978 1.67344 -2.39147 C 1.93414 0.00000 -2.39147 F 2.66433 -1.09868 -1.97765 F 2.05865 0.00794 -3.76756 F 2.67005 1.08980 -1.96461		

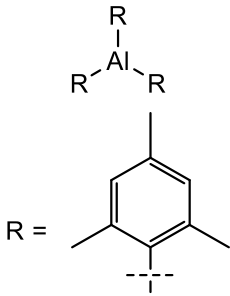
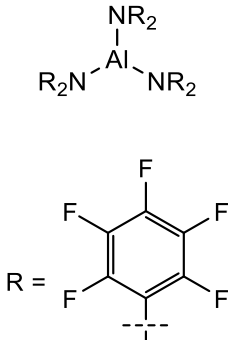
				F -0.38376 -2.85732 -1.97362 F -2.27971 -1.76482 -1.97343 F -1.02663 -1.78129 -3.76920 F -2.28658 1.75420 -1.97786 F -1.02513 1.78527 -3.76756 F -0.39602 2.85660 -1.96441		
$\text{Al}(\text{OCF}_3)_3$ 	$[(\text{OCF}_3)_3\text{AlF}]^-$	41.2	1.687	O -0.82512 -1.43858 -2.35393 O 1.64992 0.00000 -2.37380 O -0.85149 1.41396 -2.37341 C -0.54527 -2.69793 -2.50013 C -1.83284 2.18039 -2.00281 C 2.56830 0.90221 -2.55096 F 0.00000 0.00000 0.00000 F -1.48247 3.10127 -1.04437 F -2.90612 1.49479 -1.47592 F -2.33452 2.90926 -3.04885 F 2.51049 1.50547 -3.78335 F 3.83135 0.37718 -2.45844 F 2.52239 1.93052 -1.63457 F 0.00124 -2.99747 -3.72453 F 0.34841 -3.18280 -1.56946 F -1.65968 -3.49043 -2.39350 AL 0.00000 0.00000 -1.68662		
AlPh_3 	$[\text{Ph}_3\text{AlF}]^-$	44.2	1.732	F 0.00000 0.00000 0.00000 C -0.97139 -1.67112 -2.35352 C -1.83642 -2.36369 -1.46600 C -0.86267 -2.21622 -3.65900 C -2.55488 -3.51191 -1.85099 H -1.94710 -1.99180 -0.43021 C -1.57493 -3.36184 -4.06468 H -0.18557 -1.73781 -4.39289 C -2.42898 -4.01571 -3.15836 H -3.21782 -4.02104 -1.12655 H -1.46038 -3.75167 -5.09328 H -2.99030 -4.91588 -3.46821 C 1.93588 0.00000 -2.34395 C 2.96680 -0.36978 -1.44064 C 2.35821 0.34647 -3.65345 C 4.32401 -0.40519 -1.81429 H 2.69555 -0.63430 -0.40152 C 3.71011 0.31440 -4.04788 H 1.60603 0.66786 -4.39966 C 4.70227 -0.06488 -3.12578 H 5.09531 -0.69829 -1.07760 H 3.99418 0.59211 -5.08002 H 5.76538 -0.09062 -3.42660 C -0.96215 1.67101 -2.36987 C -1.11009 2.79032 -1.50921 C -1.51004 1.81715 -3.67065 C -1.74734 3.97870 -1.91502 H -0.71578 2.72701 -0.47767 C -2.14798 2.99842 -4.09715 H -1.45024 0.97169 -4.38300 C -2.26798 4.08913 -3.21720 H -1.84167 4.82664 -1.21107 H -2.55990 3.06847 -5.12116 H -2.76864 5.01884 -3.54337 AL 0.00000 0.00000 -1.73219	427	
AlAr^{F_3} 	$[\text{AlAr}^{\text{F}_3}\text{F}]^-$	45.5	1.726	F 0.00000 0.00000 0.00000 C 1.93392 -0.00000 -2.33228 C 2.94110 -0.34354 -1.39723 C 2.37568 0.31516 -3.63892 C 4.30723 -0.38094 -1.74427 H 2.65103 -0.58860 -0.36098 C 3.73781 0.27401 -4.00400 H 1.64513 0.61797 -4.40974 C 4.71245 -0.07585 -3.05459 H 5.77625 -0.10703 -3.33209 C -0.97692 1.67350 -2.31844 C -1.27194 2.66409 -1.34997 C -1.40291 1.94492 -3.64032 C -1.93734 3.86284 -1.68025 C -2.07526 3.13588 -3.98524 H -1.21567 1.20948 -4.44238 C -2.34271 4.10490 -3.00337 H -2.86444 5.03692 -3.26627 C -0.96262 -1.67967 -2.32752 C -1.70136 -2.42481 -1.37646 C -0.96163 -2.18180 -3.65067 C -2.41291 -3.59187 -1.72476 H -1.71749 -2.08742 -0.32562 C -1.66189 -3.35108 -4.01328 H -0.39538 -1.65565 -4.43939 C -2.39678 -4.06116 -3.04859 H -2.94842 -4.97138 -3.32548 C 4.15156 0.54814 -5.42912 C 5.34897 -0.68827 -0.69648 C -2.57252 3.35285 -5.39324 C -3.24095 -4.30898 -0.68652		

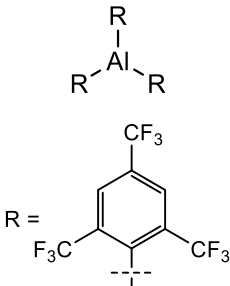
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$\text{Al}(\text{C}_5\text{F}_4\text{N})_3$ 	$[(\text{C}_5\text{F}_4\text{N})_3\text{AlF}]^-$	47.1	1.709	F 0.00000 0.00000 0.00000 C 1.93817 0.00000 -2.34151 C 2.79961 -1.01365 -1.89870 C 2.54639 0.95585 -3.16486 C 4.15686 -1.02723 -2.26744 C 3.91560 0.86756 -3.48537 C -0.97612 1.67100 -2.35244 C -0.60695 2.92404 -1.84266 C -2.04882 1.70770 -3.25252 C -1.28999 4.09344 -2.22355 C -2.67771 2.92511 -3.57986 C -0.95988 -1.67515 -2.36737 C -2.23660 -1.97618 -1.87225 C -0.45584 -2.61771 -3.27274 C -2.91377 -3.14386 -2.26847 C -1.20126 -3.76293 -3.61527 AL -0.00000 0.00000 -1.70899 N -2.30319 4.08520 -3.07225 N -2.39920 -4.01425 -3.11960 N 4.69542 -0.10175 -3.04247 F 4.96429 -2.01204 -1.82691 F 2.33857 -2.00839 -1.10723 F 1.84046 1.98585 -3.68586 F 4.47819 1.80172 -4.27772 F -3.70930 2.93276 -4.44738 F -2.50865 0.58010 -3.84287 F 0.42325 3.03711 -0.97518 F -0.91684 5.28527 -1.71722 F -2.85151 -1.14099 -1.00491 F -4.13943 -3.41061 -1.77588 F 0.75404 -2.45381 -3.85634 F -0.69168 -4.65636 -4.48648		
$\text{Al}(\text{C}_6\text{F}_5)_3$ 	$[(\text{C}_6\text{F}_5)_3\text{AlF}]^-$	47.4	1.709	F 0.00000 0.00000 0.00000 C 1.91859 -0.00000 -2.41109 C 2.81915 -0.94580 -1.90333 C 2.43530 0.85427 -3.39332 C 4.16128 -1.04542 -2.31330 C 3.76832 0.80264 -3.84264 C 4.63448 -0.15730 -3.29353 C -1.01167 1.67191 -2.28542 C -0.44794 2.92491 -2.01162 C -2.27202 1.69726 -2.89321 C -1.06958 4.14536 -2.32724 C -2.94290 2.88776 -3.23383 C -2.33277 4.11871 -2.94281 C -0.85124 -1.69683 -2.45100 C -1.41709 -2.72226 -1.68228 C -0.85823 -1.90814 -3.83517 C -1.95940 -3.89533 -2.24275 C -1.38558 -3.05614 -4.45119 C -1.93926 -4.05915 -3.63740 F 0.76287 3.00227 -1.40870 F -0.49097 5.33008 -2.04814 F -2.95577 5.27064 -3.25315 F -4.15668 2.86994 -3.82025 F -2.92221 0.54565 -3.18664 F -1.47207 -2.62925 -0.33626 F -2.49615 -4.86108 -1.46982 F -2.45165 -5.17259 -4.19367 F -1.37098 -3.21541 -5.78947 F -0.33786 -0.96455 -4.66072 F 1.64976 1.78724 -3.98071 F 4.22677 1.64630 -4.78869 F 5.91302 -0.22822 -3.70799 F 4.99368 -1.97037 -1.79508 F 2.40959 -1.83648 -0.96863 AL -0.00000 -0.00000 -1.70889	544	530 ^{2b} 536 ^{2c}

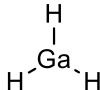
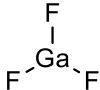
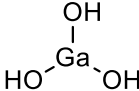
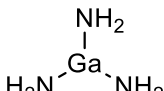
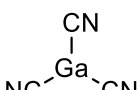
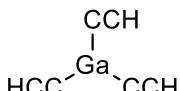
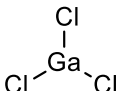
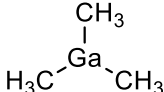
$\text{Al}(\text{C}_2\text{F}_5)_3$ 	$[(\text{C}_2\text{F}_5)_3\text{AlF}]^-$	47.5	1.708	AL -0.00000 0.00000 -1.70796 F 0.00000 0.00000 0.00000 C 1.94642 0.00000 -2.39692 C -0.80242 -1.75319 -2.44318 C -1.08006 1.66065 -2.28763 F -0.36990 2.80423 -1.91129 F -2.28149 1.71093 -1.58041 F 2.68001 -0.92887 -1.65711 F 2.01736 -0.41947 -3.72452 F 0.05491 -2.81777 -2.16009 F -0.91678 -1.70748 -3.83244 C 2.77779 1.29530 -2.33895 C -1.47093 1.89344 -3.75788 C -2.18463 -2.20893 -1.94031 F -2.16877 -2.40985 -0.60245 F -2.60068 -3.36927 -2.51594 F -3.12310 -1.27065 -2.20718 F 2.78482 1.80381 -1.08345 F 4.07584 1.10200 -2.69955 F 2.27029 2.23489 -3.16662 F -2.33671 0.94600 -4.18146 F -0.37841 1.84514 -4.55694 F -2.06396 3.10068 -3.96047	607	
$\text{Al}(\text{OC}_6\text{F}_5)_3$ 	$[(\text{OC}_6\text{F}_5)_3\text{AlF}]^-$	47.9	1.687	AL -0.00000 0.00000 -1.68726 F 0.00000 0.00000 0.00000 O 1.64533 -0.00000 -2.39153 O -0.82562 -1.41256 -2.41127 O -0.82537 1.40322 -2.42949 C 2.71584 0.76390 -2.37815 C 3.88096 0.38008 -3.10066 C 2.80860 1.97837 -1.64387 C 5.03620 1.17753 -3.12429 C 3.95902 2.78232 -1.66336 C 5.09149 2.37424 -2.38852 C -0.75929 -2.72532 -2.37779 C -1.69445 -3.50944 -3.11103 C 0.19882 -3.44728 -1.61418 C -1.64534 -4.91242 -3.11505 C 0.25543 -4.84990 -1.61370 C -0.68250 -5.59364 -2.34988 C -2.06116 1.80941 -2.62641 C -3.18258 1.28964 -1.92310 C -2.33401 2.85461 -3.55355 C -4.49189 1.73372 -2.16552 C -3.64009 3.30718 -3.79901 C -4.72652 2.76600 -3.08972 F -2.98298 0.31226 -1.01938 F -1.31889 3.40022 -4.24472 F -3.85592 4.28735 -4.69732 F -5.97943 3.20823 -3.31768 F -5.52418 1.20035 -1.48665 F -2.63459 -2.89174 -3.84593 F -2.54183 -5.61605 -3.83275 F -0.64223 -6.94111 -2.34544 F 1.18965 -5.48945 -0.88614 F 1.10339 -2.75787 -0.89446 F 3.86794 -0.76224 -3.80810 F 6.11238 0.78330 -3.83182 F 6.20492 3.13415 -2.40299 F 3.99403 3.93142 -0.96383 F 1.74011 2.38600 -0.93385	541	
$\text{Al}(\text{OTf})_3$ 	$[(\text{OTf})_3\text{AlF}]^-$	47.9	1.676	F 0.00000 0.00000 0.00000 O -0.96602 1.42072 -2.22589 O -0.85263 -1.43221 -2.38660 O 1.64542 -0.00000 -2.42372 S -0.57306 -2.97196 -2.17232 S 2.89583 0.92101 -2.12601 S -1.48730 1.94347 -3.62146 O 0.60782 -3.19795 -1.31663 O -0.75618 -3.71355 -3.42733 O -0.91154 1.19108 -4.75011 O -2.92798 2.23206 -3.55621 O 2.55767 2.00672 -1.18543 O 3.64053 1.19047 -3.36332 C 3.96338 -0.30622 -1.15299 C -2.08204 -3.40379 -1.10949 C -0.62827 3.63103 -3.62422 F -1.99662 -4.69820 -0.74725 F -2.12323 -2.64857 -0.00260 F -3.21732 -3.22604 -1.80221 F 0.70233 3.48644 -3.59810 F -0.97242 4.28270 -4.75221 F -1.01354 4.36672 -2.57064 F 3.32120 -0.74111 -0.06212 F 4.29724 -1.35455 -1.91805 F 5.09111 0.32512 -0.76989 AL -0.00000 -0.00000 -1.67628		

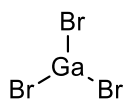
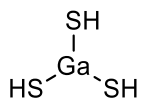
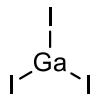
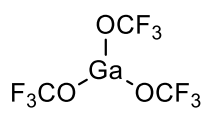
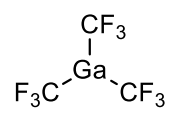
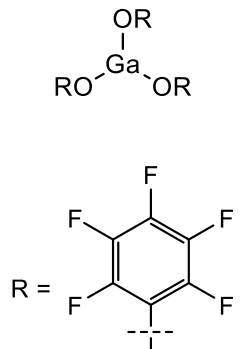
$\text{Al}(\text{OTeF}_5)_3$ 	$[(\text{OTeF}_5)_3\text{AlF}]^-$	51.5	1.678	F 0.00000 0.00000 0.00000 AL 0.00000 -0.00000 -1.67765 O 1.64343 -0.00000 -2.42773 TE 3.11964 1.14325 -2.09796 F 3.63122 0.24575 -0.47344 F 2.08128 2.41467 -1.08008 F 2.82423 2.17299 -3.69571 F 4.30588 -0.00099 -3.08594 F 4.63425 2.29356 -1.78754 O -0.82376 1.41694 -2.43445 TE -2.53998 2.16115 -2.13106 F -3.10223 0.75296 -0.93562 F -3.33733 1.22261 -3.60930 F -2.16417 3.64157 -3.29698 F -1.96607 3.21351 -0.62478 F -4.27847 2.94585 -1.85715 O -0.81758 -1.42238 -2.43288 TE -0.50016 -3.27729 -2.20425 F -1.60735 -3.40646 -0.63521 F 1.05594 -3.02021 -1.08905 F 0.62475 -3.40351 -3.76029 F -2.01562 -3.72778 -3.29547 F -0.20774 -5.17004 -1.99486		591 ^{2d}
$\text{Al}(\text{C}_6\text{Cl}_5)(\text{C}_6\text{F}_5)_2$ 	$[(\text{C}_6\text{Cl}_5)(\text{C}_6\text{F}_5)_2\text{AlF}]^-$	51.8	1.711	F 0.00000 0.00000 0.00000 C -0.93119 -1.74598 -2.21124 C -2.14237 -2.07026 -1.58481 C -0.41719 -2.72436 -3.07011 C -2.81958 -3.28674 -1.78162 C -1.05024 -3.95955 -3.30599 C -2.25936 -4.23990 -2.64895 C 1.91956 -0.00000 -2.39892 C 2.81575 -0.94363 -1.87946 C 2.45677 0.88585 -3.34024 C 4.17073 -1.01688 -2.24733 C 3.80452 0.86107 -3.74690 C 4.66471 -0.09920 -3.18983 C -0.95526 1.71086 -2.36141 C -0.59407 2.94244 -1.77396 C -1.96880 1.78212 -3.33710 C -1.22756 4.16933 -2.08078 C -2.63777 2.98264 -3.67966 C -2.26755 4.18326 -3.03592 CL -3.90094 3.00768 -4.88167 CL -0.74722 5.65754 -1.31003 CL -3.07756 5.67414 -3.42745 CL -2.43347 0.33807 -4.22700 CL 0.73152 2.99178 -0.62270 F -2.73495 -1.18145 -0.75364 F -3.98578 -3.55626 -1.16155 F -2.88432 -5.41394 -2.85626 F -0.52086 -4.87444 -4.14304 F 0.73815 -2.51340 -3.74640 F 2.38707 -1.85819 -0.97774 F 4.99878 -1.94146 -1.72192 F 5.95725 -0.14434 -3.56205 F 4.28255 1.73374 -4.65642 F 1.67871 1.82722 -3.92645 AL -0.00000 -0.00000 -1.71049		
$\text{Al}(\text{C}_6\text{Cl}_5)_2(\text{C}_6\text{F}_5)$ 	$[(\text{C}_6\text{Cl}_5)_2(\text{C}_6\text{F}_5)\text{AlF}]^-$	54.8	1.709	AL 0.00000 0.00000 -1.70939 F 0.00000 0.00000 0.00000 C -1.07550 1.59989 -2.39143 C -1.41974 2.68982 -1.57907 C -1.57715 1.64625 -3.69868 C -2.21832 3.76209 -2.02063 C -2.37860 2.69011 -4.19457 C -2.70129 3.75676 -3.33939 C -1.03383 -1.62711 -2.45681 C -2.27283 -1.96883 -1.87486 C -0.63285 -2.43225 -3.54158 C -3.05239 -3.07401 -2.29290 C -1.37343 -3.54824 -3.99863 C -2.59018 -3.87435 -3.35983 C 2.02471 0.00000 -2.12411 C 2.78402 -1.10168 -1.67392 C 2.76575 1.04528 -2.70890 C 4.18971 -1.18536 -1.79550 C 4.17488 1.01174 -2.85669 C 4.88946 -0.11413 -2.39401 CL 5.04205 2.33372 -3.59285 CL 5.07028 -2.57656 -1.22255 CL -0.81821 -4.52126 -5.33502 CL -2.92174 -0.97579 -0.57909 CL -4.56878 -3.45823 -1.52232 CL 0.84354 -2.04843 -4.41299 CL -3.51995 -5.24714 -3.89252 CL 6.62157 -0.18349 -2.55924 CL 1.94516 2.48390 -3.29810 CL 1.95921 -2.46370 -0.93158		

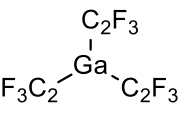
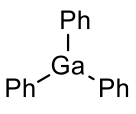
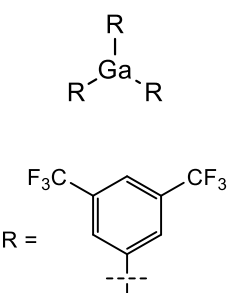
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$\text{Al}[\text{OC}(\text{CF}_3)_3]_3$   R =	$\{[\text{OC}(\text{CF}_3)_3]_3\text{AlF}\}^-$	56.8	1.690	F 0.00000 0.00000 0.00000 AL 0.00000 0.00000 -1.69017 O -0.81803 1.42217 -2.37138 O 1.63882 0.00000 -2.37590 O -0.84137 -1.41607 -2.35521 C -1.99346 2.05953 -2.53901 C 2.84617 0.60048 -2.35481 C -0.80065 -2.75357 -2.51990 C -1.67756 3.54268 -2.98154 C -2.83095 2.08973 -1.20207 C -2.85367 1.36206 -3.66980 C 3.71375 0.05737 -1.14885 C 3.58055 0.25865 -3.71052 C 2.71530 2.16826 -2.22404 C -2.27243 -3.25243 -2.80143 C -0.25216 -3.48386 -1.23244 C 0.11363 -3.13011 -3.75507 F -1.24818 3.57742 -4.26269 F -0.71035 4.06967 -2.21506 F -2.76119 4.35621 -2.89454 F -4.11503 2.48302 -1.39790 F -2.27860 2.93846 -0.30822 F -2.85837 0.86864 -0.63987 F -3.82832 2.17589 -4.15556 F -2.07002 1.00352 -4.69778 F -3.45839 0.24965 -3.20242 F 5.03741 0.32592 -1.29760 F 3.31902 0.61170 0.01764 F 3.57651 -1.27275 -1.03408 F 2.74308 0.40071 -4.74877 F 4.01957 -1.01968 -3.71071 F 4.65734 1.05537 -3.93395 F 3.89217 2.76640 -1.90881 F 2.27998 2.71367 -3.37875 F 1.82865 2.48059 -1.26228 F -2.39599 -4.60001 -2.68534 F -3.13505 -2.68817 -1.94274 F -2.66085 -2.91886 -4.05197 F 0.07040 -4.78124 -1.46458 F 0.85095 -2.86314 -0.77884 F -1.16836 -3.46484 -0.24037 F 1.42105 -3.06046 -3.42805 F -0.12263 -4.38813 -4.21220 F -0.10051 -2.27899 -4.77024	546	543 ⁵
$\text{Al}(\text{C}_6\text{Cl}_5)_3$   R =	$[(\text{C}_6\text{Cl}_5)_3\text{AlF}]^-$	59.0	1.711	F 0.00000 0.00000 0.00000 C -1.00080 -1.72405 -2.25300 C -2.21126 -2.02810 -1.59237 C -0.54841 -2.69856 -3.16432 C -2.91040 -3.24505 -1.76762 C -1.20964 -3.93300 -3.37577 C -2.39462 -4.21021 -2.66021 C 1.98631 0.00000 -2.28199 C 2.87746 -0.86881 -1.61493 C 2.57651 0.85682 -3.23224 C 4.27713 -0.85711 -1.81958 C 3.97078 0.90877 -3.47456 C 4.82711 0.05110 -2.75059 C -0.98477 1.72766 -2.27063 C -0.64048 2.93442 -1.62360 C -2.04338 1.81868 -3.19579 C -1.33086 4.15218 -1.82658 C -2.76824 3.01149 -3.43444 C -2.41309 4.18430 -2.73317 CL -0.59293 -5.11197 -4.50324 CL -4.39424 -3.57077 -0.91195 CL -4.08352 3.06126 -4.57860 CL -0.86702 5.60919 -0.98873 CL 4.64818 2.00436 -4.65027 CL 2.24022 -2.07408 -0.50943 CL 5.33014 -1.94431 -0.95397 CL 1.56466 1.89728 -4.22377 CL 0.87921 -2.39017 -4.14206 CL -3.22447 -5.72392 -2.88963 CL -2.93872 -0.83234 -0.53298 CL 6.54732 0.09945 -3.01731 CL -3.29161 5.66450 -2.99743 CL -2.48922 0.41723 -4.15817 CL 0.74520 2.96925 -0.54625 AL -0.00000 0.00000 -1.71078		
$\text{Al}[\text{C}_6\text{H}_2(\text{CH}_3)_3]_3$	$\{[\text{C}_6\text{H}_2(\text{CH}_3)_3]_3\text{AlF}\}^-$	59.9	1.760	F 0.00000 0.00000 0.00000 C -1.00435 -1.72769 -2.27091 C -2.19321 -2.07145 -1.55033 C -0.59238 -2.64510 -3.28435 C -2.89457 -3.26700 -1.82018		

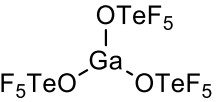
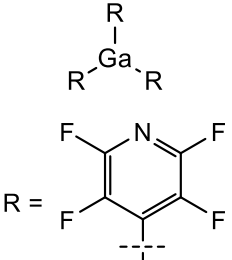
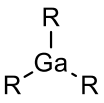
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$\text{Al}[\text{N}(\text{C}_6\text{F}_5)_2]_3$ 	$\{[\text{N}(\text{C}_6\text{F}_5)_2]_3\text{AlF}\}^-$	68.1	1.705	F 0.00000 0.00000 0.00000 N 1.67215 -0.00000 -2.62319 N -0.68447 -1.75809 -2.04110 N -1.13266 1.48796 -2.11579 C 2.48482 -1.14778 -2.44150 C 3.01814 -1.51219 -1.18226 C 2.79755 -1.99266 -3.53469 C 3.75197 -2.69799 -1.00787 C 3.55018 -3.16684 -3.38127 C 4.03476 -3.51990 -2.11078 C 2.24012 0.99530 -3.43850 C 3.53013 1.53004 -3.18002 C 1.56287 1.52532 -4.56418 C 4.11212 2.51437 -3.99430 C 2.11820 2.53227 -5.37178 C 3.40350 3.02533 -5.09517 C -1.34661 -2.44116 -0.99007 C -0.68978 -2.84747 0.19677 C -2.72430 -2.75252 -1.09084 C -1.38690 -3.45676 1.25368 C -3.43013 -3.38629 -0.05502 C -2.75512 -3.74719 1.12249 C -0.50993 -2.50103 -3.22355 C 0.10122 -3.78388 -3.21755 C -0.90492 -2.01444 -4.49487 C 0.30821 -4.52988 -4.38786 C -0.67935 -2.73690 -5.67867 C -0.09146 -4.01020 -5.62956 C -0.72846 2.77128 -2.50343 C -1.52160 3.58894 -3.35127 C 0.48484 3.34660 -2.04820 C -1.11542 4.87365 -3.74569 C 0.92389 4.61468 -2.45966	541	555 ⁵

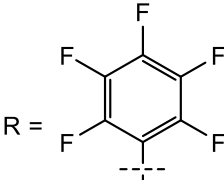
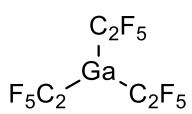
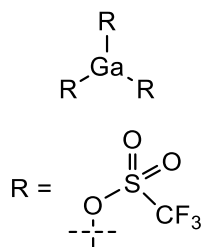
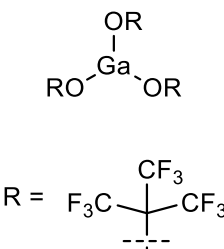
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$\text{Al}[\text{C}_6\text{H}_2(\text{CF}_3)_3]_3$ 	$\{[\text{C}_6\text{H}_2(\text{CF}_3)_3\text{AlF}]^-\}$	73.5	1.715	F 0.00000 0.00000 0.00000 C -1.02002 1.77506 -2.17280 C -0.76698 2.95669 -1.41133 C -2.09674 1.91188 -3.10176 C -1.52226 4.13845 -1.54051 C -2.85930 3.08647 -3.24193 C -2.57913 4.20847 -2.45375 H -1.27854 5.01358 -0.92137 H -3.68050 3.12408 -3.97152 C -1.02372 -1.77647 -2.15616 C -2.16369 -2.14955 -1.38109 C -0.60658 -2.78155 -3.08188 C -2.80010 -3.40136 -1.49190 C -1.23434 -4.03496 -3.20516 C -2.33231 -4.35711 -2.39913 H -3.67953 -3.62445 -0.87124 H -0.86763 -4.76229 -3.94324 C 2.04724 -0.00000 -2.17517 C 2.94891 -0.79678 -1.40538 C 2.69908 0.85583 -3.11511 C 4.34950 -0.72700 -1.53567 C 4.09726 0.93444 -3.25722 C 4.93378 0.14780 -2.45746 H 4.98850 -1.37471 -0.91868 H 4.53584 1.60959 -4.00541 C 0.32080 3.05103 -0.34511 C -2.56265 0.76739 -3.99008 C -3.35421 5.48782 -2.63925 C -2.79366 -1.24701 -0.32364 C 0.60134 -2.60704 -3.99085 C -2.96901 -5.72075 -2.48511 C 2.49204 -1.78297 -0.33385 C 1.93532 1.81180 -4.02005 C 6.43276 0.27023 -2.56010 F -2.65008 0.06948 -0.57859 F -2.29856 -1.49519 0.91060 F -4.14419 -1.46742 -0.23684 F -4.27082 -5.70658 -2.09739 F -2.33783 -6.62985 -1.69017 F -2.93066 -6.22382 -3.74793 F 0.51034 -3.38622 -5.10930 F 0.76650 -1.34072 -4.42688 F 1.75839 -2.97655 -3.37556 F -3.19268 1.22266 -5.11364 F -3.46513 -0.03308 -3.35888 F -1.55594 -0.02307 -4.41757 F -3.39385 6.23305 -1.50397 F -2.80846 6.28137 -3.60373 F -4.64015 5.25666 -3.01457 F 0.80868 4.32932 -0.25749 F -0.15168 2.74998 0.88604 F 1.38854 2.26440 -0.59103		

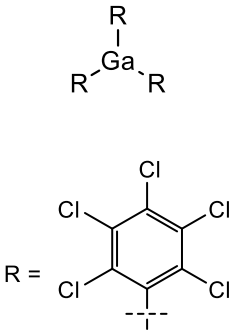
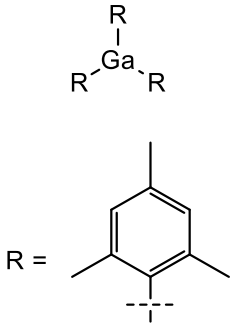
				F 1.28143 -2.32499 -0.57838 F 2.46130 -1.21531 0.89353 F 3.36295 -2.83742 -0.23748 F 6.83406 0.61984 -3.81099 F 7.06553 -0.89004 -2.24420 F 6.92600 1.22068 -1.71749 F 2.64296 2.11612 -5.14820 F 0.74999 1.32237 -4.44033 F 1.68658 3.00189 -3.40696 AL -0.00000 0.00000 -1.71535		
GaH_3 	$[\text{H}_3\text{GaF}]^-$	24.7	1.845	GA 0.00000 -0.00000 -1.84533 H 1.56562 -0.00000 -2.33636 H -0.78287 -1.35604 -2.33576 H -0.78272 1.35567 -2.33732 F 0.00000 0.00000 0.00000	302	
GaF_3 	$[\text{GaF}_4]^-$	28.9	1.802	GA -0.00000 -0.00000 -1.80157 F -0.84928 1.47025 -2.40398 F 1.69926 -0.00000 -2.39950 F 0.00000 0.00000 0.00000 F -0.84928 -1.47025 -2.40398	460	431 ^{2b} 447 ^{2c}
$\text{Ga}(\text{OH})_3$ 	$[(\text{OH})_3\text{GaF}]^-$	30.6	1.830	GA 0.00000 0.00000 -1.82947 F 0.00000 0.00000 0.00000 O 1.75923 -0.00000 -2.43198 H 1.75503 0.68159 -3.13654 O -0.84659 1.48821 -2.57754 H -1.73109 1.13385 -2.81017 O -1.02982 -1.50609 -2.24474 H -1.13630 -1.94565 -1.37458	342	
$\text{Ga}(\text{NH}_2)_3$ 	$[(\text{NH}_2)_3\text{GaF}]^-$	32.1	1.858	GA 0.00000 -0.00000 -1.85840 F 0.00000 0.00000 0.00000 N -0.92070 1.59642 -2.45503 H -1.38178 2.01488 -1.62786 H -0.19150 2.28111 -2.72142 N 1.84932 -0.00000 -2.43478 H 2.42937 0.15532 -1.59127 H 2.06914 -0.96876 -2.72600 N -0.92460 -1.59943 -2.44197 H -1.10407 -2.17496 -1.60032 H -1.86390 -1.30259 -2.76008	267	
$\text{Ga}(\text{CN})_3$ 	$[(\text{NC})_3\text{GaF}]^-$	32.7	1.798	GA 0.00000 0.00000 -1.79781 F 0.00000 0.00000 0.00000 C -0.94246 -1.63074 -2.44514 C -0.94059 1.63031 -2.44914 C 1.88258 0.00000 -2.44802 N -1.49569 2.59305 -2.83181 N 2.99431 0.00046 -2.82942 N -1.49956 -2.59398 -2.82357		
$\text{Ga}(\text{C}\equiv\text{CH})_3$ 	$[(\text{HC}\equiv\text{C})_3\text{GaF}]^-$	32.8	1.817	GA 0.00000 0.00000 -1.81687 F 0.00000 0.00000 0.00000 C -0.94475 -1.63400 -2.43084 C -0.94229 1.63381 -2.43539 C 1.88670 0.00000 -2.43343 C -1.52696 2.64838 -2.82635 H -2.04011 3.53890 -3.16803 C -1.53213 -2.64915 -2.81613 H -2.04775 -3.54024 -3.15255 C 3.05842 0.00082 -2.82212 H 4.08691 0.00154 -3.16168	377	
GaCl_3 	$[\text{Cl}_3\text{GaF}]^-$	33.3	1.796	GA -0.00000 -0.00000 -1.79600 F 0.00000 0.00000 0.00000 CL -1.05477 -1.82902 -2.51276 CL -1.05771 1.82815 -2.51119 CL 2.11284 -0.00000 -2.50886	448	432 ^{2b} 429 ^{2c}
$\text{Ga}(\text{CH}_3)_3$ 	$[(\text{CH}_3)_3\text{GaF}]^-$	33.4	1.855	GA 0.00000 0.00000 -1.85479 F 0.00000 0.00000 0.00000 C -0.97940 1.69620 -2.45468 H -0.47287 2.61783 -2.07871 H -1.02227 1.77354 -3.56913 H -2.03174 1.71701 -2.08124 C -0.98035 -1.69709 -2.45020 H -1.02603 -1.77728 -3.56431 H -0.47314 -2.61776 -2.07283 H -2.03171 -1.71661 -2.07390 C 1.95962 -0.00000 -2.45128 H 2.05112 -0.00144 -3.56547 H 2.50294 0.90079 -2.07612 H 2.50330 -0.89954 -2.07372	285	

GaBr_3 	$[\text{Br}_3\text{GaF}]^-$	34.4	1.795	GA 0.00000 -0.00000 -1.79474 F 0.00000 0.00000 0.00000 BR -1.12848 1.95685 -2.56448 BR -1.12982 -1.95597 -2.56506 BR 2.25963 -0.00000 -2.56236	448	436 ^{2b} 426 ^{2c}
$\text{Ga}(\text{SH})_3$ 	$[(\text{SH})_3\text{GaF}]^-$	34.5	1.815	GA 0.00000 0.00000 -1.81458 F 0.00000 0.00000 0.00000 S -1.18313 1.89281 -2.44188 H -0.62254 1.88241 -3.69157 S -1.00051 -1.90092 -2.67355 H 0.07790 -2.68523 -2.35412 S 2.21021 -0.00000 -2.52748 H 2.58126 0.91655 -1.57804	372	
GaI_3 	$[\text{I}_3\text{GaF}]^-$	36.0	1.795	GA -0.00000 -0.00000 -1.79497 F 0.00000 0.00000 0.00000 I -1.23231 -2.14449 -2.62274 I 2.47243 -0.00000 -2.62529 I -1.23857 2.14060 -2.62464	440	454 ^{2b}
$\text{Ga}(\text{OCF}_3)_3$ 	$[(\text{OTf})_3\text{GaF}]^-$	36.7	1.772	O -0.88977 -1.56373 -2.27931 O 1.78758 -0.00000 -2.32513 O -0.95806 1.42379 -2.52517 C -0.79746 -2.26680 -3.37431 C -1.14495 2.59304 -1.97408 C 2.27862 0.49214 -3.43115 F 0.00000 0.00000 0.00000 F -0.04554 3.07996 -1.30376 F -2.17001 2.61293 -1.05536 F -1.46947 3.53778 -2.90785 F 1.49821 0.26528 -4.53938 F 3.50484 -0.04806 -3.71096 F 2.47426 1.85268 -3.39290 F -1.08807 -1.56589 -4.51939 F 0.44596 -2.81596 -3.58414 F -1.67039 -3.32371 -3.35121 GA 0.00000 0.00000 -1.77195		
$\text{Ga}(\text{CF}_3)_3$ 	$[(\text{CF}_3)_3\text{GaF}]^-$	39.7	1.814	GA 0.00000 -0.00000 -1.81363 F 0.00000 0.00000 0.00000 C 1.95204 0.00000 -2.44246 C -0.97600 1.69162 -2.43911 C -0.97902 -1.68930 -2.44083 F 2.66932 1.09363 -2.01352 F 2.08444 -0.00075 -3.81570 F 2.67053 -1.09222 -2.01197 F -1.04825 -1.80304 -3.81395 F -0.39255 -2.85875 -2.01326 F -2.28368 -1.76248 -2.00840 F -1.04503 1.80799 -3.81207 F -2.28046 1.76680 -2.00652 F -0.38693 2.85896 -2.00921		
$\text{Ga}(\text{OC}_6\text{F}_5)_3$ 	$[(\text{OC}_6\text{F}_5)_3\text{GaF}]^-$	39.9	1.775	GA 0.00000 0.00000 -1.77469 F 0.00000 0.00000 0.00000 O -0.66249 -1.65552 -2.34714 O 1.73846 0.00000 -2.47656 O -0.82134 1.50515 -2.53792 C -2.08999 1.86725 -2.58742 C -3.14723 1.16964 -1.94453 C -2.46675 3.01353 -3.34378 C -4.48110 1.60294 -2.00040 C -3.79761 3.45556 -3.40459 C -4.81840 2.74050 -2.75295 C -0.27121 -2.36443 -3.39527 C -0.16337 -3.77952 -3.29068 C 0.03219 -1.80641 -4.66622 C 0.19202 -4.58058 -4.38726 C 0.39920 -2.59795 -5.76550 C 0.49083 -3.99350 -5.62900 C 2.43386 1.01590 -2.96199 C 2.46111 2.30712 -2.36957 C 3.25137 0.83285 -4.11152 C 3.23048 3.35598 -2.89671 C 4.03188 1.87345 -4.63972 C 4.03252 3.14057 -4.03056 F 1.71483 2.53232 -1.27239 F 3.26919 -0.36554 -4.71916 F 4.79161 1.66153 -5.73109 F 4.78533 4.13880 -4.53389 F 3.22529 4.56460 -2.30500 F -1.52007 3.71534 -3.98752 F -4.10988 4.55366 -4.11827 F -6.09727 3.16025 -2.82270 F -5.44390 0.91667 -1.35904 F -2.84397 0.07338 -1.22065 F -0.06381 -0.47313 -4.83051	481	

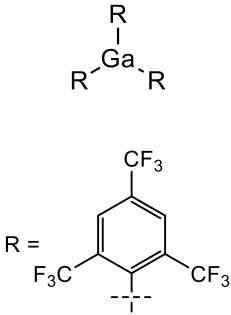
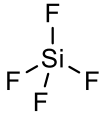
				F 0.66626 -2.02643 -6.95296 F 0.83999 -4.76162 -6.67993 F 0.27206 -5.91819 -4.24807 F -0.42693 -4.37330 -2.11438		
$\text{Ga}(\text{C}_2\text{F}_3)_3$ 	$[(\text{C}_2\text{F}_3)_3\text{GaF}]^-$	41.0	1.817	C 1.92710 -0.00000 -2.42796 C -0.86032 -1.70483 -2.49190 C -1.05243 1.58836 -2.48656 C -1.40805 2.71282 -1.83609 C -2.10791 -2.12537 -2.20723 C 2.58889 0.96194 -3.10108 F -2.70150 -3.24433 -2.66436 F -2.94551 -1.45942 -1.40167 F -0.15414 -2.51620 -3.34969 F 0.00000 0.00000 0.00000 F 2.69102 -1.09743 -2.10084 F 3.88460 0.92471 -3.46708 F 2.03396 2.11018 -3.50888 F -1.48255 1.52229 -3.79552 F -1.08099 2.98284 -0.56892 F -2.13000 3.72761 -2.35120 GA -0.00000 -0.00000 -1.81694		
GaPh_3 	$[\text{Ph}_3\text{GaF}]^-$	42.7	1.847	GA 0.00000 -0.00000 -1.84646 F 0.00000 0.00000 0.00000 C -0.94783 -1.65683 -2.54236 C -2.34184 -1.66829 -2.79171 C -0.24951 -2.86170 -2.79957 C -3.00829 -2.81491 -3.26588 H -2.92845 -0.74840 -2.61062 C -0.89982 -4.01749 -3.27398 H 0.84190 -2.89899 -2.62467 C -2.28658 -3.99761 -3.50946 H -4.09862 -2.78715 -3.44821 H -0.32194 -4.94122 -3.46279 H -2.80297 -4.90043 -3.88295 C -1.00216 1.70473 -2.31038 C -1.38734 2.07243 -3.62241 C -1.34406 2.60773 -1.27319 C -2.07031 3.27447 -3.89369 H -1.15295 1.39943 -4.46905 C -2.02644 3.81260 -1.52748 H -1.06506 2.34578 -0.23657 C -2.39249 4.15247 -2.84299 H -2.35508 3.52847 -4.93167 H -2.27743 4.49422 -0.69340 H -2.92828 5.09686 -3.04867 C 1.97639 -0.00000 -2.31513 C 2.93156 0.17215 -1.28267 C 2.48422 -0.15499 -3.62785 C 4.31509 0.19497 -1.54216 H 2.56827 0.28663 -0.24541 C 3.86557 -0.13417 -3.90435 H 1.78240 -0.30226 -4.47077 C 4.78917 0.04267 -2.85826 H 5.03270 0.33133 -0.71166 H 4.22530 -0.25841 -4.94272 H 5.87408 0.05981 -3.06791	349	
GaAr^{F_3} 	$[\text{Ar}^{\text{F}_3}\text{GaF}]^-$	45.1	1.846	GA 0.00000 0.00000 -1.84605 F 0.00000 0.00000 0.00000 C -0.96850 -1.67818 -2.43360 C -2.35991 -1.69055 -2.67118 C -0.28228 -2.90258 -2.59276 C -3.04066 -2.86736 -3.04726 H -2.94065 -0.75928 -2.55453 C -0.94992 -4.08652 -2.96877 H 0.80539 -2.94459 -2.41076 C -2.33655 -4.07348 -3.19716 H -2.86468 -4.99604 -3.47866 C -1.04792 1.71764 -2.20054 C -1.31265 2.36997 -3.43025 C -1.60621 2.31647 -1.04321 C -2.09562 3.53908 -3.50896 C -2.38774 3.47956 -1.09924 H -1.40664 1.83644 -0.06978 C -2.63952 4.09593 -2.34074 H -2.29015 4.01101 -4.48332 H -2.81260 3.90977 -0.17696 C 1.98123 0.00000 -2.26328 C 2.86999 0.12130 -1.17235 C 2.55437 -0.12999 -3.54948 C 4.26991 0.11764 -1.35272 H 2.44754 0.21217 -0.15658 C 3.95052 -0.13603 -3.73937 H 1.90560 -0.23203 -4.43372 C 4.81723 -0.01260 -2.63793 H 5.90764 -0.02577 -2.78013 C -3.44289 5.36928 -2.40124 C -0.68619 1.86842 -4.71411 C -4.52117 -2.81929 -3.33552 C -0.17291 -5.36289 -3.18090		

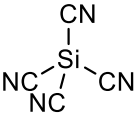
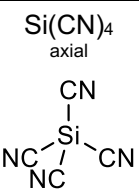
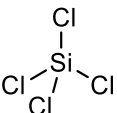
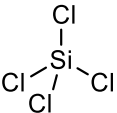
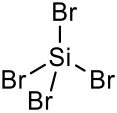
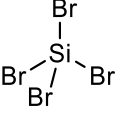
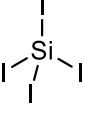
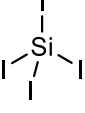
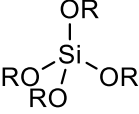
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Ga(OTeF ₅) ₃ 	[(OTeF ₅) ₃ GaF] ⁻	51.1	1.764	F 0.00000 0.00000 0.00000 GA 0.00000 0.00000 -1.76404 O 1.70763 -0.00000 -2.56595 TE 3.12602 1.18688 -2.11209 F 3.55712 0.28135 -0.46730 F 1.97656 2.40447 -1.14602 F 2.90180 2.23701 -3.71023 F 4.41056 0.09560 -3.03726 F 4.57670 2.37977 -1.68556 O -0.86776 1.47644 -2.56001 TE -2.68668 1.94866 -2.24472 F -3.03650 0.40893 -1.12841 F -3.33608 0.98853 -3.78181 F -2.51296 3.52925 -3.32552 F -2.28675 2.99496 -0.67823 F -4.52274 2.45324 -1.95195 O -0.84431 -1.46842 -2.59280 TE -0.40799 -3.29688 -2.28761 F -1.54740 -3.45343 -0.74286 F 1.09114 -2.89108 -1.13588 F 0.77431 -3.40034 -3.80406 F -1.86033 -3.87540 -3.40597 F 0.00286 -5.15806 -2.00898		
Ga(C ₅ F ₄ N) ₃ 	[(C ₅ F ₄ N) ₃ GaF] ⁻	46.2	1.809	F 0.00000 0.00000 0.00000 C -0.97666 1.69318 -2.38357 C -0.54917 2.94009 -1.90915 C -2.11081 1.72976 -3.20240 C -1.24452 4.11416 -2.25246 C -2.74566 2.95353 -3.49154 C -0.97320 -1.69402 -2.38846 C -2.24013 -1.98810 -1.86767 C -0.45450 -2.65886 -3.25940 C -2.89880 -3.18158 -2.21706 C -1.18488 -3.82729 -3.55129 C 1.94965 0.00000 -2.40378 C 2.83144 -0.97229 -1.91421 C 2.52735 0.94135 -3.26332 C 4.19019 -0.95704 -2.27998 C 3.89996 0.88074 -3.57342 N -2.37578 -4.07590 -3.03780 N 4.70493 -0.04699 -3.08858 N -2.31805 4.11196 -3.02365 F -0.81892 5.30528 -1.78863 F 0.54142 3.04379 -1.12155 F -2.62201 0.60221 -3.74639 F -3.83888 2.96884 -4.27957 F -0.66759 -4.74626 -4.39049 F 0.75009 -2.49537 -3.85232 F -2.86063 -1.13201 -1.03013 F -4.11685 -3.44851 -1.70692 F 2.39676 -1.94921 -1.09132 F 5.02414 -1.89994 -1.79983 F 1.78917 1.92273 -3.82967 F 4.43860 1.79760 -4.40142 GA -0.00000 0.00000 -1.80864		
Ga(C ₆ F ₅) ₃ 	[(C ₆ F ₅) ₃ GaF] ⁻	51.1	1.812	GA -0.00000 0.00000 -1.81187 F 0.00000 0.00000 0.00000 C -0.97318 1.69251 -2.40187 C -0.44288 2.65692 -3.26470 C -2.25171 1.95673 -1.89569 C -1.12806 3.83679 -3.61265 C -2.98038 3.11731 -2.21216 C -2.40531 4.06539 -3.07558 C 1.96014 0.00000 -2.37145 C 2.56419 -0.97302 -3.17363 C 2.80246 1.00757 -1.88551 C 3.93772 -0.96744 -3.48423 C 4.17915 1.06192 -2.16681 C 4.74740 0.05845 -2.97015	454	447 ^{2b} 453 ^{2c}

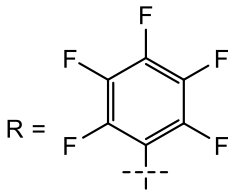
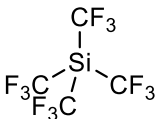
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$\text{Ga}(\text{C}_2\text{F}_5)_3$ 	$[(\text{C}_2\text{F}_5)_3\text{GaF}]^-$	46.9	1.810	GA -0.00000 -0.00000 -1.80991 F 0.00000 0.00000 0.00000 C -0.92286 -1.77877 -2.32803 C 1.96041 0.00000 -2.46394 C -0.96584 1.72091 -2.42328 F -0.38941 -2.83058 -1.59852 F -2.27036 -1.71962 -1.99356 F -0.66880 2.01767 -3.74796 F -0.51349 2.79443 -1.66919 F 2.02621 -0.08105 -3.85019 F 2.61967 -1.11914 -1.97356 C -0.87813 -2.23182 -3.79920 C -2.50265 1.77053 -2.32611 C 2.84564 1.20112 -2.08171 F 0.38272 -2.54694 -4.16757 F -1.31812 -1.24672 -4.61769 F -1.65253 -3.32565 -4.03395 F 4.12856 1.05723 -2.51686 F 2.36584 2.34245 -2.62470 F 2.89385 1.36285 -0.74191 F -2.91735 1.49504 -1.06990 F -3.00142 2.99438 -2.65551 F -3.06793 0.87223 -3.16230	514	
$\text{Ga}(\text{OTf})_3$ 	$[(\text{OTf})_3\text{GaF}]^-$	48.7	1.763	GA 0.00000 0.00000 -1.76307 F 0.00000 0.00000 0.00000 O -1.06161 1.47298 -2.28440 O -0.91614 -1.49490 -2.48648 O 1.69911 0.00000 -2.58861 S -0.47444 -2.98487 -2.17993 S 2.85111 1.01125 -2.17748 S -1.46589 1.86074 -3.76749 O 0.76349 -3.02919 -1.37544 O -0.64151 -3.83197 -3.36937 O -0.85476 0.96058 -4.76324 O -2.89276 2.21357 -3.82922 O 2.34710 2.06318 -1.27105 O 3.67774 1.33985 -3.34724 C 3.92763 -0.13072 -1.11237 C -1.87997 -3.48931 -1.01117 C -0.53657 3.50632 -3.90976 F -1.64917 -4.74202 -0.57369 F -1.94525 -2.66849 0.04580 F -3.05837 -3.46945 -1.65360 F 0.78476 3.31508 -3.81560 F -0.81187 4.04883 -5.11193 F -0.92915 4.36138 -2.95384 F 3.23816 -0.60323 -0.06842 F 4.39087 -1.15634 -1.83983 F 4.97622 0.58218 -0.65440	490	
$\text{Ga}[\text{OC}(\text{CF}_3)_3]$ 	$\{[\text{OC}(\text{CF}_3)_3]_3\text{GaF}\}^-$	56.3	1.777	GA 0.00000 0.00000 -1.77679 F 0.00000 0.00000 0.00000 O -0.81540 -1.59058 -2.29759 O 1.71033 0.00000 -2.51632 O -0.88338 1.47677 -2.50138 C 2.93152 0.48503 -2.17484 C -1.99136 2.20253 -2.20041 C -0.79392 -2.45789 -3.33835 C 3.94919 -0.06610 -3.25061 C 3.39963 -0.00097 -0.74213 C 2.95114 2.06102 -2.21138 C -2.11719 3.30156 -3.32785 C -1.87650 2.92684 -0.79635 C -3.29474 1.31393 -2.20199 C -1.97840 -3.47474 -3.09453 C -1.01738 -1.73546 -4.72228 C 0.56463 -3.27299 -3.39816 F 4.74943 0.06230 -0.59324 F 2.85716 0.75474 0.23425	501	

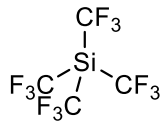
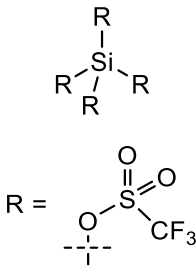
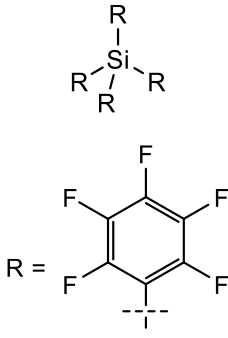
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$\text{Ga}(\text{C}_6\text{Cl}_5)_3$ 	$[(\text{C}_6\text{Cl}_5)_3\text{GaF}]^-$	58.1	1.813	GA -0.00000 0.00000 -1.81251 F 0.00000 0.00000 0.00000 C -0.99806 1.73181 -2.32329 C -0.53102 2.68864 -3.24346 C -2.20293 2.04493 -1.66015 C -1.18138 3.92724 -3.46400 C -2.88848 3.26848 -1.84906 C -2.36325 4.22120 -2.74977 C 2.00650 0.00000 -2.29172 C 2.62424 -0.89858 -3.18093 C 2.86319 0.89771 -1.62107 C 4.02745 -0.96018 -3.36264 C 4.27002 0.87477 -1.77179 C 4.85488 -0.07284 -2.64058 C -1.00522 -1.73119 -2.31247 C -0.68113 -2.92553 -1.63516 C -2.07019 -1.80885 -3.22920 C -1.40857 -4.12737 -1.80616 C -2.82845 -2.98800 -3.43139 C -2.50003 -4.15146 -2.70226 CL -2.93875 0.86716 -0.59266 CL -4.36949 3.61640 -0.99766 CL -3.17872 5.74070 -2.99257 CL -0.55383 5.09012 -4.60190 CL 0.89128 2.35381 -4.21769 CL 1.64739 -1.97831 -4.16286 CL 2.18496 2.14240 -0.59213 CL 5.29032 1.99622 -0.91115 CL 6.58447 -0.13324 -2.83474 CL 4.74915 -2.10579 -4.46157 CL -2.48314 -0.42023 -4.22190 CL 0.70991 -2.97247 -0.57220 CL -0.97825 -5.57651 -0.93771 CL -3.42214 -5.61242 -2.92139 CL -4.15352 -3.03010 -4.56427		
$\text{Ga}[\text{C}_6\text{H}_2(\text{CH}_3)_3]_3$ 	$\{[\text{C}_6\text{H}_2(\text{CH}_3)_3]_3\text{GaF}\}^-$	59.0	1.891	F 0.00000 0.00000 0.00000 C -1.01453 -1.73945 -2.32530 C -2.18460 -2.06953 -1.57547 C -0.60244 -2.66492 -3.32715 C -2.87384 -3.27995 -1.80936 C -1.31392 -3.86773 -3.53971 C -2.45090 -4.20269 -2.78340 H -3.77663 -3.50633 -1.21011 H -0.96700 -4.56565 -4.32571 C 2.01272 -0.00000 -2.33090 C 2.89522 -0.82784 -1.57192 C 2.59689 0.81299 -3.34506 C 4.28772 -0.80460 -1.80759 C 3.99398 0.81272 -3.55968 C 4.86383 0.01741 -2.79313 H 4.94441 -1.45677 -1.20025 H 4.41551 1.45638 -4.35545 C -1.00259 1.74419 -2.33713 C -0.72058 2.92513 -1.58481 C -1.99678 1.84364 -3.35313 C -1.42829 4.12281 -1.82900 C -2.68638 3.05717 -3.57656 C -2.42561 4.21138 -2.81720 H -1.18643 5.01961 -1.22685 H -3.45285 3.10082 -4.37400 C -2.73743 -1.11479 -0.53372 H -1.92654 -0.76077 0.13960 H -3.15234 -0.19854 -1.01625 H -3.55234 -1.58385 0.06259 C 0.60132 -2.39188 -4.21142		

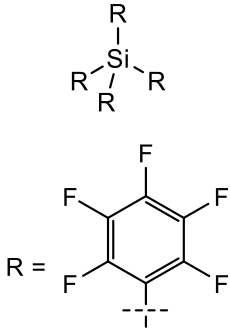
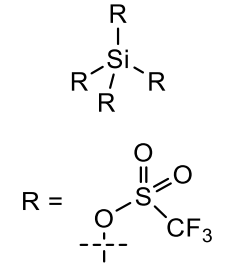
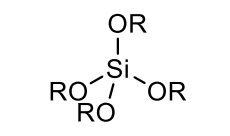
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$\text{Ga}[\text{N}(\text{C}_6\text{F}_5)_2]_3$ $\text{R} = \text{C}_6\text{F}_5$	$\{[\text{N}(\text{C}_6\text{F}_5)_2]_3\text{GaF}\}^-$	69.2	1.804	GA 0.00000 -0.00000 -1.80382 F 0.00000 0.00000 0.00000 N 1.84865 -0.00000 -2.43291 N -0.95637 -1.68229 -2.10290 N -0.91378 1.72842 -2.17666 C 2.55126 1.18252 -2.69964 C 2.58067 2.26470 -1.78507 C 3.28102 1.36100 -3.90531 C 3.26241 3.46106 -2.05937 C 3.99822 2.53657 -4.17811 C 3.98489 3.59747 -3.25642 C 2.59003 -1.19424 -2.51285 C 3.67487 -1.43538 -1.63329 C 2.29122 -2.21112 -3.44751 C 4.41019 -2.63018 -1.66932 C 2.99476 -3.42598 -3.47609 C 4.06679 -3.63320 -2.59250 C -1.49832 -2.18235 -3.29835 C -1.17561 -3.48637 -3.75416 C -2.39687 -1.44320 -4.10226 C -1.70619 -4.02048 -4.93774 C -2.91012 -1.94702 -5.30857 C -2.57542 -3.24587 -5.72532 C -1.24721 -2.43880 -0.94896 C -0.23107 -2.90864 -0.08408 C -2.58138 -2.73873 -0.57756 C -0.52113 -3.61870 1.09041 C -2.88755 -3.48143 0.57423 C -1.85440 -3.91545 1.42082 C -1.24044 2.43385 -0.99465 C -0.64220 3.67140 -0.66817 C -2.13057 1.88143 -0.04659 C -0.91897 4.33836 0.53359 C -2.40018 2.52224 1.17286 C -1.79263 3.75422 1.46646 C -1.16620 2.29982 -3.41457 C -0.71182 1.66038 -4.60078 C -1.94378 3.47113 -3.65831 C -0.89459 2.16842 -5.89147 C -2.12460 4.00749 -4.94489 C -1.62420 3.35348 -6.07983 F -2.75753 0.72854 -0.31177 F -3.25189 1.97472 2.05454 F -2.05685 4.37843 2.62547 F -0.34487 5.52173 0.80638 F 0.19493 4.25033 -1.54557 F 1.95116 2.15024 -0.60738 F 3.26966 4.45761 -1.16223 F 4.65566 4.73090 -3.51963 F 4.67478 2.66573 -5.33220 F 3.29407 0.38447 -4.82819 F 1.31985 -2.02294 -4.35148 F 4.00340 -0.50964 -0.72036 F 5.42641 -2.83278 -0.81398 F 4.75860 -4.78320 -2.62683 F 2.68364 -4.37018 -4.37729 F -0.31566 -4.23770 -3.04660 F -1.36646 -5.25615 -5.34006	458	472 ⁵

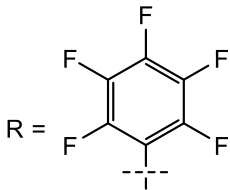
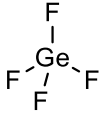
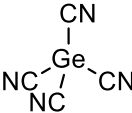
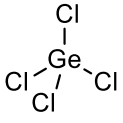
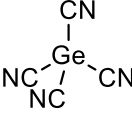
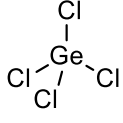
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$\text{Ga}[\text{C}_6\text{H}_2(\text{CF}_3)_3]_3$ 	$\{[\text{C}_6\text{H}_2(\text{CF}_3)_3]_3\text{GaF}\}^-$	72.9	1.820	F 0.00000 0.00000 0.00000 C 2.05195 -0.00000 -2.21707 C 2.93357 -0.80276 -1.43584 C 2.70561 0.86682 -3.14170 C 4.33584 -0.72411 -1.54568 C 4.10560 0.94981 -3.26018 C 4.93078 0.15950 -2.45212 H 4.96843 -1.37369 -0.92433 H 4.55395 1.63176 -3.99619 C -1.02632 1.77690 -2.21769 C -0.77486 2.94113 -1.43462 C -2.10208 1.91003 -3.14441 C -1.54549 4.11540 -1.54392 C -2.87505 3.08022 -3.26276 C -2.60644 4.18896 -2.45222 H -1.30170 4.98719 -0.92044 H -3.68840 3.12769 -4.00037 C -1.02604 -1.77640 -2.22267 C -2.16313 -2.14076 -1.44387 C -0.60400 -2.77153 -3.15275 C -2.80004 -3.39162 -1.56255 C -1.23581 -4.02293 -3.27965 C -2.33490 -4.34406 -2.47534 H -3.67985 -3.61572 -0.94294 H -0.87061 -4.74884 -4.01947 C 2.46772 -1.80267 -0.37872 C 1.95009 1.82714 -4.04956 C 6.43081 0.28814 -2.53220 C 0.32183 3.03809 -0.37525 C -2.55347 0.77637 -4.05439 C -3.47011 5.42210 -2.53275 C -2.79230 -1.24270 -0.37993 C 0.60775 -2.59612 -4.05728 C -2.97945 -5.70410 -2.56441 GA -0.00000 -0.00000 -1.82000 F 1.39879 2.27082 -0.62834 F -0.14200 2.73243 0.85661 F 0.79241 4.32524 -0.28908 F -2.79827 6.54503 -2.16799 F -4.55684 5.33845 -1.71533 F -3.94909 5.62950 -3.78833 F -3.19968 1.24676 -5.16255 F -1.53995 0.01041 -4.50716 F -3.43874 -0.05032 -3.43284 F 2.68053 2.15313 -5.15731 F 1.67768 3.00623 -3.42591 F 0.77957 1.33389 -4.50293 F 6.84983 0.61860 -3.78274 F 6.90541 1.25584 -1.69893 F 7.06428 -0.86298 -2.18674 F 3.34634 -2.85447 -0.29345 F 2.43365 -1.25053 0.85412 F 1.26456 -2.35045 -0.63430 F -2.66753 0.07437 -0.63118 F -2.29086 -1.49365 0.84937 F -4.14181 -1.47914 -0.28897 F -4.30040 -5.66770 -2.24835 F -2.40321 -6.59893 -1.71392 F -2.87829 -6.23786 -3.81060 F 0.52732 -3.38953 -5.16683 F 0.76770 -1.33515 -4.50816 F 1.76326 -2.95139 -3.43132		
SiF_4 	$[\text{SiF}_5]^-$	37.9	1.693	SI 0.00000 0.00000 -1.69278 F 0.00000 0.00000 0.00000 F -0.83144 -1.44659 -1.69462 F 0.00186 0.00323 -3.38556 F -0.83997 1.44189 -1.69186 F 1.66871 0.00000 -1.69186	310	
$\text{Si}(\text{CN})_4$ equatorial	$[(\text{NC})_4\text{SiF}]^-$ equatorial	43.2	1.667	SI -0.00000 -0.00000 -1.66744 F 0.00000 0.00000 0.00000 C 0.00335 -1.57573 -2.72477 C -0.00338 1.58720 -2.70630 C 1.95854 -0.00000 -1.59633 C -1.95853 -0.00834 -1.59634		

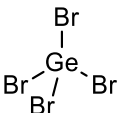
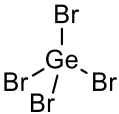
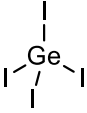
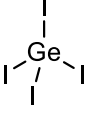
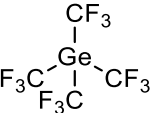
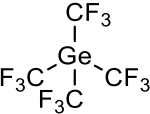
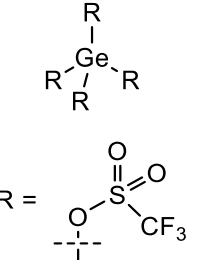
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	[(NC) ₄ SiF] ⁻ axial	44.2	1.691	Si 0.00000 0.00000 -1.69096 F 0.00000 0.00000 0.00000 C 1.89808 0.00000 -1.71294 C -0.94953 1.64350 -1.71294 C 0.00020 0.00034 -3.66201 C -0.94882 -1.64397 -1.71319 N -1.53696 2.66068 -1.70258 N 0.00030 0.00052 -4.83872 N -1.53597 -2.66130 -1.70273 N 3.07269 0.00022 -1.70258		
	[Cl ₄ SiF] ⁻ equatorial	44.6	1.657	Si 0.00000 -0.00000 -1.65720 F 0.00000 0.00000 0.00000 Cl 0.00000 2.22334 -1.62044 Cl 1.86345 -0.00000 -2.72504 Cl -1.86345 0.00000 -2.72504 Cl 0.00000 -2.22334 -1.62044	328	
	[Cl ₄ SiF] ⁻ axial	46.0	1.673	Si -0.00000 0.00000 -1.67323 Cl -1.08386 -1.87243 -1.66063 Cl 2.16350 0.00000 -1.66063 Cl 0.00066 -0.00115 -3.88780 Cl -1.08064 1.87416 -1.66145 F 0.00000 0.00000 0.00000	328	
	[Br ₄ SiF] ⁻ equatorial	46.7	1.654	Si -0.00000 0.00000 -1.65379 Br -0.00000 -2.00236 -2.82276 Br -0.00000 2.00236 -2.82276 Br -2.42845 0.00000 -1.57272 Br 2.42845 0.00000 -1.57272 F 0.00000 0.00000 0.00000	344	
	[Br ₄ SiF] ⁻ axial	48.3	1.670	Si -0.00000 0.00000 -1.67019 F 0.00000 0.00000 0.00000 Br -1.16461 -2.03013 -1.65194 Br 2.34045 0.00000 -1.65194 Br -0.00147 0.00254 -4.09683 Br -1.17331 2.02575 -1.64967	344	
	[I ₄ SiF] ⁻ equatorial	49.4	1.652	Si 0.00000 0.00000 -1.65165 F 0.00000 0.00000 0.00000 I 0.00000 2.71130 -1.46991 I 2.18200 0.00000 -2.99765 I -2.18200 0.00000 -2.99765 I 0.00000 -2.71130 -1.46991	352	
	[I ₄ SiF] ⁻ axial	51.3	1.668	Si -0.00000 -0.00000 -1.66810 I 2.58734 -0.00000 -1.63712 I -1.28881 2.24351 -1.63712 I -0.00170 -0.00293 -4.40963 I -1.29632 -2.23967 -1.63438 F 0.00000 0.00000 0.00000	352	
	[(OC ₆ F ₅) ₃ SiF] ⁻ axial	54.5	1.665	Si 0.00000 0.00000 -1.66454 F 0.00000 0.00000 0.00000 O 1.72196 0.00000 -1.65872 O -0.83473 -1.53032 -1.71645 O -0.74622 1.56634 -1.61885 O -0.02792 -0.01918 -3.46343 C -1.10637 2.41867 -2.58194 C -0.17676 3.01938 -3.46680 C -2.45476 2.84955 -2.67076 C -0.58058 3.95441 -4.43471 C -2.86260 3.79079 -3.63073 C -1.92318 4.36210 -4.50551 C -0.81994 -0.60014 -4.35618 C -2.23193 -0.69686 -4.23584	431	

 R =				C -0.26082 -1.09891 -5.56461 C -3.02296 -1.32004 -5.21519 C -1.04408 -1.71959 -6.55037 C -2.43627 -1.81771 -6.39010 C -1.27504 -2.24768 -0.67204 C -0.64428 -3.46730 -0.32927 C -2.39751 -1.85538 0.09565 C -1.13011 -4.27712 0.71154 C -2.88318 -2.65549 1.14302 C -2.24790 -3.86903 1.45809 C 2.66484 -0.15662 -2.59151 C 3.65339 0.84490 -2.75961 C 2.80298 -1.33915 -3.35651 C 4.71088 0.68530 -3.66995 C 3.85555 -1.50311 -4.27150 C 4.82217 -0.49543 -4.42365 F 1.11824 2.68348 -3.39942 F -3.36932 2.34015 -1.83744 F -4.15043 4.17268 -3.69694 F -2.31001 5.27188 -5.41795 F 0.32388 4.49602 -5.26869 F 0.43396 -3.87131 -1.01447 F -3.02017 -0.70440 -0.18194 F -3.95608 -2.26411 1.85248 F -2.71478 -4.63943 2.45753 F -0.51817 -5.43781 1.00786 F -2.84587 -0.19078 -3.15278 F -4.35499 -1.40310 -5.05058 F -3.19329 -2.40224 -7.33757 F -0.46751 -2.19413 -7.66915 F 1.06324 -1.00176 -5.76921 F 1.90583 -2.32490 -3.22047 F 3.95362 -2.63314 -4.99164 F 5.83811 -0.65276 -5.29214 F 5.63400 1.65417 -3.80999 F 3.58310 1.97282 -2.03929		
Si(CF₃)₄ equatorial 	[(CF₃)₄SiF]⁻ equatorial	54.6	1.688	Si 0.00000 -0.00000 -1.65331 F 0.00000 0.00000 0.00000 O -1.78622 -0.03470 -1.69453 O -0.00604 -1.40430 -2.64996 O 1.77898 -0.00000 -1.72492 O -0.01945 1.55505 -2.39019 C -2.69817 -0.59814 -0.91853 C -2.53113 -1.81638 -0.20676 C -3.95985 0.04470 -0.77526 C -3.56634 -2.36949 0.56713 C -5.00008 -0.50694 -0.01272 C -4.80258 -1.71334 0.68091 C 2.60498 0.76191 -1.00748 C 3.06482 0.35132 0.27200 C 3.13336 1.97526 -1.52231 C 3.95754 1.13615 1.02071 C 4.02872 2.76185 -0.77688 C 4.45519 2.33967 0.49314 C -1.05424 2.36494 -2.66099 C -1.55597 3.26302 -1.69222 C -1.65134 2.38159 -3.94225 C -2.58497 4.16878 -1.99617 C -2.68004 3.28528 -4.25541 C -3.15709 4.17653 -3.27917 C 1.03054 -2.10519 -3.13446 C 1.45069 -1.93379 -4.47411 C 1.70192 -3.07609 -2.35485 C 2.47707 -2.71984 -5.02462 C 2.73127 -3.86297 -2.89777 C 3.12612 -3.68388 -4.23483 F -1.37360 -2.49005 -0.29005 F -3.37058 -3.53300 1.21320 F -5.79337 -2.24439 1.42313 F -6.18100 0.13146 0.08271 F -4.17289 1.20986 -1.41225 F 2.64280 -0.80929 0.78821 F 4.36728 0.72396 2.23440 F 5.32001 3.08755 1.20373 F 4.50519 3.91165 -1.28945 F 2.77813 2.39623 -2.74330 F -1.22446 1.52810 -4.88181 F -3.22455 3.29168 -5.48497 F -4.14288 5.04181 -3.57655 F -3.03811 5.01945 -1.05925 F -1.03472 3.25720 -0.45654 F 0.85620 -1.00982 -5.23961 F 1.34849 -3.25961 -1.07763 F 3.34829 -4.78693 -2.14080 F 2.85095 -2.54637 -6.30466 F 4.10813 -4.43969 -4.75847		
Si(CF₃)₄ axial	[(CF₃)₄SiF]⁻ axial	57.4	1.708	Si 0.00000 0.00000 -1.70814 F 0.00000 0.00000 0.00000 C -0.99830 1.72390 -1.65830 C 0.00256 -0.00134 -3.74757		

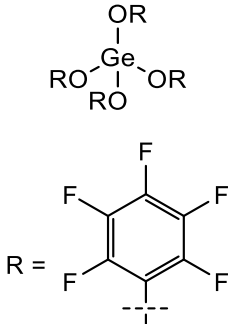
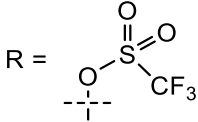
				C -1.00306 -1.72087 -1.65183 C 1.99256 0.00000 -1.65379 F -2.34948 1.47838 -1.55018 F -0.67355 2.50047 -0.58375 F -0.85308 2.53656 -2.74751 F -1.23389 0.24794 -4.29761 F 0.83728 0.94474 -4.29674 F 0.40543 -1.19733 -4.29598 F 2.45672 1.29142 -1.53190 F 2.62707 -0.52237 -2.74572 F 2.49858 -0.68025 -0.58401 F -0.12379 -2.77035 -1.49874 F -1.75420 -2.02225 -2.75275 F -1.86498 -1.79927 -0.59585		
Si(OTf)₄ equatorial 	[(OTf)₄SiF]⁻ equatorial	61.9	1.646	Si 0.00000 0.00000 -1.64575 S -2.28058 0.05195 -2.51515 O -2.92405 -1.06331 -1.75409 O -2.96352 1.36241 -2.67739 S -0.10924 -2.40445 -1.61458 O -0.71138 -3.10448 -2.78418 O 1.30626 -2.69817 -1.20748 S 2.23924 0.00000 -2.51501 O 2.11420 1.08890 -3.53491 O 3.25841 0.05807 -1.43514 C -1.15403 -3.07432 -0.07944 C -2.10715 -0.60238 -4.35243 C 2.78578 -1.50973 -3.63532 F -2.75075 -1.75821 -4.50137 F -0.79747 -0.76563 -4.62223 F -2.61570 0.30041 -5.20084 F -1.64081 -2.09432 0.68720 F -0.33746 -3.84146 0.66253 F -2.15966 -3.82647 -0.53740 F 3.52702 -2.37869 -2.95367 F 1.72107 -2.12102 -4.17019 F 3.52968 -0.99163 -4.62924 F 0.00000 0.00000 0.00000 S 0.13675 2.38931 -1.52610 O -1.09286 2.73200 -0.75126 O 1.46486 2.90374 -1.09303 C -0.16411 3.19316 -3.28297 F 0.93420 3.82795 -3.69851 F -1.16829 4.07426 -3.19036 F -0.49586 2.24226 -4.17742	519	
Si(C₆F₅)₄ axial 	[(C₆F₅)₄SiF]⁻ axial	63.9	1.713	Si -0.00000 -0.00000 -1.71341 F 0.00000 0.00000 0.00000 C -1.65668 1.13249 -1.53931 C -1.93270 2.39299 -2.09955 C -2.68164 0.64791 -0.69379 C -3.11832 3.11991 -1.86486 C -3.88357 1.33135 -0.43988 C -4.10130 2.58835 -1.02246 C 0.32272 0.50098 -3.68519 C 1.05512 1.67882 -3.92760 C 0.05002 -0.24905 -4.84162 C 1.45693 2.12257 -5.19768 C 0.42540 0.15038 -6.14075 C 1.13160 1.34697 -6.32123 C -0.64222 -1.82833 -1.87602 C 0.00862 -2.88801 -1.21972 C -1.86242 -2.16137 -2.48809 C -0.47479 -4.20994 -1.22647 C -2.38887 -3.46349 -2.51010 C -1.68846 -4.49643 -1.86818 C 1.98533 -0.00000 -1.55358 C 2.66250 0.90482 -0.72059 C 2.79426 -0.91490 -2.24236 C 4.06070 0.90321 -0.56669 C 4.19378 -0.96247 -2.11201 C 4.82985 -0.04298 -1.26335 F 1.99035 1.85937 -0.04904 F 4.67358 1.79789 0.23244 F 6.16774 -0.06313 -1.12383 F 4.92680 -1.87287 -2.78127 F 2.24077 -1.82261 -3.08050 F -2.60706 -1.21553 -3.09566 F 1.15931 -2.69221 -0.54872 F 0.19894 -5.19452 -0.60404 F -2.17295 -5.74970 -1.87422 F -3.55982 -3.72825 -3.11747 F -2.58724 -0.55370 -0.09228 F -1.06317 3.01936 -2.91805 F -3.30440 4.32698 -2.43149 F -5.23781 3.26442 -0.78365 F -4.82436 0.79786 0.36164 F -0.58164 -1.44263 -4.79048 F 1.42919 2.46778 -2.89260 F 2.14530 3.26932 -5.35309 F 1.49879 1.74373 -7.55248 F 0.12610 -0.61285 -7.20985	336	

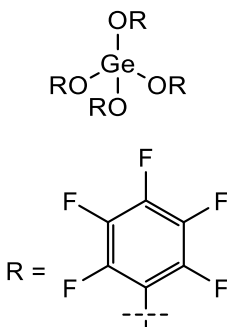
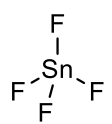
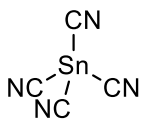
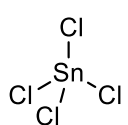
$\text{Si}(\text{C}_6\text{F}_5)_4$ equatorial  R =	$[(\text{C}_6\text{F}_5)_4\text{SiF}]^-$ equatorial	65.4	1.667	Si 0.00000 0.00000 -1.66719 F 0.00000 0.00000 0.00000 C -1.68387 0.00154 -2.63401 C -1.83222 0.62382 -3.88266 C -2.85502 -0.50989 -2.05366 C -3.06721 0.72095 -4.54652 C -4.11340 -0.41895 -2.67293 C -4.21624 0.19809 -3.93035 C 1.68430 0.00000 -2.63288 C 2.85340 0.51896 -2.05523 C 1.83461 -0.62605 -3.87932 C 4.11146 0.43313 -2.67571 C 3.06942 -0.71913 -4.54403 C 4.21626 -0.18796 -3.93093 C -0.18631 2.06744 -1.54597 C -1.17543 2.57540 -0.68209 C 0.51917 3.05378 -2.25348 C -1.42693 3.94518 -0.48580 C 0.31088 4.43828 -2.09359 C -0.67128 4.88761 -1.20022 C 0.18666 -2.06697 -1.54503 C 1.18176 -2.57236 -0.68651 C -0.52205 -3.05503 -2.24679 C 1.43759 -3.94146 -0.49120 C -0.31035 -4.43905 -2.08685 C 0.67895 -4.88582 -1.20002 F -0.76655 1.17895 -4.49687 F -2.80642 -1.13795 -0.86368 F -5.21433 -0.92134 -2.08595 F -5.40907 0.28781 -4.54238 F -3.16679 1.31551 -5.74912 F -1.98598 1.73847 0.00560 F 1.47304 2.73355 -3.16208 F -2.38754 4.36595 0.36095 F 1.03355 5.33498 -2.79411 F -0.89168 6.20457 -1.03427 F 2.80290 1.15016 -0.86700 F 0.77109 -1.18831 -4.49064 F 3.17081 -1.31737 -5.74463 F 5.40892 -0.27356 -4.54387 F 5.21013 0.94410 -2.09196 F 1.99430 -1.73301 -0.00398 F -1.48196 -2.73713 -3.14968 F -1.03611 -5.33782 -2.78157 F 0.90317 -6.20225 -1.03482 F 2.40502 -4.35973 0.34904	336	
$\text{Si}(\text{OTf})_4$ axial  R =	$[(\text{OTf})_4\text{SiF}]^-$ axial	66.8	1.663	Si -0.00000 0.00000 -1.66272 F 0.00000 0.00000 0.00000 S -0.77028 -2.21901 -1.64193 O -1.65434 -2.52893 -2.79764 O 0.40393 -3.07771 -1.31446 S 2.37491 -0.00000 -1.75873 O 2.89731 -0.38275 -0.42046 O 2.81689 -0.69787 -2.99765 S -0.13785 0.11036 -4.07678 O -1.56347 0.16293 -4.51082 O 0.77394 1.26820 -4.36860 S -1.45123 1.90974 -1.47883 O -2.84753 1.39183 -1.48365 O -0.92136 2.67640 -0.31666 C 0.60614 -1.38228 -5.12763 C 2.96060 1.85068 -1.95320 C -1.94307 -2.37251 -0.09962 C -1.44176 3.28605 -2.86553 F -2.71138 -3.46115 -0.27827 F -2.72721 -1.29191 -0.00657 F -1.23903 -2.51795 1.02734 F 3.96245 2.07260 -1.08856 F 3.38591 2.09895 -3.19037 F 1.93350 2.66126 -1.64698 F 0.93559 -2.41390 -4.34490 F 1.68439 -0.95679 -5.79359 F -0.32427 -1.77535 -6.00880 F -0.20905 3.74947 -3.08394 F -1.99362 2.88649 -4.00683 F -2.19317 4.27843 -2.34545	519	
$\text{Si}(\text{OC}_6\text{F}_5)_3$ equatorial  R =	$[(\text{OC}_6\text{F}_5)_3\text{SiF}]^-$ equatorial	67.6	1.653	Si 0.00000 -0.00000 -1.65331 F 0.00000 0.00000 0.00000 O -1.78622 -0.03470 -1.69453 O -0.00604 -1.40430 -2.64996 O 1.77898 -0.00000 -1.72492 O -0.01945 1.55505 -2.39019 C -2.69817 -0.59814 -0.91853 C -2.53113 -1.81638 -0.20676 C -3.95985 0.04470 -0.77526 C -3.56634 -2.36949 0.56713 C -5.00008 -0.50694 -0.01272 C -4.80258 -1.71334 0.68091 C 2.60498 0.76191 -1.00748 C 3.06482 0.35132 0.27200	431	

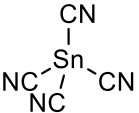
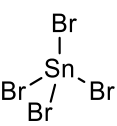
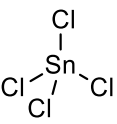
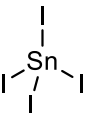
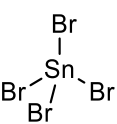
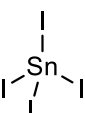
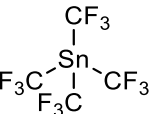
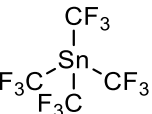
				C 3.13336 1.97526 -1.52231 C 3.95754 1.13615 1.02071 C 4.02872 2.76185 -0.77688 C 4.45519 2.33967 0.49314 C -1.05424 2.36494 -2.66099 C -1.55597 3.26302 -1.69222 C -1.65134 2.38159 -3.94225 C -2.58497 4.16878 -1.99617 C -2.68004 3.28528 -4.25541 C -3.15709 4.17653 -3.27917 C 1.03054 -2.10519 -3.13446 C 1.45069 -1.93379 -4.47411 C 1.70192 -3.07609 -2.35485 C 2.47707 -2.71984 -5.02462 C 2.73127 -3.86297 -2.89777 C 3.12612 -3.68388 -4.23483 F -1.37360 -2.49005 -0.29005 F -3.37058 -3.53300 1.21320 F -5.79337 -2.24439 1.42313 F -6.18100 0.13146 0.08271 F -4.17289 1.20986 -1.41225 F 2.64280 -0.80929 0.78821 F 4.36728 0.72396 2.23440 F 5.32001 3.08755 1.20373 F 4.50519 3.91165 -1.28945 F 2.77813 2.39623 -2.74330 F -1.22446 1.52810 -4.88181 F -3.22455 3.29168 -5.48497 F -4.14288 5.04181 -3.57655 F -3.03811 5.01945 -1.05925 F -1.03472 3.25720 -0.45654 F 0.85620 -1.00982 -5.23961 F 1.34849 -3.25961 -1.07763 F 3.34829 -4.78693 -2.14080 F 2.85095 -2.54637 -6.30466 F 4.10813 -4.43969 -4.75847		
GeF_4 	$[\text{GeF}_5]^-$	37.2	1.693	F 0.00000 0.00000 0.00000 F 1.77626 -0.00000 -1.80332 F -0.01150 0.00000 -3.59524 F -0.87995 -1.54347 -1.79482 F -0.87994 1.54347 -1.79482 GE 0.00000 -0.00000 -1.79764	355	
$\text{Ge}(\text{CN})_4$ equatorial 	$[(\text{NC})_4\text{GeF}]^-$ equatorial	41.7	1.792	F 0.00000 0.00000 0.00000 C -1.62315 0.00005 -2.91880 C 1.65022 0.00000 -2.87527 C -0.01030 -2.03314 -1.65362 C -0.01024 2.03314 -1.65362 N 2.65887 0.00005 -3.47679 N -0.01820 3.20657 -1.57826 N -2.61355 0.00014 -3.55012 N -0.01830 -3.20657 -1.57827 GE -0.00000 0.00000 -1.79194		
GeCl_4 equatorial 	$[\text{Cl}_4\text{GeF}]^-$ equatorial	42.6	1.777	F 0.00000 0.00000 0.00000 CL -0.00000 -2.29914 -1.72133 CL -1.94477 0.00000 -2.89803 CL 1.94477 0.00000 -2.89803 CL -0.00000 2.29914 -1.72133 GE -0.00000 0.00000 -1.77716	323	
$\text{Ge}(\text{CN})_4$ axial 	$[(\text{NC})_4\text{GeF}]^-$ axial	42.7	1.823	F 0.00000 0.00000 0.00000 C -0.98358 1.70529 -1.79797 C -0.98358 -1.70529 -1.79797 C -0.00123 -0.00000 -3.88072 C 1.96864 -0.00000 -1.79873 N -1.57037 -2.72192 -1.76755 N -0.00239 -0.00000 -5.05720 N 3.14247 -0.00000 -1.76875 N -1.57037 2.72192 -1.76755 GE 0.00000 -0.00000 -1.82245		
GeCl_4 axial 	$[\text{Cl}_4\text{GeF}]^-$ axial	44.2	1.794	CL 2.24956 -0.00000 -1.76862 CL -1.12987 1.94523 -1.76862 CL 0.00176 0.00306 -4.10127 CL -1.12214 -1.94947 -1.77085 F 0.00000 0.00000 0.00000 GE -0.00000 -0.00000 -1.79388	323	
GeBr_4 equatorial	$[\text{Br}_4\text{GeF}]^-$ equatorial	44.4	1.777	BR -0.00000 -2.08996 -2.98805 BR -0.00000 2.08996 -2.98805 BR -2.48902 -0.00000 -1.68444 BR 2.48902 -0.00000 -1.68444	321	

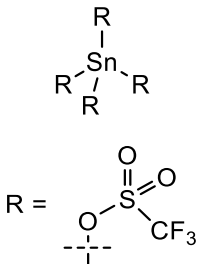
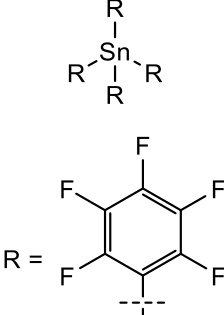
				F 0.00000 0.00000 0.00000 GE -0.00000 0.00000 -1.77743		
GeBr₄ axial 	[Br ₄ GeF] ⁻ axial	46.3	1.794	F 0.00000 0.00000 0.00000 BR -1.20992 -2.09505 -1.75751 BR 2.41933 -0.00000 -1.75751 BR -0.00010 0.00016 -4.30594 BR -1.20948 2.09518 -1.75741 GE 0.00000 -0.00000 -1.79349	321	
GeI₄ equatorial 	[I ₄ GeF] ⁻ equatorial	46.9	1.779	F 0.00000 0.00000 0.00000 I -2.75517 0.00000 -1.58829 I 0.00000 2.26961 -3.16140 I 0.00000 -2.26961 -3.16140 I 2.75517 0.00000 -1.58829 GE 0.00000 0.00000 -1.77908	299	
GeI₄ axial 	[I ₄ GeF] ⁻ axial	49.1	1.794	I -1.30904 -2.31526 -1.73905 I 2.65970 0.00000 -1.73905 I -0.00635 0.01088 -4.60315 I -1.34073 2.29822 -1.72980 F 0.00000 0.00000 0.00000 GE -0.00000 0.00000 -1.79431	299	
Ge(CF₃)₄ equatorial 	[(CF ₃) ₄ GeF] ⁻ equatorial	51.8	1.825	C 0.01028 -2.09117 -1.62645 C 1.68099 0.00000 -3.06451 C -1.79914 0.00493 -2.85689 F 0.98755 -2.56855 -0.79823 F -1.17435 -2.55905 -1.11327 F 0.18005 -2.75375 -2.81866 F -2.85476 0.00363 -1.98854 F -1.96833 -1.08218 -3.66636 F -1.96627 1.09634 -3.66079 F 1.35307 0.04593 -4.39347 F 2.46632 -1.10539 -2.90334 F 2.50307 1.06701 -2.83586 F 0.00000 0.00000 0.00000 C 0.02095 2.09131 -1.62739 F 0.21165 2.75016 -2.81867 F -1.16825 2.56695 -1.13188 F 0.98870 2.56523 -0.78656 GE 0.00000 0.00000 -1.82528		
Ge(CF₃)₄ axial 	[(CF ₃) ₄ GeF] ⁻ axial	54.6	1.851	F 0.00000 0.00000 0.00000 C 2.05754 -0.00000 -1.77473 C -0.00244 -0.00410 -3.98408 C -1.01712 1.78779 -1.76748 C -1.03652 -1.77748 -1.76548 F 2.53688 1.28415 -1.70569 F 2.55895 -0.65266 -0.69362 F 2.65471 -0.56980 -2.86415 F 0.84940 0.92634 -4.52938 F 0.37779 -1.20835 -4.52608 F -1.23548 0.26728 -4.52688 F -0.17063 -2.83571 -1.64739 F -1.80016 -2.03413 -2.86938 F -1.88197 -1.85617 -0.70428 F -2.36624 1.57048 -1.64122 F -0.86214 2.57381 -2.87447 F -0.65443 2.56163 -0.71050 GE -0.00000 -0.00000 -1.85127		
Ge(OTf)₄ equatorial 	[(OTf) ₄ GeF] ⁻ equatorial	60.6	1.782	S -0.06154 -2.45710 -2.54446 O 0.91280 -3.19818 -1.69161 O -1.41755 -3.00410 -2.83128 S 2.52519 -0.00000 -1.65508 O 3.26136 -0.91318 -2.57804 O 2.84319 1.46619 -1.61832 S -0.01617 2.39219 -2.70848 O -1.21742 2.26658 -3.59582 O 0.09202 3.48871 -1.70763 C 3.05109 -0.60738 0.12488 C 0.76767 -2.36861 -4.32139 C 1.39720 2.75093 -4.01856 F 1.93523 -3.00730 -4.33547 F 0.95269 -1.06915 -4.63239 F -0.05122 -2.91628 -5.22903 F 2.43378 -1.74563 0.44862 F 2.78083 0.33084 1.03771	524	

				F 4.37997 -0.82117 0.09806 F 2.34227 3.53825 -3.51307 F 1.93036 1.59228 -4.43873 F 0.83042 3.36812 -5.06931 F 0.00000 0.00000 0.00000 S -2.51936 0.14896 -1.63955 O -2.88721 -1.09143 -0.89469 O -3.03906 1.47486 -1.20195 C -3.25414 -0.13524 -3.43378 F -3.88643 0.95959 -3.85963 F -4.11716 -1.15707 -3.40001 F -2.25001 -0.43292 -4.27912 GE 0.00000 0.00000 -1.78147		
$\text{Ge}(\text{C}_6\text{F}_5)_4$ equatorial R =	$[(\text{C}_6\text{F}_5)_4\text{GeF}]^-$ equatorial	61.8	1.866	F 0.00000 0.00000 0.00000 C 0.27401 0.20691 -4.01736 C -0.31133 -0.58408 -5.01855 C 1.20213 1.14884 -4.49806 C -0.04135 -0.44058 -6.39423 C 1.50874 1.33361 -5.85899 C 0.87732 0.52907 -6.81851 C -0.87372 -1.81344 -1.80928 C -0.25507 -2.88785 -1.15252 C -2.19965 -2.01782 -2.21583 C -0.88557 -4.13412 -0.97880 C -2.87068 -3.24114 -2.05007 C -2.20798 -4.30441 -1.41682 C 2.01760 -0.00000 -1.65742 C 2.66882 0.95856 -0.87062 C 2.81200 -0.99944 -2.22802 C 4.05734 0.93092 -0.65308 C 4.20271 -1.07019 -2.02563 C 4.82488 -0.09731 -1.22733 C -1.40720 1.47446 -1.69626 C -2.51096 1.25311 -0.84781 C -1.34201 2.75011 -2.27547 C -3.51036 2.21725 -0.62437 C -2.31500 3.74764 -2.06683 C -3.40423 3.48023 -1.22715 F -1.18380 -1.57561 -4.72641 F 1.88569 1.95530 -3.65340 F 2.40147 2.26250 -6.25209 F 1.15226 0.68332 -8.12569 F -0.64259 -1.23124 -7.30497 F 1.98670 1.98399 -0.32949 F 2.26018 -1.95287 -3.01145 F 4.66469 1.87327 0.09258 F 4.93910 -2.05286 -2.57747 F 6.15326 -0.14089 -1.02207 F 0.99547 -2.78384 -0.66732 F -2.89953 -1.02709 -2.80459 F -4.14106 -3.39876 -2.46415 F -2.83088 -5.48264 -1.24382 F -0.24978 -5.15158 -0.36938 F -2.69834 0.07824 -0.22489 F -0.31943 3.10580 -3.07578 F -2.19688 4.95631 -2.64664 F -4.34351 4.41625 -1.01149 F -4.55941 1.94996 0.17451 GE 0.00000 0.00000 -1.86581	278	
$\text{Ge}(\text{C}_6\text{F}_5)_4$ axial R =	$[(\text{C}_6\text{F}_5)_4\text{GeF}]^-$ axial	61.9	1.868	F 0.00000 0.00000 0.00000 C -0.73972 -1.89657 -1.70388 C -1.92016 -2.37159 -2.29359 C -0.08424 -2.80437 -0.84765 C -2.42090 -3.67230 -2.08795 C -0.54425 -4.11513 -0.62655 C -1.72996 -4.54810 -1.24016 C -0.27123 0.15670 -4.02441 C -1.50557 0.60382 -4.53105 C 0.70759 -0.05643 -5.00812 C -1.77661 0.79640 -5.89855 C 0.48956 0.11959 -6.38923 C -0.76603 0.54985 -6.83892 C 2.01333 -0.00000 -1.78795 C 2.70445 1.03456 -1.13970 C 2.77716 -1.11398 -2.16300 C 4.09795 1.00906 -0.94427 C 4.16781 -1.18613 -1.97447 C 4.83027 -0.11702 -1.35093 C -0.90020 1.80318 -1.65511 C -2.04749 1.95217 -0.86521 C -0.36174 2.96425 -2.21846 C -2.64172 3.20541 -0.63674 C -0.91886 4.23868 -2.00532 C -2.06537 4.35539 -1.20372 F -2.66007 0.88017 -0.33099 F -3.75427 3.32277 0.11249 F -2.61850 5.56207 -0.98793 F -0.36983 5.34019 -2.55087 F 0.73560 2.90208 -3.00512 F 2.19660 -2.18382 -2.74277	278	

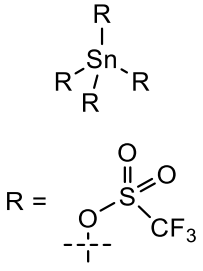
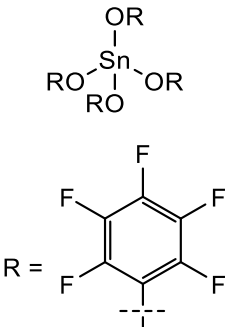
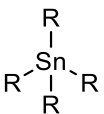
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$\text{Ge}(\text{OC}_6\text{F}_5)_4$ equatorial  R =	$[(\text{OC}_6\text{F}_5)_4\text{GeF}]^-$ equatorial	62.0	1.762	F 0.00000 0.00000 0.00000 O -1.89505 0.02634 -1.82307 O -0.02802 -1.60126 -2.66065 O 1.89286 0.00000 -1.82957 O 0.04059 1.51784 -2.81277 C -2.75119 -0.37084 -0.88547 C -2.62028 -1.55881 -0.11669 C -3.93030 0.39238 -0.66258 C -3.57011 -1.92295 0.85249 C -4.89018 0.02747 0.29422 C -4.72435 -1.14678 1.04720 C 2.73217 1.01478 -1.99620 C 2.65702 2.24036 -1.28330 C 3.80679 0.88387 -2.91755 C 3.60554 3.26087 -1.46041 C 4.76698 1.89326 -3.09015 C 4.66324 3.09619 -2.37086 C -0.97562 2.32536 -3.15237 C -1.63869 3.14790 -2.21206 C -1.37182 2.43065 -4.50772 C -2.63127 4.05871 -2.60512 C -2.35881 3.34555 -4.91056 C -2.99952 4.15601 -3.95786 C 1.04138 -2.31476 -3.05024 C 1.45695 -2.30553 -4.40231 C 1.75863 -3.13949 -2.15140 C 2.50983 -3.11985 -4.85034 C 2.81600 -3.95241 -2.58945 C 3.20150 -3.93750 -3.94131 F -1.55320 -2.35255 -0.28611 F -3.39940 -3.04853 1.56875 F -5.64549 -1.50842 1.96033 F -5.98542 0.78778 0.47584 F -4.12845 1.51737 -1.37156 F 1.66274 2.43166 -0.40233 F 3.50424 4.40465 -0.75979 F 5.57697 4.07107 -2.53790 F 5.77743 1.72411 -3.96238 F 3.92287 -0.24854 -3.63223 F -0.78158 1.66061 -5.43163 F -2.70547 3.44030 -6.20656 F -3.94834 5.02881 -4.34070 F -3.24271 4.83101 -1.69245 F -1.31319 3.05551 -0.91530 F 0.82733 -1.51310 -5.27978 F 1.42044 -3.15091 -0.85537 F 3.47449 -4.73788 -1.71887 F 2.87611 -3.10442 -6.14368 F 4.21238 -4.71707 -4.36463 GE -0.00000 0.00000 -1.76175	436	
$\text{Ge}(\text{OTf})_4$ axial  R =	$[(\text{OTf})_4\text{GeF}]^-$ axial	63.4	1.797	F 0.00000 0.00000 0.00000 S 2.47859 -0.00000 -1.69927 O 3.00138 -0.73008 -2.89126 O 3.00838 1.34158 -1.32161 S -0.87077 2.34499 -1.89898 O -0.74702 2.93726 -0.53962 O -0.36095 3.05266 -3.10534 S 0.06293 -0.18735 -4.40968 O 0.46734 -1.49798 -4.99927 O -1.30429 0.36952 -4.69347 S -1.45221 -2.04616 -1.53852 O -0.53112 -3.21707 -1.47520 O -2.42025 -1.76588 -0.44158 C 1.30162 1.09633 -5.25292 C -2.80092 2.19225 -2.15311 C 2.93813 -1.15370 -0.20175 C -2.62843 -2.45795 -3.03614 F 4.20106 -1.58117 -0.37589 F 2.11685 -2.21000 -0.17950 F 2.85790 -0.49114 0.95481 F -3.41301 3.06470 -1.33936 F -3.14313 2.44787 -3.41403 F -3.17453 0.94553 -1.81948 F 1.96119 1.78625 -4.31400 F 0.60438 1.94044 -6.02210	524	

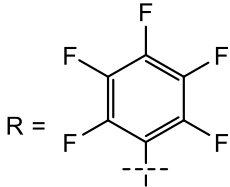
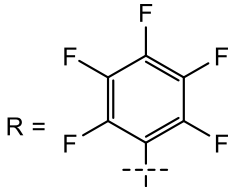
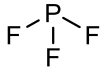
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$\text{Ge}(\text{OC}_6\text{F}_5)_4$ axial 	$[(\text{OC}_6\text{F}_5)_4\text{GeF}]^-$ axial	67.0	1.775	F 0.00000 0.00000 0.00000 O -0.05527 -1.89381 -1.80787 O -0.01503 1.88890 -1.82644 O 1.65598 0.00000 -2.57109 O -1.42553 -0.01106 -2.94336 C 2.44372 -1.06422 -2.79239 C 3.22405 -1.64120 -1.76334 C 2.56738 -1.61355 -4.09104 C 4.12237 -2.68835 -2.02092 C 3.46742 -2.65811 -4.35924 C 4.23830 -3.20856 -3.32094 C -2.03515 1.07963 -3.43580 C -1.67379 1.60826 -4.69835 C -3.09594 1.70976 -2.74156 C -2.36580 2.69259 -5.26274 C -3.79067 2.79613 -3.29780 C -3.42081 3.29734 -4.55807 C 0.53916 2.67625 -0.90245 C -0.16641 3.04797 0.27212 C 1.84262 3.21436 -1.06757 C 0.38321 3.92962 1.21627 C 2.39575 4.10236 -0.12861 C 1.67631 4.44774 1.02749 C -0.54952 -2.70230 -0.87604 C 0.14319 -3.90118 -0.55599 C -1.77261 -2.47856 -0.19069 C -0.34801 -4.81576 0.38909 C -2.26315 -3.38007 0.76762 C -1.55953 -4.56209 1.05447 F 3.11163 -1.17019 -0.51276 F 1.82867 -1.11775 -5.09209 F 3.58134 -3.15133 -5.60533 F 5.09678 -4.21221 -3.57507 F 4.85949 -3.21090 -1.02641 F -1.40439 2.57786 0.47155 F 2.55712 2.90889 -2.15858 F 3.62701 4.61016 -0.32164 F 2.20772 5.29187 1.93104 F -0.31585 4.27289 2.31323 F -0.65834 1.06007 -5.37700 F -2.01381 3.16804 -6.47044 F -4.08626 4.33552 -5.09525 F -4.80449 3.36971 -2.62643 F -3.45595 1.25536 -1.53550 F -2.48052 -1.36850 -0.45217 F -3.42432 -3.12884 1.39734 F -2.03591 -5.43716 1.96029 F 0.33843 -5.94061 0.66093 F 1.30959 -4.16915 -1.16862 GE -0.00000 0.00000 -1.77488	436	
SnF_4 	$[\text{SnF}_5]^-$	36.3	1.982	F 0.00000 0.00000 0.00000 F -0.97041 1.71605 -1.99325 F 0.01094 -0.01935 -3.96427 F 1.97160 -0.00000 -1.97675 F -1.01619 -1.68955 -1.97676 SN 0.00000 -0.00000 -1.98220	412	
$\text{Sn}(\text{CN})_4$ equatorial 	$[(\text{NC})_4\text{SnF}]^-$ equatorial	39.3	1.980	F 0.00000 0.00000 0.00000 C -1.80310 0.00004 -3.19354 C 1.83099 -0.00000 -3.14794 C -0.01096 -2.20872 -1.83158 C -0.01091 2.20873 -1.83158 N 2.84428 0.00005 -3.74273 N -0.01870 3.38287 -1.76564 N -2.79911 0.00012 -3.81698 N -0.01878 -3.38287 -1.76564 SN 0.00000 -0.00000 -1.97960		
SnCl_4 equatorial 	$[\text{Cl}_4\text{SnF}]^-$ equatorial	39.7	1.975	F 0.00000 0.00000 0.00000 CL -2.45010 0.00000 -1.90952 CL 0.00000 2.09804 -3.18724 CL 0.00000 -2.09804 -3.18724 CL 2.45010 0.00000 -1.90952 SN 0.00000 0.00000 -1.97468	360	
$\text{Sn}(\text{CN})_4$ axial	$[(\text{NC})_4\text{SnF}]^-$ axial	40.8	1.997	F 0.00000 0.00000 0.00000 C -1.08638 -1.87535 -1.95796 C 2.16729 0.00000 -1.95796 C 0.00126 -0.00218 -4.22733 C -1.08228 1.87773 -1.95968		

				N 3.34171 -0.00041 -1.92567 N 0.00230 -0.00399 -5.40370 N -1.66876 2.89526 -1.92861 N -1.67472 -2.89177 -1.92567 SN -0.00000 0.00000 -1.99693		
SnBr₄ equatorial 	[Br ₄ SnF] ⁻ equatorial	41.1	1.976	BR 0.00000 -2.26199 -3.24184 BR -0.00000 2.26199 -3.24184 BR -2.62489 -0.00000 -1.90154 BR 2.62489 -0.00000 -1.90154 F 0.00000 0.00000 0.00000 SN 0.00000 0.00000 -1.97632	364	
SnCl₄ axial 	[Cl ₄ SnF] ⁻ axial	41.8	1.984	CL -1.22449 -2.09156 -1.94483 CL 2.42363 0.00000 -1.94483 CL 0.00473 -0.00825 -4.44019 CL -1.20536 2.10240 -1.95073 F 0.00000 0.00000 0.00000 SN -0.00000 0.00000 -1.98360	360	
SnI₄ equatorial 	[I ₄ SnF] ⁻ equatorial	43.1	1.981	F 0.00000 0.00000 0.00000 I 2.86982 0.00000 -1.83004 I 0.00000 -2.44524 -3.39839 I 0.00000 2.44524 -3.39839 I -2.86982 0.00000 -1.83004 SN 0.00000 -0.00000 -1.98093	331	
SnBr₄ axial 	[Br ₄ SnF] ⁻ axial	43.5	1.984	F 0.00000 0.00000 0.00000 BR -1.29167 -2.24382 -1.93569 BR 2.58904 0.00000 -1.93569 BR -0.00129 0.00222 -4.62524 BR -1.29592 2.24130 -1.93364 SN -0.00000 0.00000 -1.98406	364	
SnI₄ axial 	[I ₄ SnF] ⁻ axial	45.9	1.988	I -1.36388 -2.46517 -1.91682 I 2.81731 -0.00000 -1.91682 I -0.01324 0.02246 -4.89479 I -1.43147 2.42793 -1.89777 F 0.00000 0.00000 0.00000 SN 0.00000 -0.00000 -1.98780	331	
Sn(CF₃)₄ equatorial 	[(CF ₃) ₄ SnF] ⁻ equatorial	47.1	2.013	C 0.01687 -2.28597 -1.83099 C 1.88000 0.00000 -3.32302 C -1.99746 0.00285 -3.10983 F 0.98638 -2.78460 -1.00831 F -1.17115 -2.77348 -1.35029 F 0.20588 -2.90063 -3.04523 F -3.05302 -0.00118 -2.24143 F -2.16540 -1.08607 -3.91974 F -2.16792 1.09629 -3.91280 F 1.59178 0.05032 -4.66233 F 2.65460 -1.11086 -3.14360 F 2.69553 1.06704 -3.06940 F 0.00000 0.00000 0.00000 C 0.02520 2.28608 -1.83200 F 0.23389 2.89756 -3.04481 F -1.16746 2.77939 -1.36879 F 0.98498 2.78243 -0.99704 SN 0.00000 -0.00000 -2.01283		
Sn(CF₃)₄ axial 	[(CF ₃) ₄ SnF] ⁻ axial	50.0	2.029	F 0.00000 0.00000 0.00000 C 2.26102 -0.00000 -1.95446 C 0.00021 -0.00524 -4.35546 C -1.12336 1.96206 -1.95547 C -1.13774 -1.95394 -1.95175 F 2.75733 1.27664 -1.88712 F 2.77007 -0.66399 -0.88201 F 2.83230 -0.57097 -3.05776 F 0.87627 0.90284 -4.89820 F 0.35022 -1.21979 -4.89332 F -1.22513 0.29724 -4.89765 F -0.28573 -3.02517 -1.86794 F -1.90822 -2.16835 -3.06081 F -1.97822 -2.05112 -0.88659 F -2.47774 1.75961 -1.88360 F -0.91483 2.73988 -3.06061		

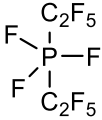
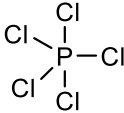
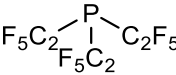
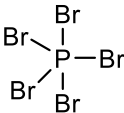
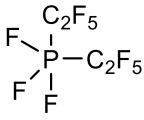
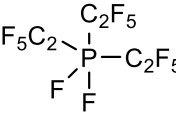
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$\text{Sn}(\text{OTf})_4$ equatorial 	$[(\text{OTf})_4\text{SnF}]^-$ equatorial	55.5	1.982	S -0.16550 -2.65032 -2.78550 O 0.60386 -3.56103 -1.88677 O -1.54467 -2.99575 -3.24268 S 2.72751 -0.00000 -1.79728 O 3.42290 -1.00857 -2.65527 O 3.14643 1.43935 -1.81835 S -0.03611 2.59469 -2.94541 O -1.25467 2.54048 -3.81587 O 0.17591 3.71442 -1.98376 C 3.16464 -0.57739 0.01575 C 0.85668 -2.60822 -4.46300 C 1.40090 2.77678 -4.26575 F 2.02709 -3.22742 -4.33306 F 1.06082 -1.31084 -4.78355 F 0.14903 -3.18566 -5.44242 F 2.52178 -1.71355 0.30598 F 2.84722 0.36739 0.90401 F 4.49091 -0.79965 0.06706 F 2.41000 3.50306 -3.79433 F 1.83302 1.54271 -4.59404 F 0.90712 3.36474 -5.36628 F 0.00000 0.00000 0.00000 S -2.72559 0.18657 -1.87802 O -3.20797 -1.04946 -1.19149 O -3.20861 1.53265 -1.45151 C -3.34961 -0.01763 -3.73090 F -3.96455 1.09248 -4.14141 F -4.19331 -1.05044 -3.81249 F -2.28007 -0.25488 -4.51558 SN -0.00000 0.00000 -1.98164	519	
$\text{Sn}(\text{C}_6\text{F}_5)_4$ axial 	$[(\text{C}_6\text{F}_5)_4\text{SnF}]^-$ axial	56.6	2.026	F 0.00000 0.00000 0.00000 C -0.72583 -2.10489 -1.81310 C -1.93840 -2.59079 -2.31161 C 0.03482 -2.99717 -1.04300 C -2.37606 -3.91305 -2.10338 C -0.35912 -4.32860 -0.81650 C -1.58164 -4.78191 -1.33960 C -0.46754 0.12581 -4.30290 C -1.75860 0.50619 -4.69243 C 0.44573 -0.06731 -5.34515 C -2.14920 0.66625 -6.03461 C 0.10774 0.07911 -6.70474 C -1.20206 0.44863 -7.04818 C 2.20391 0.00000 -2.06975 C 2.93417 1.03079 -1.46788 C 2.92915 -1.09847 -2.54319 C 4.33975 1.01408 -1.39529 C 4.33232 -1.16097 -2.48450 C 5.03715 -0.09859 -1.89380 C -0.87158 2.03536 -1.81054 C -1.99142 2.27604 -1.01006 C -0.25935 3.13663 -2.41102 C -2.50006 3.57242 -0.81116 C -0.72917 4.45104 -2.23386 C -1.85376 4.66353 -1.41879 F -2.65640 1.25844 -0.43067 F -3.58813 3.78896 -0.04872 F -2.32330 5.90962 -1.23300 F -0.12074 5.50006 -2.81828 F 0.82089 2.96915 -3.20861 F 2.29534 -2.15213 -3.09772 F 2.31316 2.10486 -0.94307 F 5.02093 2.02808 -0.83180 F 6.37813 -0.13942 -1.82093 F 5.00567 -2.22491 -2.95765 F 1.21017 -2.62473 -0.50354 F -2.76094 -1.79828 -3.02979 F -3.54924 -4.34489 -2.60186 F -1.98060 -6.04645 -1.12210 F 0.40310 -5.16698 -0.09105 F 1.73368 -0.40100 -5.10034 F -2.71601 0.75217 -3.76784 F -3.40400 1.02748 -6.36316 F -1.54699 0.59537 -8.33933 F 1.01877 -0.11911 -7.67714 SN -0.00000 0.00000 -2.02621	332	

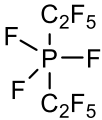
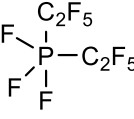
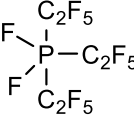
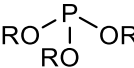
$\text{Sn}(\text{OTf})_4$ axial	$[(\text{OTf})_4\text{SnF}]^-$ axial	57.0	1.991	F 0.00000 0.00000 0.00000 S -0.86416 -2.57365 -1.76576 O -1.74076 -2.78187 -2.96559 O 0.12954 -3.60984 -1.35290 S 2.70455 -0.00000 -2.27225 O 3.31828 0.15888 -0.92284	519	
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				O 3.16175 -1.06343 -3.21221 S -0.74364 -0.20306 -4.71973 O -2.13979 -0.16142 -5.25159 O 0.24314 0.86193 -5.12742 S -1.12861 2.46407 -1.64045 O -2.50201 2.22515 -1.10234 O -0.16824 3.35942 -0.92938 C 0.02276 -1.83018 -5.51193 C 3.12921 1.68467 -3.17124 C -2.14253 -2.50822 -0.29940 C -1.47379 3.40421 -3.30913 F -3.01775 -3.51809 -0.43806 F -2.80810 -1.34319 -0.35686 F -1.52809 -2.61970 0.88002 F 4.25545 2.18587 -2.64595 F 3.29448 1.49231 -4.47897 F 2.12148 2.54498 -2.95778 F 0.81822 -2.42447 -4.60893 F 0.75634 -1.48482 -6.58076 F -0.93981 -2.67018 -5.89200 F -0.33072 3.73767 -3.91308 F -2.21618 2.64413 -4.11970 F -2.15545 4.52311 -3.00709 SN 0.00000 0.00000 -1.99116		
$\text{Sn}(\text{OC}_6\text{F}_5)_4$ equatorial 	$[(\text{OC}_6\text{F}_5)_4\text{SnF}]^-$ equatorial	58.6	1.960	F 0.00000 0.00000 0.00000 O 0.04856 -2.07638 -2.20770 O 1.88954 -0.00000 -2.80615 O 0.01559 2.06621 -2.28295 O -2.09163 -0.02142 -2.20521 C -0.22844 -2.89586 -1.19380 C 0.67125 -3.09409 -0.11139 C -1.44018 -3.63662 -1.15730 C 0.40653 -4.01590 0.91271 C -1.70941 -4.56937 -0.14243 C -0.79721 -4.74306 0.91231 C -0.95929 2.88282 -1.88716 C -0.93330 3.50832 -0.61139 C -2.05906 3.19219 -2.73063 C -1.91358 4.43798 -0.22736 C -3.04460 4.11721 -2.35334 C -2.98725 4.72708 -1.08766 C -2.67134 -0.51295 -3.29251 C -4.04582 -0.86977 -3.28112 C -1.98565 -0.70699 -4.51498 C -4.68041 -1.36981 -4.42923 C -2.59771 -1.21762 -5.66607 C -3.96254 -1.55152 -5.62550 C 2.62980 1.09109 -3.00492 C 2.86294 1.58318 -4.31583 C 3.25645 1.78417 -1.93642 C 3.72176 2.66866 -4.55197 C 4.10803 2.87608 -2.16191 C 4.33401 3.33077 -3.47350 F 1.82427 -2.41222 -0.08834 F 1.28937 -4.19578 1.91079 F -1.05506 -5.62749 1.89288 F -2.85506 -5.27381 -0.15434 F -2.33882 -3.47847 -2.14279 F 0.07661 3.24729 0.22780 F -1.84781 5.03553 0.97523 F -3.93185 5.61037 -0.71846 F -4.06229 4.40413 -3.18385 F -2.14290 2.61240 -3.93889 F -0.66441 -0.38385 -4.54762 F -1.89833 -1.38301 -6.79981 F -4.57758 -2.03550 -6.72063 F -5.98554 -1.69080 -4.38770 F -4.75809 -0.72133 -2.15411 F 2.27064 0.98482 -5.35888 F 3.03586 1.37490 -0.67951 F 4.70093 3.50245 -1.13084 F 3.94293 3.09857 -5.80733 F 5.15315 4.37417 -3.69642 SN 0.00000 -0.00000 -1.95981	332	
$\text{Sn}(\text{C}_6\text{F}_5)_4$ equatorial 	$[(\text{C}_6\text{F}_5)_4\text{SnF}]^-$ equatorial	58.7	1.986	C 0.00000 0.00000 0.00000 F 0.05627 1.99194 -2.99424 C -0.07881 2.19978 -4.36968 C 0.28601 3.11900 -2.19932 C 0.01326 3.47868 -4.94897 C 0.38293 4.41634 -2.73455 C 0.24344 4.59092 -4.12167 C -0.04197 -1.95534 -3.07198 C 0.67764 -3.04556 -2.56978 C -0.83349 -2.18391 -4.20232 C 0.65256 -4.31316 -3.18019 C -0.88598 -3.43343 -4.84787 C -0.13826 -4.50259 -4.32619 C 2.30112 -0.00000 -1.95055 C 3.14357 -0.01799 -0.83022 C 2.93416 0.02516 -3.19723	492	

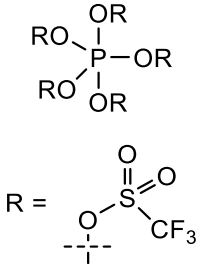
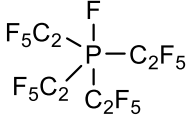
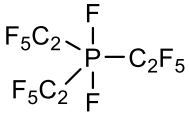
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$\text{Sn}(\text{OC}_6\text{F}_5)_4$ axial 	$[(\text{OC}_6\text{F}_5)_4\text{SnF}]^-$ axial	65.4	1.981	F 0.00000 0.00000 0.00000 O -2.02635 0.53790 -1.94557 O 2.08658 0.00000 -2.00842 O -0.38871 -1.97053 -2.42556 O 0.09670 0.96488 -3.81178 C -1.38924 -2.62428 -1.82123 C -1.20172 -3.27691 -0.57538 C -2.67843 -2.70644 -2.40843 C -2.22521 -4.03208 0.02030 C -3.70675 -3.45885 -1.81856 C -3.49005 -4.10450 -0.58872 C 1.20796 1.15056 -4.52541 C 1.79523 0.11109 -5.29307 C 1.83491 2.42294 -4.57889 C 2.90735 0.34050 -6.11731 C 2.94308 2.66378 -5.40662 C 3.49604 1.61679 -6.16447 C 2.82255 -0.22794 -0.91944 C 3.07138 0.78887 0.03853 C 3.40268 -1.49988 -0.67402 C 3.91073 0.57514 1.14190 C 4.25212 -1.72052 0.42263 C 4.48591 -0.69115 1.35073 C -2.50189 1.40727 -1.06501 C -3.82804 1.28398 -0.57010 C -1.75167 2.51122 -0.58641 C -4.36369 2.21766 0.33197 C -2.26431 3.43742 0.33107 C -3.58659 3.29729 0.78910 F -0.00686 -3.21266 0.02748 F -2.91106 -2.08934 -3.57275 F -4.91205 -3.54118 -2.40788 F -4.47479 -4.82149 -0.01850 F -2.01227 -4.66430 1.18779 F 2.51992 1.99808 -0.13829 F 3.17771 -2.50301 -1.53322 F 4.81506 -2.92693 0.61318 F 5.28976 -0.90269 2.40830 F 4.14711 1.56508 2.02055 F 1.26406 -1.11760 -5.23991 F 3.43029 -0.65906 -6.84861 F 4.56087 1.84215 -6.95470 F 3.50023 3.88699 -5.45759 F 1.34136 3.42951 -3.84367 F -0.47985 2.64817 -1.03167 F -1.51331 4.46481 0.75941 F -4.10441 4.18827 1.65531 F -5.62719 2.07892 0.77204 F -4.59075 0.25613 -0.97551 SN -0.00000 0.00000 -1.98109	492	
PF_3 	$[\text{PF}_4]^-$ trans	29.6	1.754	P 0.00000 -0.00000 -1.75439 F 0.17772 1.70033 -2.14829 F 1.67222 -0.00000 -1.61606 F 0.00000 0.00000 0.00000 F 0.34766 -1.42454 -2.85313	200	
PF_3	$[\text{PF}_4]^-$ cis	36.3	1.678	P 0.00000 0.00000 -1.67793 F -1.08282 1.37276 -1.53330 F 0.00000 0.00000 0.00000	200	

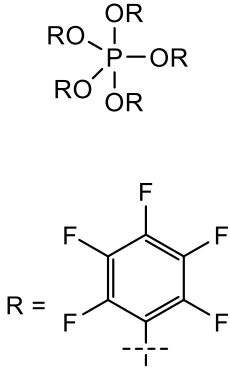
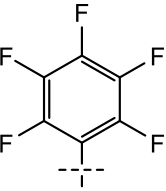
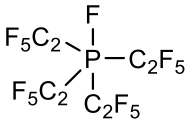
$\begin{array}{c} \text{F} \\ \\ \text{P} \\ \\ \text{F} \end{array}$				F -1.08282 -1.37276 -1.53330 F 1.81437 0.00000 -1.42204		
PF_5 $\begin{array}{c} \text{F} \\ \\ \text{F}-\text{P}-\text{F} \\ \\ \text{F} \end{array}$	$[\text{PF}_6]^-$	38.4	1.653	P 0.00000 -0.00000 -1.65304 F 0.00000 0.00000 0.00000 F 1.65304 -0.00000 -1.65304 F 0.00000 -1.65304 -1.65304 F -1.65304 -0.00000 -1.65304 F 0.00000 1.65304 -1.65304 F 0.00000 -0.00000 -3.30608	384	394 ^{2b} 380 ^{2c}
$\text{P}(\text{C}_2\text{F}_5)\text{F}_4$ $\begin{array}{c} \text{F} \\ \\ \text{F}-\text{P}-\text{C}_2\text{F}_5 \\ \\ \text{F} \end{array}$	$[(\text{C}_2\text{F}_5)\text{PF}_5]^-$ <i>trans</i>	38.5	1.658	P -0.00000 0.00000 -1.64787 F 0.01353 1.65742 -1.65563 F 0.00000 0.00000 0.00000 F -1.66118 -0.00025 -1.66339 F 0.01435 -1.65737 -1.65538 C -0.06943 0.00137 -3.59832 C 1.26073 0.00615 -4.39930 F 2.00453 1.10245 -4.15424 F 0.99307 0.00869 -5.74114 F -0.75060 -1.10062 -4.06348 F -0.75643 1.10095 -4.06054 F 2.00921 -1.08815 -4.15952 F 1.66443 0.00000 -1.65985		
PCl_3 $\begin{array}{c} \text{Cl} \\ \\ \text{P} \\ \\ \text{Cl} \end{array}$	$[\text{Cl}_3\text{PF}]^-$	42.0	1.637	F 0.00000 0.00000 0.00000 CL -0.13758 -2.12637 -1.97339 CL 2.40652 0.00000 -1.58202 CL -2.38604 0.31150 -1.57876 P 0.00000 -0.00000 -1.63664	265	
PBr_3 $\begin{array}{c} \text{Br} \\ \\ \text{P} \\ \\ \text{Br} \end{array}$	$[\text{Br}_3\text{PF}]^-$	45.0	1.630	F 0.00000 0.00000 0.00000 P 0.00000 -0.00000 -1.63035 BR -1.26391 -2.19161 -1.65815 BR -1.26846 2.18909 -1.65612 BR 2.53029 -0.00000 -1.65634	286	
PI_3 $\begin{array}{c} \text{I} \\ \\ \text{P} \\ \\ \text{I} \end{array}$	$[\text{I}_3\text{PF}]^-$	45.9	1.632	F 0.00000 0.00000 0.00000 I 2.75684 -0.00000 -1.78011 I -1.37857 -2.38895 -1.77408 I -1.36741 2.39482 -1.77683 P -0.00000 0.00000 -1.63203		
$\text{P}(\text{CF}_3)_3$ $\begin{array}{c} \text{F}_3\text{C} \\ \\ \text{P} \\ \\ \text{F}_3\text{C} \end{array}$	$[(\text{CF}_3)_3\text{PF}]^-$	46.4	1.823	F 0.00000 0.00000 0.00000 P -0.00000 0.00000 -1.82275 C 0.25066 0.38080 -3.80913 C -0.64011 1.80826 -1.52144 C 1.91852 0.00000 -1.54725 F 0.73981 -0.76591 -4.39627 F -1.00198 0.54570 -4.36066 F 1.01123 1.40304 -4.32479 F -1.85288 1.74245 -0.89304 F 0.15912 2.56553 -0.72834 F -0.85941 2.55924 -2.64194 F 2.39984 1.09677 -0.90432 F 2.26574 -1.07540 -0.78186 F 2.66703 -0.11832 -2.68494		
$\text{P}(\text{C}_2\text{F}_5)\text{F}_4$ $\begin{array}{c} \text{F} \\ \\ \text{F}-\text{P}-\text{F} \\ \\ \text{F} \end{array}$	$[(\text{C}_2\text{F}_5)\text{PF}_5]^-$ <i>cis</i>	47.5	1.657	P -0.00000 -0.00000 -1.65744 F -0.01526 -0.02788 -3.31464 F 1.64786 0.00000 -1.66491 F -0.01558 1.66112 -1.67150 F 0.00000 0.00000 0.00000 C -1.95043 0.06941 -1.65059 C -2.75138 -1.26073 -1.64023 F -2.51126 -2.01400 -2.73114 F -4.09322 -0.99311 -1.63901 F -2.41062 0.76010 -0.55244 F -2.41766 0.74687 -2.75396 F -2.50662 -1.99972 -0.54058 F -0.01191 -1.66437 -1.64298		
$\text{P}(\text{CN})_5$ $\begin{array}{c} \text{CN} \\ \\ \text{NC}-\text{P}-\text{CN} \\ \\ \text{NC} \end{array}$	$[(\text{NC})_5\text{PF}]^-$	48.0	1.668	P 0.00000 -0.00000 -1.66845 F 0.00000 0.00000 0.00000 C -1.88045 -0.00000 -1.65363 C 0.00000 1.88045 -1.65363 C 0.00000 -1.88045 -1.65363 C 1.88045 0.00000 -1.65363 C 0.00000 0.00000 -3.53803 N 3.05398 -0.00000 -1.60628 N 0.00000 0.00000 -4.71240 N 0.00000 3.05398 -1.60628 N -3.05398 -0.00000 -1.60628 N 0.00000 -3.05398 -1.60628		

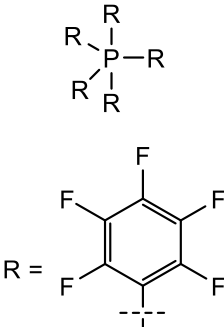
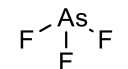
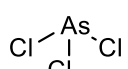
$\text{P}(\text{C}_2\text{F}_5)_2\text{F}_3$ 	$[(\text{C}_2\text{F}_5)_2\text{PF}_4]^-$ <i>cis/trans</i>	49.5	1.659	P 0.00000 0.00000 -1.65874 C 0.08304 1.97217 -1.55745 C -1.21305 2.75300 -1.20312 F 1.66368 0.00000 -1.69717 F 0.00000 0.00000 0.00000 F -1.67166 0.01113 -1.66228 F 0.53806 2.54006 -2.72707 F 0.98704 2.32792 -0.58781 F -1.75524 2.33687 -0.04320 F -0.92184 4.08001 -1.05132 F -2.14524 2.67008 -2.16928 F -0.00178 -1.66358 -1.64260 C -0.07171 -0.03411 -3.62927 C -0.45998 -1.37714 -4.31867 F -1.01274 0.86454 -4.07816 F 1.12445 0.31190 -4.20577 F -0.60948 -1.16438 -5.66077 F 0.49652 -2.31573 -4.18495 F -1.62653 -1.87537 -3.87292		
PCl_5 	$[\text{Cl}_5\text{PF}]^-$	49.6	1.642	P 0.00000 0.00000 -1.64233 F 0.00000 0.00000 0.00000 Cl -2.20394 0.00000 -1.63050 Cl 0.00000 2.20394 -1.63050 Cl 2.20394 -0.00000 -1.63050 Cl 0.00000 -2.20394 -1.63050 Cl 0.00000 -0.00000 -3.84765	396	393 ^{2c}
$\text{P}(\text{C}_2\text{F}_5)_3$ 	$[(\text{C}_2\text{F}_5)_3\text{PF}]^-$	51.6	1.788	F 0.00000 0.00000 0.00000 C 1.94703 0.00000 -1.54921 C -0.72409 -1.80863 -1.50567 C 0.16883 -0.00736 -3.91933 F 2.64402 0.16354 -2.71878 F 2.22590 1.11337 -0.78733 F -0.04290 -2.48631 -0.52927 F -1.99866 -1.58554 -1.01974 F -1.16466 0.11397 -4.30146 F 0.70727 1.27154 -4.04114 C 0.82550 -0.80810 -5.08458 C -0.92269 -2.86715 -2.62164 C 2.67688 -1.18067 -0.83948 F 1.06245 -0.02121 -6.17761 F 0.02537 -1.81354 -5.51182 F 2.01135 -1.35665 -4.74381 F -1.76616 -2.44184 -3.57691 F -1.46508 -3.99771 -2.08920 F 0.24957 -3.22049 -3.18393 F 2.29651 -1.37209 0.42940 F 4.01737 -0.92693 -0.81787 F 2.50421 -2.32950 -1.52722 P 0.00000 -0.00000 -1.78821	271	
PBr_5 	$[\text{Br}_5\text{PF}]^-$	52.5	1.642	P -0.00000 0.00000 -1.64177 F 0.00000 0.00000 0.00000 Br -2.40817 -0.00000 -1.61256 Br -0.00000 2.40817 -1.61256 Br 2.40817 0.00000 -1.61256 Br 0.00000 -2.40817 -1.61256 Br -0.00000 0.00000 -4.06007	406	
$\text{P}(\text{C}_2\text{F}_5)_2\text{F}_3$ 	$[(\text{C}_2\text{F}_5)_2\text{PF}_4]^-$ <i>cis/cis</i>	52.7	1.664	P -0.00000 0.00000 -1.66413 C -1.97108 -0.12227 -1.58344 C -2.74874 -0.45411 -2.88737 F 0.00000 0.00000 0.00000 F 0.01605 -1.65822 -1.70243 F -0.01153 0.04203 -3.33525 F -2.55016 1.03099 -1.10154 F -2.31723 -1.11592 -0.70208 F -2.32152 -1.59712 -3.45621 F -4.07415 -0.62544 -2.59975 F -2.67538 0.53407 -3.79700 F 1.66365 0.00000 -1.66628 C 0.01502 1.97190 -1.69031 C 1.35124 2.68304 -2.06256 F -0.88813 2.43368 -2.62073 F -0.33628 2.51725 -0.48116 F 1.12547 4.02612 -2.18102 F 2.29129 2.53636 -1.10940 F 1.85349 2.26919 -3.23909		
$\text{P}(\text{C}_2\text{F}_5)_3\text{F}_2$ 	$[(\text{C}_2\text{F}_5)_3\text{PF}_3]^-$ <i>fac</i>	54.8	1.668	P 0.00000 0.00000 -1.66761 F 0.02450 1.66885 -1.69692 F 0.00000 0.00000 0.00000 F 1.67855 0.00000 -1.65318 C 0.24611 -2.03041 -1.60475 C -2.01269 0.13188 -1.40826 C 0.02364 0.07836 -3.65621 C 1.36931 0.41279 -4.37209 C -0.85861 -3.13518 -1.70623 C -3.12117 0.33596 -2.49025		388 ^{2c}

				F -2.22200 1.18210 -0.55231 F -2.40422 -1.00162 -0.73054 F -4.34244 0.13750 -1.91781 F -3.12536 1.59052 -2.97823 F -3.02697 -0.52925 -3.51683 F 0.90311 -2.32201 -0.43837 F 1.11930 -2.33924 -2.62227 F -1.46501 -3.35705 -0.52381 F -0.28882 -4.31795 -2.07081 F -1.79836 -2.85368 -2.62872 F -0.82427 1.07953 -4.06852 F -0.43707 -1.07681 -4.23640 F 1.12910 0.55188 -5.71042 F 2.29642 -0.54826 -4.24557 F 1.88643 1.57743 -3.94299		
$P(C_2F_5)_2F_3$ 	$[(C_2F_5)_2PF_4]^-$ <i>trans/trans</i>	56.6	1.664	P 0.00000 0.00000 -1.66392 C -0.08006 -1.94883 -1.66581 C 0.07982 1.94885 -1.66010 C -1.25136 2.74916 -1.63326 C 1.25111 -2.74954 -1.67851 F 1.67340 0.00000 -1.66407 F 0.00000 0.00000 0.00000 F -1.67343 -0.00006 -1.66422 F 0.00001 0.00004 -3.32766 F -0.77531 -2.39930 -2.76174 F -0.75805 -2.40406 -0.56113 F 2.00129 -2.50875 -0.58655 F 0.98198 -4.08898 -1.68329 F 1.98682 -2.49765 -2.77782 F 0.74751 2.40676 -2.76996 F 0.78503 2.39702 -0.56962 F -1.97895 2.49124 -0.53002 F -0.98250 4.08863 -1.62346 F -2.00941 2.51398 -2.72105		
$P(C_2F_5)_2F_3$ 	$[(C_2F_5)_2PF_4]^-$ <i>trans/cis</i>	59.1	1.673	P -0.00000 0.00000 -1.67343 C 0.00182 1.94883 -1.59331 C -0.00376 -1.94885 -1.75332 C -0.03081 -2.74920 -0.42218 C 0.01475 2.74958 -2.92444 F 0.00046 0.00006 -3.34684 F -1.66392 -0.00004 -1.67374 F 0.00000 0.00000 0.00000 F 1.66374 0.00000 -1.67315 F 1.09762 2.39930 -0.89784 F -1.10299 2.40400 -0.91550 F -1.07707 2.50879 -3.67483 F 0.01945 4.08901 -2.65527 F 1.11420 2.49774 -3.65997 F 1.10624 -2.40671 -2.42082 F -1.09409 -2.39702 -2.45874 F -1.13420 -2.49134 0.30522 F -0.04053 -4.08866 -0.69108 F 1.05683 -2.51402 0.33609		
$P(C_2F_5)_3F_2$ 	$[(C_2F_5)_3PF_3]^-$ <i>mer/cis-1</i>	59.3	1.669	P 0.00000 0.00000 -1.66893 F 0.00000 0.00000 0.00000 F 1.68544 -0.00000 -1.67628 F -0.04659 0.00011 -3.34778 C 0.10714 1.97870 -1.70285 C -2.00269 -0.00040 -1.54344 C -2.92560 -0.00190 -2.80371 C 0.10853 -1.97877 -1.70022 C 1.43436 -2.62713 -2.21594 F -2.39997 1.09801 -0.81821 F -2.39914 -1.09797 -0.81653 F -2.76004 -1.08975 -3.57465 F -2.76164 1.08489 -3.57656 F -4.22805 -0.00244 -2.39104 F -0.86335 -2.49762 -2.52006 F -0.07688 -2.52472 -0.45763 F 1.81730 -2.15229 -3.41352 F 1.23611 -3.97038 -2.36714 F 2.44831 -2.48759 -1.34256 F -0.86711 2.49527 -2.52140 F -0.07590 2.52681 -0.46089 C 1.43095 2.62763 -2.22313 F 2.44666 2.49213 -1.35111 F 1.23021 3.97000 -2.37811 F 1.81259 2.14987 -3.41985		388 ^{2c}
$P[OC(CF_3)_3]_3$ 	$\{[OC(CF_3)_3]_3PF\}^-$	61.9	1.630	O 1.72575 0.00000 -1.70168 • 0.22771 -1.96936 -1.56995 O 0.18387 1.96798 -1.55613 C 2.61861 -0.00179 -2.75087 C 3.92515 -0.66682 -2.16461 C 2.94183 1.48227 -3.19663 C 2.14883 -0.83147 -4.00954 C -0.72502 -2.93525 -1.56068 C 0.03267 -4.31604 -1.42635	319	

$R = \begin{array}{c} \text{CF}_3 \\ \\ \text{F}_3\text{C}-\text{C}-\text{CF}_3 \\ \\ - \end{array}$				C -1.57033 -2.95970 -2.89921 C -1.71334 -2.78416 -0.33653 C -0.79703 2.90176 -1.64301 C -1.92854 2.68158 -0.56160 C -0.11714 4.30309 -1.37626 C -1.46371 2.93933 -3.07981 F -2.55127 -1.73757 -0.53496 F -1.04139 -2.55697 0.80104 F -2.48802 -3.88471 -0.13892 F -2.03031 -1.73176 -3.20468 F -2.64635 -3.78782 -2.83966 F -0.80658 -3.37209 -3.93682 F -0.76910 -5.38668 -1.67835 F 1.06702 -4.38044 -2.27966 F 0.52643 -4.47536 -0.17824 F 0.00000 0.00000 0.00000 F -2.69979 1.61870 -0.89958 F -2.75648 3.75147 -0.42902 F -1.39960 2.43096 0.64476 F 0.20347 4.44300 -0.07083 F -0.92312 5.34962 -1.70480 F 1.01546 4.43128 -2.08523 F -2.59743 3.68767 -3.12455 F -0.60955 3.45683 -3.99172 F -1.78654 1.69989 -3.49373 F 4.10451 1.54725 -3.90034 F 3.06837 2.27819 -2.13327 F 1.96527 1.96580 -3.98857 F 2.23481 -2.15202 -3.79577 F 0.87247 -0.53575 -4.32366 F 2.91026 -0.54366 -5.09437 F 4.81435 -0.97248 -3.14180 F 4.54066 0.17205 -1.30399 F 3.63240 -1.79107 -1.50380 P -0.00000 0.00000 -1.63006		
$\text{P}(\text{C}_2\text{F}_5)_4\text{F}$	$[(\text{C}_2\text{F}_5)_4\text{PF}_2]^-$ <i>cis-1</i>	62.8	1.681	P -0.00000 -0.00000 -1.68100 C -0.32131 -2.06115 -1.55329 C -0.07215 -0.14575 -3.76574 C -0.07667 1.99466 -1.62058 C 2.05431 0.00000 -1.36932 F 0.00000 0.00000 0.00000 F 2.27681 -1.14038 -0.63982 F 2.33420 1.04801 -0.52868 F 0.83237 2.50093 -2.52286 F 0.26062 2.49848 -0.39686 F -1.37626 -0.34092 -4.12618 F 0.62214 -1.29743 -4.06620 F -1.02119 -2.24951 -0.39310 F -1.17753 -2.39644 -2.56965 C 0.73540 -3.22686 -1.54296 C -1.44844 2.69474 -1.91228 C 0.42756 0.85699 -4.86622 C 3.24761 0.05179 -2.37859 F 0.11447 -4.39139 -1.88040 F 1.26018 -3.42146 -0.31735 F 1.74160 -3.05447 -2.41927 F 3.42973 1.29604 -2.85866 F 4.39299 -0.28403 -1.72302 F 3.12204 -0.80043 -3.40890 F -2.29289 2.54078 -0.87619 F -1.23209 4.03345 -2.05597 F -2.06157 2.27453 -3.02928 F -0.27503 2.00333 -4.89285 F 0.25413 0.26650 -6.08146 F 1.73150 1.15986 -4.76523 F -1.68680 0.01642 -1.66935		
$\text{P}(\text{CF}_3)_5$	$[(\text{CF}_3)_5\text{PF}]^-$	63.9	1.700	P 0.00000 -0.00000 -1.69966 C 0.03229 2.01132 -1.45705 C -0.07733 0.04934 -3.73143 C 2.03290 -0.00000 -1.73679 C 0.07176 -2.02871 -1.46189 C -2.03887 -0.06040 -1.68065 F 0.00000 0.00000 0.00000 F -2.55729 -0.26419 -0.44741 F -2.49172 -1.07938 -2.47399 F -2.64886 1.05583 -2.16646 F -1.05389 -2.50654 -0.86297 F 1.08791 -2.33767 -0.60757 F 0.27008 -2.79742 -2.56352 F 1.10166 0.37598 -4.32490 F -0.46758 -1.12078 -4.29862 F -0.97771 0.97826 -4.15945 F 2.60351 -0.09030 -0.51336 F 2.57069 1.10638 -2.32368 F 2.49776 -1.06026 -2.46573 F 1.07544 2.35621 -0.65051 F 0.16481 2.75898 -2.58656 F -1.07308 2.47406 -0.81361		

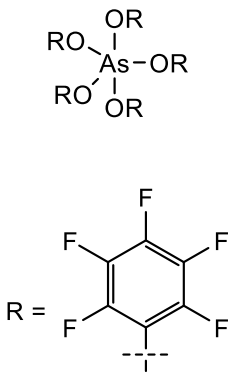
P(OTf)_5 	$[(\text{OTf})_5\text{PF}]^-$	66.4	1.651	P 0.00000 0.00000 -1.65140 S 2.46097 0.00000 -1.21819 O 2.82214 0.96957 -0.15364 • 2.72262 -1.45931 -1.03447 S -2.46619 0.07691 -1.22854 • -2.74292 -0.94990 -0.18856 O -2.65865 1.52512 -0.92109 S 0.15654 2.48785 -1.69454 O 0.14790 3.01055 -0.30479 O 1.40277 2.52514 -2.53391 S -0.17559 -2.45670 -1.64130 • 0.15994 -3.04836 -0.32416 • -1.48787 -2.70076 -2.30005 S -0.40257 0.15456 -4.24475 • -0.70453 -1.16922 -4.87613 O -1.50552 1.16615 -4.03878 C -0.98389 3.79403 -2.67659 C 3.63201 0.45643 -2.71588 C 0.63920 0.98892 -5.69937 C -3.82998 -0.28489 -2.61592 F 0.00000 0.00000 0.00000 F 2.99345 0.29619 -3.88272 F 4.08853 1.69894 -2.60707 F 4.66839 -0.39662 -2.67256 F -0.24833 1.28338 -6.66380 F 1.27218 2.10226 -5.33593 F 1.52206 0.10269 -6.17920 F -3.39009 -1.06313 -3.59436 F -4.26309 0.87750 -3.10354 F -4.84109 -0.89722 -1.97888 C 1.11650 -3.22863 -2.90700 F -2.28086 3.54062 -2.65590 F -0.54768 3.88463 -3.93380 F -0.75161 4.96149 -2.04972 F 1.74115 -2.26712 -3.60041 F 0.44048 -4.01266 -3.75074 F 2.00662 -3.96238 -2.24182	557	
$\text{P(C}_2\text{F}_5)_4\text{F}$ 	$[(\text{C}_2\text{F}_5)_4\text{PF}_2]^-$ <i>trans/trans</i>	67.4	1.683	P 0.00000 0.00000 -1.68345 C -2.02299 0.03840 -1.84288 C 0.02126 2.02893 -1.46116 C 2.04836 0.00000 -1.87643 C 0.10134 -2.02305 -1.40526 F 0.00000 0.00000 0.00000 F -1.09330 -2.34952 -0.80814 F 1.05576 -2.28185 -0.46304 F 2.33629 -1.24883 -2.40703 F 2.68995 0.07763 -0.67756 F 1.18938 2.25222 -0.75842 F 0.14205 2.65641 -2.67160 F -2.60199 0.35202 -0.64202 F -2.23615 1.10263 -2.69092 C -2.92958 -1.08905 -2.46348 C -0.98454 2.90405 -0.62358 C 2.85814 0.91499 -2.87228 C 0.32191 -3.09375 -2.55875 F -3.98422 -0.52828 -3.11265 F -3.45490 -1.90427 -1.53136 F -2.26415 -1.83304 -3.36890 F 1.47944 -3.76819 -2.37654 F -0.67008 -4.02066 -2.54034 F 0.34975 -2.56356 -3.79026 F 2.92649 2.21338 -2.53631 F 4.14619 0.46122 -2.89453 F 2.38710 0.83048 -4.12784 F -2.17985 3.10480 -1.20365 F -0.42916 4.14227 -0.47159 F -1.18252 2.40587 0.60766 F -0.02238 0.02229 -3.36280		
$\text{P(C}_2\text{F}_5)_3\text{F}_2$ 	$[(\text{C}_2\text{F}_5)_3\text{PF}_3]^-$ <i>mer/trans</i>	67.7	1.685	P 0.00000 -0.00000 -1.68545 F 1.66891 0.00000 -1.69273 F 0.00000 0.00000 0.00000 F -1.67904 -0.00011 -1.72472 C -0.03346 -1.97870 -1.57817 C 0.11675 0.00040 -3.68867 C -1.14753 0.00190 -4.60607 C -0.03082 1.97877 -1.57679 C -0.54076 2.62713 -0.24872 F 0.84024 -1.09801 -4.08911 F 0.84192 1.09797 -4.08829 F -1.91774 1.08975 -4.43716 F -1.91966 -1.08489 -4.43875 F -0.74055 0.00244 -5.91031 F -0.85490 2.49762 -2.54508 F 1.21095 2.52472 -1.76762		388 ^{2c}

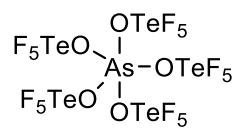
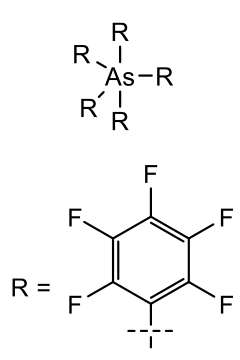
				F -1.73666 2.15229 0.13943 F -0.69282 3.97038 -0.44631 F 0.33704 2.48759 0.76141 F -0.85625 -2.49527 -2.54884 F 1.20769 -2.52681 -1.76662 C -0.54796 -2.62763 -0.25211 F 0.32848 -2.49213 0.75980 F -0.70382 -3.97000 -0.45216 F -1.74300 -2.14987 0.13476		
$P(OC_6F_5)_5$  R = 	$[(OC_6F_5)_5PF]^-$	71.3	1.647	P 0.00000 -0.00000 -1.64665 O -1.73705 0.04588 -1.61686 • -0.03402 -1.74758 -1.62572 • -0.00430 -0.04139 -3.40168 O 1.75656 0.00000 -1.69663 O -0.00268 1.76499 -1.66009 C 2.56847 0.72395 -0.90080 C 3.16040 1.91360 -1.39359 C 2.92651 0.31983 0.41045 C 4.07673 2.65751 -0.63383 C 3.84083 1.06472 1.17658 C 4.41412 2.23813 0.66285 C -0.77179 2.52174 -0.84947 C -0.27275 2.99325 0.39149 C -2.07432 2.95043 -1.21752 C -1.02389 3.83674 1.22693 C -2.83023 3.79492 -0.38434 C -2.31136 4.24090 0.84136 C -2.59881 -0.86359 -2.10283 C -3.21280 -0.68757 -3.36674 C -3.02176 -1.95964 -1.31095 C -4.17423 -1.59793 -3.83834 C -3.97822 -2.87355 -1.78267 C -4.57072 -2.68490 -3.04270 C 0.66922 -2.58283 -2.41340 C 0.13884 -3.07903 -3.63033 C 1.91682 -3.10939 -1.99509 C 0.84680 -3.99504 -4.42559 C 2.62956 -4.02627 -2.78604 C 2.08931 -4.48743 -3.99680 C 0.76545 0.68996 -4.23146 C 0.32442 1.93561 -4.74407 C 1.99426 0.18807 -4.72855 C 1.10124 2.66721 -5.65903 C 2.77349 0.91460 -5.64325 C 2.32162 2.15322 -6.12476 F 0.00000 0.00000 0.00000 F 2.45567 -2.73116 -0.83397 F -1.05889 -2.66781 -4.06578 F 0.32004 -4.43198 -5.58255 F 2.76256 -5.37639 -4.74621 F 3.81740 -4.49573 -2.36675 F 2.45548 -1.00179 -4.32099 F 3.94130 0.41417 -6.08241 F 3.05673 2.84643 -7.01033 F 0.66007 3.85049 -6.11985 F -0.84377 2.45235 -4.36231 F 2.86446 2.34714 -2.62671 F 4.62567 3.77613 -1.13831 F 5.28825 2.94523 1.39865 F 2.41493 -0.78279 0.95836 F 4.16555 0.65591 2.41514 F 0.95903 2.65472 0.79504 F -0.50981 4.26515 2.39251 F -3.03502 5.05145 1.63180 F -4.05999 4.18332 -0.76381 F -2.62482 2.57561 -2.37210 F -2.50123 -2.14527 -0.09457 F -2.87163 0.33807 -4.14979 F -4.73590 -1.42021 -5.04693 F -5.49735 -3.54985 -3.49036 F -4.35921 -3.91232 -1.01768	453	
$P(C_2F_5)_4F$ 	$[(C_2F_5)_4PF_2]^-$ <i>trans/cis</i>	72.9	1.680	P 0.00000 0.00000 -1.67965 C -2.02073 -0.03376 -1.49278 C 0.01612 -2.03172 -1.87526 C 2.05075 0.00000 -1.51400 C 0.09979 2.01905 -1.98599 F -0.02246 -0.02231 -3.36280 F -1.10236 2.33907 -2.57142 F 1.04183 2.26415 -2.94419 F 2.34708 1.25539 -1.00390 F 2.67621 -0.09431 -2.72018 F 1.17451 -2.26577 -2.59048 F 0.15237 -2.64326 -0.65832 F -2.61603 -0.36255 -2.68155 F -2.22369 -1.08639 -0.62793 C -2.91775 1.10295 -0.87517 C -1.00170 -2.91661 -2.68767		

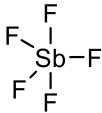
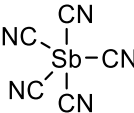
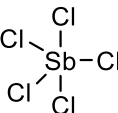
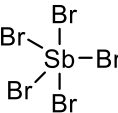
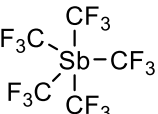
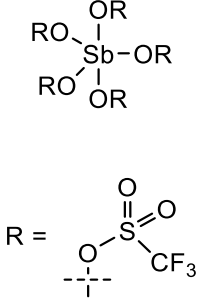
				C 2.87277 -0.90272 -0.51698 C 0.33688 3.10467 -0.84985 F -3.96423 0.55215 -0.20461 F -3.45458 1.90640 -1.81094 F -2.23949 1.85804 0.01135 F 1.49260 3.77520 -1.05641 F -0.65428 4.03250 -0.86733 F 0.38058 2.59082 0.38811 F 2.93523 -2.20553 -0.83657 F 4.16148 -0.45030 -0.51791 F 2.41861 -0.80099 0.74351 F -2.18939 -3.10816 -2.08912 F -0.44973 -4.15743 -2.83061 F -1.21556 -2.43455 -3.92267 F 0.00000 0.00000 0.00000		
$P(C_6F_5)_5$ 	$[(C_6F_5)_5PF]^-$	77.8	1.702	P -0.00000 -0.00000 -1.70179 C 1.99250 -0.00000 -1.51300 C 2.64389 0.81416 -0.56514 C 2.81934 -0.97492 -2.10798 C 4.01951 0.71207 -0.27467 C 4.18893 -1.11667 -1.83519 C 4.79732 -0.27094 -0.89719 C -0.10363 2.03701 -1.52240 C -0.81726 2.61506 -0.44025 C 0.51305 2.98845 -2.35508 C -0.90928 4.00261 -0.21855 C 0.43877 4.38317 -2.16790 C -0.27322 4.90189 -1.08287 C -0.00077 0.00092 -3.76018 C -1.14700 -0.25935 -4.56162 C 1.14480 0.26266 -4.56197 C -1.16641 -0.25546 -5.97099 C 1.16283 0.26266 -5.97147 C -0.00212 0.00445 -6.69535 C 0.10421 -2.03707 -1.52281 C 0.81748 -2.61511 -0.44038 C -0.51070 -2.98876 -2.35660 C 0.91068 -4.00266 -0.21944 C -0.43581 -4.38351 -2.16971 C 0.27579 -4.90212 -1.08439 C -1.99254 -0.00093 -1.51214 C -2.64320 -0.81626 -0.56473 C -2.82041 0.97370 -2.10617 C -4.01901 -0.71616 -0.27444 C -4.19024 1.11359 -1.83344 C -4.79786 0.26644 -0.89626 F -2.34164 1.83038 -3.03578 F -2.00313 -1.76733 0.13836 F -4.58156 -1.53648 0.63159 F -4.92125 2.05442 -2.45825 F -6.10658 0.38134 -0.61802 F 0.00000 0.00000 0.00000 F -1.49948 1.89430 0.46746 F 1.24960 2.63426 -3.42514 F 1.06174 5.21602 -3.02207 F -0.35353 6.22671 -0.87902 F -1.60852 4.47462 0.82983 F 2.00473 1.76571 0.13809 F 4.58293 1.53107 0.63199 F 6.10587 -0.38767 -0.61877 F 4.91889 -2.05777 -2.46074 F 2.33953 -1.83038 -3.03815 F -1.24406 -2.63493 -3.42895 F -1.05689 -5.21651 -3.02516 F 0.35734 -6.22694 -0.88120 F 1.60994 -4.47452 0.82895 F 1.49845 -1.89431 0.46829 F 2.35648 0.56564 -4.06408 F 2.30741 0.52962 -6.62426 F -2.35785 -0.56474 -4.06309 F -2.31152 -0.52093 -6.62338 F -0.00284 0.00602 -8.03633	335	
AsF_3 	$[AsF_4]^-$	19.2	1.942	F -0.91483 -1.58546 -2.59108 F 0.00000 0.00000 0.00000 F 1.83046 0.00000 -2.59108 F -0.91590 1.58591 -2.58806 AS -0.00000 0.00000 -1.94212	244	
$AsCl_3$ 	$[Cl_3AsF]^-$	34.1	1.773	F 0.00000 0.00000 0.00000 CL -1.21651 2.11185 -1.75549 CL -1.22009 -2.10986 -1.75323 CL 2.43740 -0.00000 -1.75515 AS -0.00000 0.00000 -1.77255	276	
$AsBr_3$	$[Br_3AsF]^-$	34.4	1.771	F 0.00000 0.00000 0.00000 BR 2.60402 -0.00000 -1.82963 BR -1.29985 -2.25613 -1.82821 BR -1.30371 2.25449 -1.82943	286	

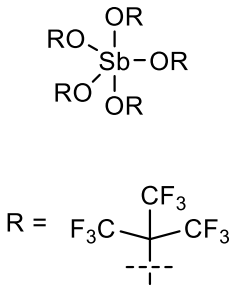
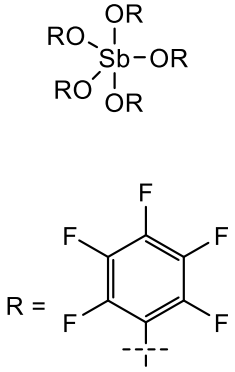
$\begin{array}{c} \text{Br} \quad \text{As} \quad \text{Br} \\ \\ \text{Br} \end{array}$				AS -0.00000 0.00000 -1.77115		
AsI_3 $\begin{array}{c} \text{As} \\ \\ \text{I} \quad \text{I} \quad \text{I} \end{array}$	$[\text{I}_3\text{AsF}]^-$	34.5	1.773	F 0.00000 0.00000 0.00000 I 2.82061 -0.00000 -1.95739 I -1.41714 -2.44561 -1.94646 I -1.38013 2.46251 -1.95447 AS 0.00000 0.00000 -1.77332		
$\text{As}(\text{CF}_3)_3$ $\begin{array}{c} \text{As} \\ \\ \text{F}_3\text{C} \quad \text{CF}_3 \\ \\ \text{F}_3\text{C} \end{array}$	$[(\text{CF}_3)_3\text{AsF}]^-$	35.3	1.933	F 0.00000 0.00000 0.00000 P -0.00000 0.00000 -1.82275 C 0.25066 0.38080 -3.80913 C -0.64011 1.80826 -1.52144 C 1.91852 0.00000 -1.54725 F 0.73981 -0.76591 -4.39627 F -1.00198 0.54570 -4.36066 F 1.01123 1.40304 -4.32479 F -1.85288 1.74245 -0.89304 F 0.15912 2.56553 -0.72834 F -0.85941 2.55924 -2.64194 F 2.39984 1.09677 -0.90432 F 2.26574 -1.07540 -0.78186 F 2.66703 -0.11832 -2.68494		
AsF_5 $\begin{array}{c} \text{F} \\ \\ \text{F} \quad \text{As} \quad \text{F} \\ \\ \text{F} \quad \text{F} \end{array}$	$[\text{AsF}_6]^-$	35.6	1.774	F 0.00000 0.00000 0.00000 F -1.77414 0.00000 -1.77414 F -0.00000 1.77414 -1.77414 F 1.77414 0.00000 -1.77414 F 0.00000 -1.77414 -1.77414 F 0.00000 -0.00000 -3.54828 AS -0.00000 0.00000 -1.77414	439	426 ^{2b} 434 ^{2c}
$\text{As}(\text{C}_2\text{F}_5)_3$ $\begin{array}{c} \text{As} \\ \\ \text{F}_5\text{C}_2 \quad \text{C}_2\text{F}_5 \\ \\ \text{F}_5\text{C}_2 \end{array}$	$[(\text{C}_2\text{F}_5)_3\text{AsF}]^-$	43.3	1.915	F 0.00000 0.00000 0.00000 C 2.06594 -0.00000 -1.62031 C -0.70284 -1.94162 -1.56397 C 0.26092 -0.07140 -4.17096 F 2.76986 0.16093 -2.78534 F 2.31514 1.11975 -0.86196 F -0.01438 -2.56906 -0.56636 F -1.98680 -1.72958 -1.10276 F -1.05820 0.05466 -4.60383 F 0.81596 1.20302 -4.29411 C 0.95162 -0.90180 -5.27759 C -0.85107 -2.99790 -2.68115 C 2.76686 -1.17910 -0.89254 F 1.08893 -0.19442 -6.44184 F 0.23522 -2.00688 -5.58932 F 2.19123 -1.30499 -4.92554 F -1.64970 -2.55706 -3.67011 F -1.41627 -4.13530 -2.18709 F 0.34572 -3.34160 -3.19451 F 2.35679 -1.34903 0.36936 F 4.11258 -0.95246 -0.84936 F 2.58193 -2.33135 -1.57245 AS -0.00000 0.00000 -1.91497	267	
$\text{As}(\text{CN})_5$ $\begin{array}{c} \text{CN} \\ \\ \text{NC} \quad \text{As} \quad \text{CN} \\ \\ \text{NC} \quad \text{CN} \end{array}$	$[(\text{NC})_5\text{AsF}]^-$	44.4	1.799	F 0.00000 0.00000 0.00000 C -1.99775 -0.00000 -1.77376 C 0.00000 1.99775 -1.77376 C 0.00000 -1.99775 -1.77376 C 1.99775 0.00000 -1.77376 C 0.00000 -0.00000 -3.78969 N 3.17138 -0.00000 -1.72489 N 0.00000 0.00000 -4.96408 N 0.00000 3.17138 -1.72489 N -3.17138 -0.00000 -1.72489 N 0.00000 -3.17138 -1.72489 AS 0.00000 0.00000 -1.79854		
AsCl_5 $\begin{array}{c} \text{Cl} \\ \\ \text{Cl} \quad \text{As} \quad \text{Cl} \\ \\ \text{Cl} \quad \text{Cl} \end{array}$	$[\text{Cl}_5\text{AsF}]^-$	45.1	1.779	F 0.00000 0.00000 0.00000 CL -2.29555 -0.00000 -1.75576 CL 0.00000 2.29555 -1.75576 CL 2.29555 0.00000 -1.75576 CL 0.00000 -2.29555 -1.75576 CL 0.00000 0.00000 -4.08521 AS 0.00000 0.00000 -1.77879	401	
AsBr_5 $\begin{array}{c} \text{Br} \\ \\ \text{Br} \quad \text{As} \quad \text{Br} \\ \\ \text{Br} \quad \text{Br} \end{array}$	$[\text{Br}_5\text{AsF}]^-$	47.4	1.779	F 0.00000 0.00000 0.00000 BR -2.49194 0.00000 -1.73968 BR 0.00000 2.49194 -1.73968 BR 2.49194 0.00000 -1.73968 BR 0.00000 -2.49194 -1.73968 BR 0.00000 0.00000 -4.29461 AS 0.00000 0.00000 -1.77934	393	

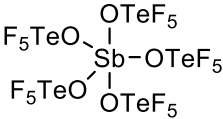
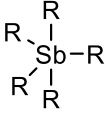
$\text{As}[\text{OC}(\text{CF}_3)_3]_3$ $\text{R} = \text{C}_6\text{F}_5$	$\{[\text{OC}(\text{CF}_3)_3]_3\text{AsF}\}^-$	52.3	1.764	O 0.23616 1.85806 -1.78777 O 2.08365 0.00000 -1.69940 O -2.02921 0.47366 -1.68743 C 0.33482 2.75150 -2.82616 C 1.07876 4.00614 -2.22148 C -1.10182 3.18868 -3.32608 C 1.16816 2.21560 -4.05517 C 2.94438 -1.04470 -1.67548 C 4.40501 -0.44822 -1.57787 C 2.85166 -1.91596 -2.99420 C 2.69807 -1.98187 -0.42711 C -3.09805 -0.35452 -1.75296 C -3.05102 -1.46355 -0.62852 C -4.39307 0.52522 -1.53853 C -3.20923 -1.06327 -3.16578 F 1.55316 -2.69184 -0.59918 F 2.56653 -1.26600 0.69668 F 3.69848 -2.88060 -0.22610 F 1.56310 -2.20706 -3.28076 F 3.51945 -3.09487 -2.91885 F 3.35015 -1.23912 -4.05262 F 5.36926 -1.37348 -1.83901 F 4.56905 0.56024 -2.44829 F 4.64712 0.03934 -0.34112 F 0.00000 0.00000 0.00000 F -2.08551 -2.37510 -0.92054 F -4.21774 -2.14619 -0.49350 F -2.75409 -0.93004 0.56348 F -4.50628 0.91257 -0.24920 F -5.53683 -0.14107 -1.85876 F -4.34994 1.63538 -2.29144 F -4.09317 -2.09288 -3.19095 F -3.59038 -0.18465 -4.11866 F -2.00930 -1.55917 -3.54119 F -1.05540 4.34062 -4.04876 F -1.92128 3.39188 -2.29284 F -1.63538 2.23748 -4.12100 F 2.48201 2.18709 -3.79220 F 0.77714 0.95928 -4.37190 F 0.98700 2.98093 -5.15829 F 1.48890 4.86369 -3.19034 F 0.26248 4.69204 -1.39346 F 2.15401 3.63118 -1.52006 AS 0.00000 0.00000 -1.76412	341	
$\text{As}(\text{CF}_3)_5$ 	$[(\text{CF}_3)_5\text{AsF}]^-$	59.1	1.838	C -2.10966 0.01747 -1.58437 C -0.06235 -0.07032 -3.97649 C 0.00003 2.13110 -1.87266 C 2.12144 0.07032 -1.59400 C 0.06960 -2.13280 -1.82562 F 0.00000 0.00000 0.00000 F 0.29130 -2.66216 -0.60226 F 1.08317 -2.56328 -2.63848 F -1.05843 -2.72362 -2.30720 F 2.59210 -1.05920 -0.99946 F 2.44149 1.09467 -0.75758 F 2.86304 0.25214 -2.71831 F -0.43197 1.10882 -4.54551 F 1.11985 -0.41639 -4.54782 F -0.96809 -0.99737 -4.39699 F 0.10614 2.70165 -0.65217 F -1.11544 2.65637 -2.45246 F 1.05594 2.58265 -2.61612 F -2.47292 1.07398 -0.80794 F -2.83542 0.11574 -2.73322 F -2.55634 -1.08853 -0.93344 AS 0.00000 -0.00000 -1.83802		
$\text{As}(\text{OTf})_5$ $\text{R} = \text{SO}_2\text{CF}_3$	$[(\text{OTf})_5\text{AsF}]^-$	60.3	1.793	S 2.54718 0.00000 -1.26588 O 2.94750 0.93453 -0.18239 • 2.76238 -1.47392 -1.11978 S -2.55018 0.00757 -1.28395 • -2.79679 -1.06162 -0.27936 O -2.78856 1.44180 -0.94675 S 0.18598 2.59099 -1.71736 O 0.07211 3.09976 -0.32595 O 1.47971 2.67672 -2.47583 S -0.13797 -2.57725 -1.75831 • 0.17020 -3.25274 -0.47312 • -1.44188 -2.77427 -2.45790 S -0.45032 0.14318 -4.48797 • -0.74236 -1.14362 -5.19661 O -1.55188 1.15028 -4.25633 C -0.96943 3.82940 -2.74328 C 3.70953 0.45313 -2.76907 C 0.66860 1.05161 -5.82739	598	

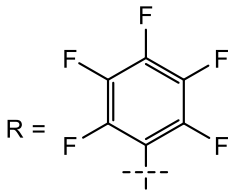
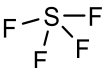
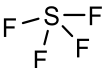
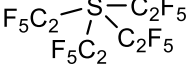
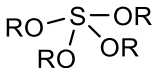
				C -3.87427 -0.36421 -2.70385 F 0.00000 0.00000 0.00000 F 3.04207 0.29297 -3.92225 F 4.16260 1.69852 -2.67202 F 4.74777 -0.39724 -2.75007 F -0.14555 1.43495 -6.82381 F 1.28764 2.12271 -5.33052 F 1.57461 0.19123 -6.31141 F -3.38182 -1.12179 -3.67441 F -4.31379 0.79432 -3.19487 F -4.89190 -1.00494 -2.10732 C 1.16639 -3.28406 -3.04508 F -2.25601 3.52385 -2.68331 F -0.55807 3.87464 -4.01124 F -0.77149 5.03335 -2.17735 F 1.71976 -2.27347 -3.73378 F 0.52056 -4.09146 -3.89157 F 2.11127 -3.97418 -2.41071 AS -0.00000 -0.00000 -1.79268		
$\text{As}(\text{OC}_6\text{F}_5)_5$  R =	$[(\text{OC}_6\text{F}_5)_5\text{AsF}]^-$	66.0	1.779	O -1.88004 0.05012 -1.73504 • -0.04261 -1.88844 -1.76492 • -0.00564 -0.04701 -3.69111 O 1.89992 0.00000 -1.84286 O 0.00258 1.90525 -1.78548 C 2.65799 0.77510 -1.04982 C 3.15955 2.01491 -1.52227 C 3.03013 0.38207 0.26184 C 4.01394 2.81110 -0.74462 C 3.88418 1.17682 1.04501 C 4.36645 2.40007 0.55167 C -0.76950 2.61837 -0.94705 C -0.29593 3.01699 0.32991 C -2.06698 3.06059 -1.31920 C -1.06715 3.81413 1.19127 C -2.84150 3.86043 -0.46159 C -2.34879 4.23416 0.79977 C -2.68827 -0.85213 -2.31150 C -3.23979 -0.63046 -3.59899 C -3.09597 -2.01696 -1.61218 C -4.14939 -1.53909 -4.16540 C -4.00068 -2.92868 -2.17836 C -4.53103 -2.69112 -3.45820 C 0.67490 -2.67380 -2.58418 C 0.15198 -3.12988 -3.82119 C 1.94643 -3.17008 -2.19694 C 0.87698 -3.99816 -4.65224 C 2.67538 -4.04028 -3.02384 C 2.13996 -4.46401 -4.25134 C 0.79719 0.69653 -4.46742 C 0.39150 1.96954 -4.94712 C 2.04968 0.20500 -4.91876 C 1.20791 2.72045 -5.80893 C 2.86930 0.95211 -5.77860 C 2.44843 2.21387 -6.23022 F 0.00000 0.00000 0.00000 F 2.47755 -2.81283 -1.02610 F -1.06021 -2.73022 -4.22584 F 0.35767 -4.40675 -5.82261 F 2.83139 -5.30580 -5.03719 F 3.87990 -4.49163 -2.63403 F 2.47735 -1.00223 -4.52624 F 4.05256 0.46039 -6.18474 F 3.22508 2.92908 -7.06074 F 0.79899 3.92302 -6.24847 F -0.78732 2.47874 -4.58835 F 2.84158 2.43647 -2.75362 F 4.48443 3.97451 -1.22616 F 5.18100 3.15910 1.30331 F 2.59344 -0.76834 0.77520 F 4.23195 0.77713 2.28003 F 0.92927 2.65687 0.73333 F -0.58248 4.18130 2.38975 F -3.09003 5.00079 1.61711 F -4.06369 4.26969 -0.84332 F -2.57835 2.73765 -2.50721 F -2.62125 -2.25680 -0.38696 F -2.90359 0.45523 -4.29774 F -4.66195 -1.31006 -5.38682 F -5.40336 -3.55864 -3.99885 F -4.37549 -4.02633 -1.49761 AS -0.00000 0.00000 -1.77894	509	
$\text{As}(\text{OTeF}_5)_5$	$[(\text{OTeF}_5)_5\text{AsF}]^-$	69.0	1.757	AS -0.00000 0.00000 -1.75687 O 0.02101 1.85858 -1.83097 TE 1.36198 3.20550 -1.40684 F 2.58644 4.63824 -1.03148 F 0.60055 4.31760 -2.77274 F 0.17451 4.01295 -0.13315		593 ^{2b}

				F 2.20665 2.23236 0.01527 F 2.65905 2.57435 -2.67419 O -1.85433 0.10170 -1.86580 TE -3.13587 1.37681 -1.11971 F -4.50181 2.54599 -0.44089 F -2.00148 2.03218 0.28159 F -2.62453 2.83104 -2.26159 F -4.39349 0.78313 -2.43993 F -3.83111 0.04665 0.07651 • -0.11622 -1.85413 -1.84405 TE -0.77993 -3.15388 -0.54445 F -1.38819 -4.55006 0.62747 F -2.21852 -3.63970 -1.71797 F 0.32423 -4.46710 -1.40204 F 0.60375 -2.81251 0.74127 F -1.95910 -1.96809 0.39608 • 0.15030 -0.04874 -3.61984 TE -1.12797 -0.45812 -5.03737 F -2.27572 -0.80873 -6.53750 F -0.13098 0.72340 -6.17616 F -0.03763 -1.91343 -5.64991 F -2.20210 -1.69827 -4.04318 F -2.31381 0.99238 -4.60732 O 1.85633 0.00000 -1.73819 TE 3.21607 -1.21396 -2.42390 F 4.68145 -2.31964 -2.99232 F 4.46283 -0.30315 -1.28658 F 2.90063 -2.50645 -1.03819 F 2.10903 -2.21769 -3.62410 F 3.67085 -0.02130 -3.85534 F 0.00000 0.00000 0.00000		
As(C₆F₅)₅  R =	[(C ₆ F ₅) ₅ AsF] ⁻	73.5	1.836	C 2.09346 -0.00000 -1.61996 C 2.73279 0.81847 -0.67382 C 2.90441 -0.97860 -2.21920 C 4.10594 0.70592 -0.37583 C 4.27290 -1.12726 -1.94195 C 4.87885 -0.28121 -1.00122 C -0.09829 2.12786 -1.63447 C -0.82825 2.70850 -0.57369 C 0.57134 3.04684 -2.45567 C -0.89084 4.09911 -0.35762 C 0.52750 4.44272 -2.27447 C -0.20645 4.97678 -1.20913 C -0.00159 0.00293 -4.00380 C -1.15577 -0.24555 -4.78548 C 1.15063 0.25517 -4.78709 C -1.17696 -0.23884 -6.19458 C 1.16706 0.26013 -6.19641 C -0.00617 0.01378 -6.91493 C 0.09870 -2.12794 -1.63655 C 0.82371 -2.70876 -0.57253 C -0.56532 -3.04666 -2.46256 C 0.88234 -4.09922 -0.35453 C -0.52543 -4.44239 -2.27927 C 0.20136 -4.97657 -1.20909 C -2.09347 -0.00212 -1.61744 C -2.73055 -0.82321 -0.67202 C -2.90685 0.97624 -2.21379 C -4.10363 -0.71378 -0.37256 C -4.27538 1.12189 -1.93502 C -4.87891 0.27320 -0.99514 F -2.41029 1.83410 -3.13286 F -2.08131 -1.78476 0.00663 F -4.67174 -1.53447 0.52944 F -5.00816 2.06693 -2.55118 F -6.18598 0.39301 -0.71082 F 0.00000 0.00000 0.00000 F -1.54797 1.98968 0.30410 F 1.33135 2.64538 -3.49341 F 1.19508 5.26209 -3.10757 F -0.26027 6.30389 -1.01045 F -1.60730 4.59574 0.66724 F 2.08559 1.78042 0.00621 F 4.67647 1.52395 0.52703 F 6.18609 -0.40370 -0.71873 F 5.00333 -2.07249 -2.56055 F 2.40543 -1.83368 -3.13948 F -1.31372 -2.64532 -3.50874 F -1.18797 -5.26165 -3.11651 F 0.25162 -6.30355 -1.00863 F 1.59282 -4.59611 0.67435 F 1.54134 -1.99040 0.30724 F 2.35631 0.53259 -4.26300 F 2.31132 0.51335 -6.85467 F -2.35886 -0.53080 -4.25944 F -2.32307 -0.48805 -6.85103 F -0.00845 0.01933 -8.25604 AS 0.00000 -0.00000 -1.83638	325	

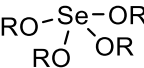
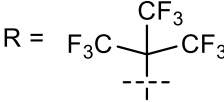
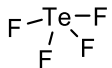
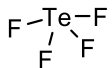
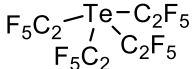
SbF_5 	$[\text{SbF}_6]^-$	37.4	1.952	F 0.00000 0.00000 0.00000 F -1.95175 0.00000 -1.95175 F 0.00000 1.95175 -1.95175 F 1.95175 -0.00000 -1.95175 F 0.00000 -1.95175 -1.95175 F 0.00000 0.00000 -3.90349 SB 0.00000 0.00000 -1.95175	496	489 ^{2b} 495 ^{2c}
$\text{Sb}(\text{CN})_5$ 	$[(\text{NC})_5\text{SbF}]^-$	43.4	1.971	F 0.00000 0.00000 0.00000 C -2.18400 -0.00000 -1.95723 C 0.00000 2.18400 -1.95723 C 0.00000 -2.18400 -1.95723 C 2.18400 -0.00000 -1.95723 C 0.00000 -0.00000 -4.15405 N 3.35883 -0.00000 -1.94848 N 0.00000 -0.00000 -5.32879 N 0.00000 3.35883 -1.94848 N -3.35883 -0.00000 -1.94848 N 0.00000 -3.35883 -1.94848 SB 0.00000 -0.00000 -1.97097		
SbCl_5 	$[\text{Cl}_5\text{SbF}]^-$	45.0	1.963	F 0.00000 0.00000 0.00000 Cl -2.43533 -0.00000 -1.93328 Cl 0.00000 2.43533 -1.93328 Cl 2.43533 -0.00000 -1.93328 Cl 0.00000 -2.43533 -1.93328 Cl -0.00000 -0.00000 -4.40840 SB 0.00000 -0.00000 -1.96291	438	
SbBr_5 	$[\text{Br}_5\text{SbF}]^-$	46.9	1.966	F 0.00000 0.00000 0.00000 BR -2.61877 -0.00000 -1.93047 BR 0.00000 2.61877 -1.93047 BR 2.61877 0.00000 -1.93047 BR 0.00000 -2.61877 -1.93047 BR 0.00000 -0.00000 -4.60778 SB 0.00000 0.00000 -1.96582	413	
$\text{Sb}(\text{CF}_3)_5$ 	$[(\text{CF}_3)_5\text{SbF}]^-$	55.4	2.010	C -0.01722 2.28961 -1.80927 C -0.03065 0.10397 -4.33673 C 2.30262 0.00000 -2.06669 C 0.05591 -2.29775 -1.82155 C -2.30239 -0.08574 -2.04795 F 0.00000 0.00000 0.00000 F -2.87147 -0.31510 -0.84027 F -2.70187 -1.10225 -2.87349 F -2.87396 1.04822 -2.54001 F -1.04673 -2.76205 -1.16995 F 1.13205 -2.68536 -1.08134 F 0.12872 -2.98325 -2.99343 F 1.10400 0.66991 -4.83851 F -0.16413 -1.09925 -4.95689 F -1.06959 0.87458 -4.77188 F 2.89410 -0.18056 -0.86139 F 2.81867 1.14871 -2.58647 F 2.73689 -1.01504 -2.87567 F 1.04401 2.72410 -1.07558 F 0.03825 2.95040 -3.00024 F -1.13227 2.73551 -1.16904 SB -0.00000 0.00000 -2.01008		
$\text{Sb}(\text{OTf})_5$ 	$[(\text{OTf})_5\text{SbF}]^-$	60.1	1.976	S 0.17042 -2.68593 -1.35861 • 1.06155 -3.04701 -0.22371 • -1.30076 -2.97508 -1.30448 S -0.47951 2.67086 -1.42939 O -1.43409 2.74285 -0.28946 O 0.88969 3.25652 -1.32886 S 2.74394 0.00000 -1.74194 O 3.19643 0.31005 -0.35892 • 3.01547 -1.33269 -2.37561 S -2.74232 -0.19645 -1.93543 • -3.49099 -0.58087 -0.71045 O -2.99957 1.11411 -2.61976 S 0.18205 0.42757 -4.85138 O -1.10119 0.50942 -5.61846 O 1.08180 1.62852 -4.73495 C 3.79110 1.25122 -2.83701 C 0.76022 -3.82435 -2.82634 C 1.24900 -0.78623 -5.96847 C -1.34057 3.73962 -2.85179 F 0.00000 0.00000 0.00000 F 0.48894 -3.20830 -3.99167 F 2.06047 -4.09118 -2.74817 F 0.06637 -4.97078 -2.77277 F 1.73421 -0.07836 -6.99892 F 2.26478 -1.30481 -5.27218	594	

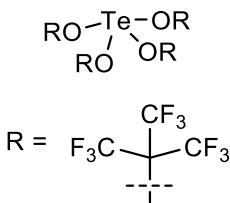
				F 0.47503 -1.77223 -6.43914 F -1.38152 3.07093 -4.00019 F -0.60929 4.85214 -3.00674 F -2.57098 4.06904 -2.46329 C -3.26798 -1.51124 -3.29222 F 3.27415 2.47306 -2.79681 F 3.85788 0.81128 -4.09520 F 5.02768 1.26987 -2.31243 F -2.17176 -1.90307 -3.96509 F -4.12238 -0.93332 -4.14213 F -3.85092 -2.56348 -2.72306 SB -0.00000 0.00000 -1.97559		
$\text{Sb}[\text{OC}(\text{CF}_3)_3]_3$  $\text{R} = \text{F}_3\text{C}-\text{CH}_2-\text{CF}_3$	$\{[\text{OC}(\text{CF}_3)_3]_3\text{SbF}\}^-$	61.9	1.959	O 2.08049 -0.00000 -1.99064 • 0.25946 -2.19328 -1.85679 O 0.20356 2.19747 -1.86777 C 2.98988 0.03067 -3.00878 C 4.38225 -0.33738 -2.36216 C 3.07957 1.47331 -3.64909 C 2.66819 -1.01998 -4.14359 C -0.52847 -3.23752 -1.52538 C 0.21694 -4.55961 -1.96698 C -1.92089 -3.18012 -2.27165 C -0.79442 -3.30326 0.03407 C -0.56889 3.23354 -1.48067 C -0.65442 3.34721 0.09711 C 0.08201 4.55891 -2.04614 C -2.03569 3.11505 -2.05719 F -1.72569 -2.39060 0.39754 F 0.32654 -3.04662 0.71786 F -1.25502 -4.52059 0.43730 F -2.44761 -1.93054 -2.18288 F -2.84652 -4.03761 -1.78185 F -1.77703 -3.44668 -3.58920 F -0.59928 -5.64899 -1.97743 F 0.72560 -4.42806 -3.20329 F 1.24194 -4.83493 -1.13139 F 0.00000 0.00000 0.00000 F -1.53247 2.44877 0.59785 F -1.06934 4.57789 0.51086 F 0.54078 3.11354 0.65222 F 1.18056 4.89570 -1.33606 F -0.76576 5.62324 -2.00698 F 0.45953 4.39442 -3.32486 F -2.92311 3.96261 -1.48682 F -2.05380 3.34364 -3.39003 F -2.50991 1.85497 -1.87277 F 4.18403 1.62817 -4.42519 F 3.11095 2.41447 -2.70253 F 1.99993 1.69845 -4.43543 F 2.91235 -2.27472 -3.73664 F 1.35685 -0.94484 -4.48537 F 3.38421 -0.80553 -5.27283 F 5.32030 -0.61735 -3.30444 F 4.85174 0.68611 -1.61822 F 4.26997 -1.40621 -1.56377 SB 0.00000 0.00000 -1.95847	402	
$\text{Sb}(\text{OC}_6\text{F}_5)_5$  $\text{R} = \text{C}_6\text{F}_5$	$[(\text{OC}_6\text{F}_5)_5\text{SbF}]^-$	63.3	1.966	-2.08457 0.05020 -1.92385 O -0.06265 -2.08982 -2.00997 • 0.01756 -0.02601 -4.08436 O 2.09850 0.00000 -2.05102 O 0.03518 2.10018 -1.93791 C 2.83697 0.79526 -1.27168 C 3.27197 2.06779 -1.72730 C 3.23220 0.40201 0.03471 C 4.09933 2.88618 -0.94487 C 4.06115 1.21634 0.82215 C 4.47878 2.47026 0.34338 C -0.69978 2.80409 -1.07102 C -0.20487 3.14530 0.21598 C -1.99836 3.27222 -1.41102 C -0.94705 3.93788 1.10520 C -2.74374 4.06804 -0.52627 C -2.22806 4.38850 0.74191 C -2.85943 -0.81984 -2.57740 C -3.35828 -0.53419 -3.87641 C -3.25517 -2.04606 -1.97936 C -4.23273 -1.41555 -4.53154 C -4.12541 -2.93123 -2.63289 C -4.60666 -2.62347 -3.91778 C 0.63960 -2.82858 -2.87365 C 0.10439 -3.20567 -4.13364 C 1.93532 -3.31166 -2.54730 C 0.81258 -4.03486 -5.01572 C 2.64756 -4.14386 -3.42472 C 2.09399 -4.49665 -4.66786 C 0.85561 0.71135 -4.81475 C 0.50602 2.01891 -5.25066	543	

				C 2.12065 0.20917 -5.22304 C 1.36198 2.76921 -6.07168 C 2.98095 0.95579 -6.04089 C 2.60921 2.24654 -6.45605 F 0.00000 0.00000 0.00000 F 2.48388 -2.99198 -1.37270 F -1.11634 -2.78217 -4.48683 F 0.27812 -4.38546 -6.19756 F 2.77456 -5.29354 -5.50765 F 3.86569 -4.60026 -3.08835 F 2.49821 -1.01883 -4.84263 F 4.16691 0.45144 -6.42175 F 3.42939 2.96518 -7.24000 F 1.00290 3.99658 -6.48414 F -0.66993 2.54169 -4.89765 F 2.91657 2.48834 -2.94889 F 4.51299 4.07804 -1.40753 F 5.26801 3.25179 1.09845 F 2.84319 -0.77963 0.51780 F 4.44086 0.81500 2.04677 F 1.01700 2.73943 0.58518 F -0.44569 4.26070 2.30917 F -2.94239 5.14782 1.58930 F -3.96218 4.51318 -0.87752 F -2.51719 2.98115 -2.60548 F -2.80814 -2.35808 -0.75935 F -3.01253 0.60264 -4.48429 F -4.70526 -1.11895 -5.75405 F -5.44073 -3.46906 -4.54533 F -4.49680 -4.08091 -2.04329 SB 0.00000 0.00000 -1.96601		
$\text{Sb}(\text{OTeF}_5)_5$ 	$[(\text{OTeF}_5)_5\text{SbF}]^-$	67.5	1.933	O 2.03979 0.00000 -2.02202 TE 3.36999 -1.27641 -1.42608 F 4.76666 -2.47707 -0.87764 F 4.58810 -0.56559 -2.72691 F 4.06633 -0.02987 -0.14437 F 2.27574 -2.06295 -0.05786 F 2.84327 -2.63152 -2.68084 O 0.05184 2.03351 -2.08364 TE 1.26390 3.37149 -1.37588 F 2.39952 4.77378 -0.71577 F 2.70931 2.89372 -2.54263 F 0.61303 4.60877 -2.68892 F -0.07063 4.01433 -0.15526 F 1.98302 2.24770 0.00566 O -2.03922 0.06775 -2.02146 TE -3.34126 0.69529 -0.72768 F -4.71652 1.28040 0.47978 F -3.90387 2.10333 -1.90273 F -4.64462 -0.45807 -1.53439 F -2.92841 -0.66527 0.56229 F -2.15427 1.91871 0.15737 • -0.02354 -0.15474 -3.97334 TE -0.48360 1.09391 -5.38472 F -0.89916 2.24488 -6.86560 F 0.74458 0.17518 -6.53870 F -1.88491 -0.05883 -6.00699 F -1.76489 2.09115 -4.36142 F 0.90606 2.34293 -4.93486 • 0.03017 -2.03928 -1.93668 TE -1.15392 -3.38602 -2.66726 F -2.26060 -4.81616 -3.31624 F -0.25241 -4.68828 -1.58489 F -2.45082 -3.13558 -1.27242 F -2.15259 -2.21860 -3.81620 F 0.04816 -3.77654 -4.11030 F 0.00000 0.00000 0.00000 SB 0.00000 -0.00000 -1.93297	633 ^{2b}	
$\text{Sb}(\text{C}_6\text{F}_5)_5$ 	$[(\text{C}_6\text{F}_5)_5\text{SbF}]^-$	69.5	1.998	C -2.26242 0.00327 -1.76941 C -2.90176 -0.83853 -0.84897 C -3.06328 0.98185 -2.37283 C -4.27964 -0.74407 -0.56912 C -4.43849 1.11378 -2.11847 C -5.04846 0.24558 -1.19906 C 0.07286 -2.28477 -1.81644 C 0.82643 -2.89382 -0.79816 C -0.66970 -3.15272 -2.62504 C 0.85397 -4.28859 -0.60434 C -0.66771 -4.55134 -2.46788 C 0.09887 -5.12271 -1.44238 C -0.00000 -0.00171 -4.32948 C 1.16096 0.22971 -5.09481 C -1.16061 -0.23467 -5.09488 C 1.18250 0.22820 -6.50342 C -1.18120 -0.23712 -6.50359 C 0.00089 -0.00537 -7.21720 C -0.07337 2.28494 -1.81886	384	

				C -0.82378 2.89485 -0.79878 C 0.66550 3.15216 -2.63148 C -0.85054 4.28981 -0.60622 C 0.66398 4.55091 -2.47581 C -0.09875 5.12320 -1.44792 C 2.26260 -0.00000 -1.76855 C 2.90069 0.84569 -0.85083 C 3.06539 -0.97817 -2.37005 C 4.27916 0.75584 -0.57246 C 4.44121 -1.10596 -2.11665 C 5.04994 -0.23344 -1.20052 F 2.54258 -1.85608 -3.25546 F 2.23710 1.81333 -0.19302 F 4.86086 1.59663 0.30149 F 5.17564 -2.05355 -2.72659 F 6.36339 -0.33550 -0.93966 F 0.00000 0.00000 0.00000 F 1.59534 -2.18464 0.04585 F -1.45594 -2.68118 -3.61495 F -1.39870 -5.33947 -3.27698 F 0.11561 -6.45419 -1.26819 F 1.59566 -4.83141 0.37765 F -2.23988 -1.80656 -0.19008 F -4.86249 -1.58071 0.30803 F -6.36133 0.35195 -0.93706 F -5.17100 2.06144 -2.73055 F -2.53929 1.85592 -3.26129 F 1.44730 2.67948 -3.62446 F 1.39139 5.33832 -3.28879 F -0.11489 6.45485 -1.27484 F -1.58857 4.83357 0.37806 F -1.58964 2.18643 0.04841 F -2.35749 -0.48483 -4.53696 F -2.32696 -0.46666 -7.16738 F 2.35734 0.48230 -4.53687 F 2.32860 0.45653 -7.16699 F 0.00141 -0.00714 -8.55854 SB -0.00000 0.00000 -1.99779		
SF_4 	$[SF_5]^-$ axial	33.5	1.662 1.772	S 0.00000 -0.00000 -1.77226 F 0.13172 -1.65186 -1.63970 F 1.77223 -0.00000 -1.76099 F 0.02239 -0.28085 -3.52199 F 0.00000 0.00000 0.00000 F -1.74983 -0.28085 -1.76099	223	
SF_4 	$[SF_5]^-$ equatorial	40.8	1.662 1.772	S 0.00000 0.00000 -1.66240 F 0.00000 0.00000 0.00000 F 0.00000 -1.76662 -1.52108 F -1.76662 0.00000 -1.52108 F 1.76662 0.00000 -1.52108 F 0.00000 1.76662 -1.52108	233	
$S(C_2F_5)_4$ 	$[(C_2F_5)_4SF]^-$	64.8	1.773	S -0.00000 -0.00000 -1.77271 F 0.00000 0.00000 0.00000 C 2.17656 0.00000 -1.55682 C 2.77514 0.51764 -2.88760 C -0.03506 2.16894 -1.35518 C -0.50742 2.98806 -2.61483 C -0.02710 -2.11988 -1.34187 C 0.22575 -2.97203 -2.61372 C -2.21589 0.05321 -1.56116 C -2.98341 -0.62269 -2.73201 F -2.73908 -0.39259 -0.39039 F -2.59075 1.37262 -1.68605 F -4.28210 -0.19959 -2.76101 F -3.02695 -1.96527 -2.66267 F -2.42878 -0.27660 -3.91399 F -0.82984 2.17801 -3.64601 F -1.58263 3.76212 -2.34427 F 0.46853 3.81897 -3.05859 F -0.16270 -4.26486 -2.42707 F -0.48056 -2.48860 -3.65997 F 1.52190 -2.99855 -2.97158 F 2.43557 -0.32052 -3.89391 F 4.13530 0.56645 -2.84108 F 2.34712 1.75023 -3.22354 F -1.26705 -2.46951 -0.89369 F 0.84453 -2.52600 -0.38319 F 2.69873 -1.26114 -1.43527 F 2.68710 0.71697 -0.52401 F 1.20236 2.64080 -1.03283 F -0.83300 2.47987 -0.30504	166	
$S[OC(CF_3)_3]_4$ 	$\{[OC(CF_3)_3]_4SF\}^-$	82.2	1.708	S 0.00000 0.00000 -1.70766 F 0.00000 0.00000 0.00000 O 0.01448 0.29106 -3.67524 C -0.10616 -0.66598 -4.64937 C 0.35652 -2.11075 -4.21306 C 0.81143 -0.22025 -5.86356 C -1.60354 -0.76141 -5.16099 F -0.00765 -3.05607 -5.11269	319	

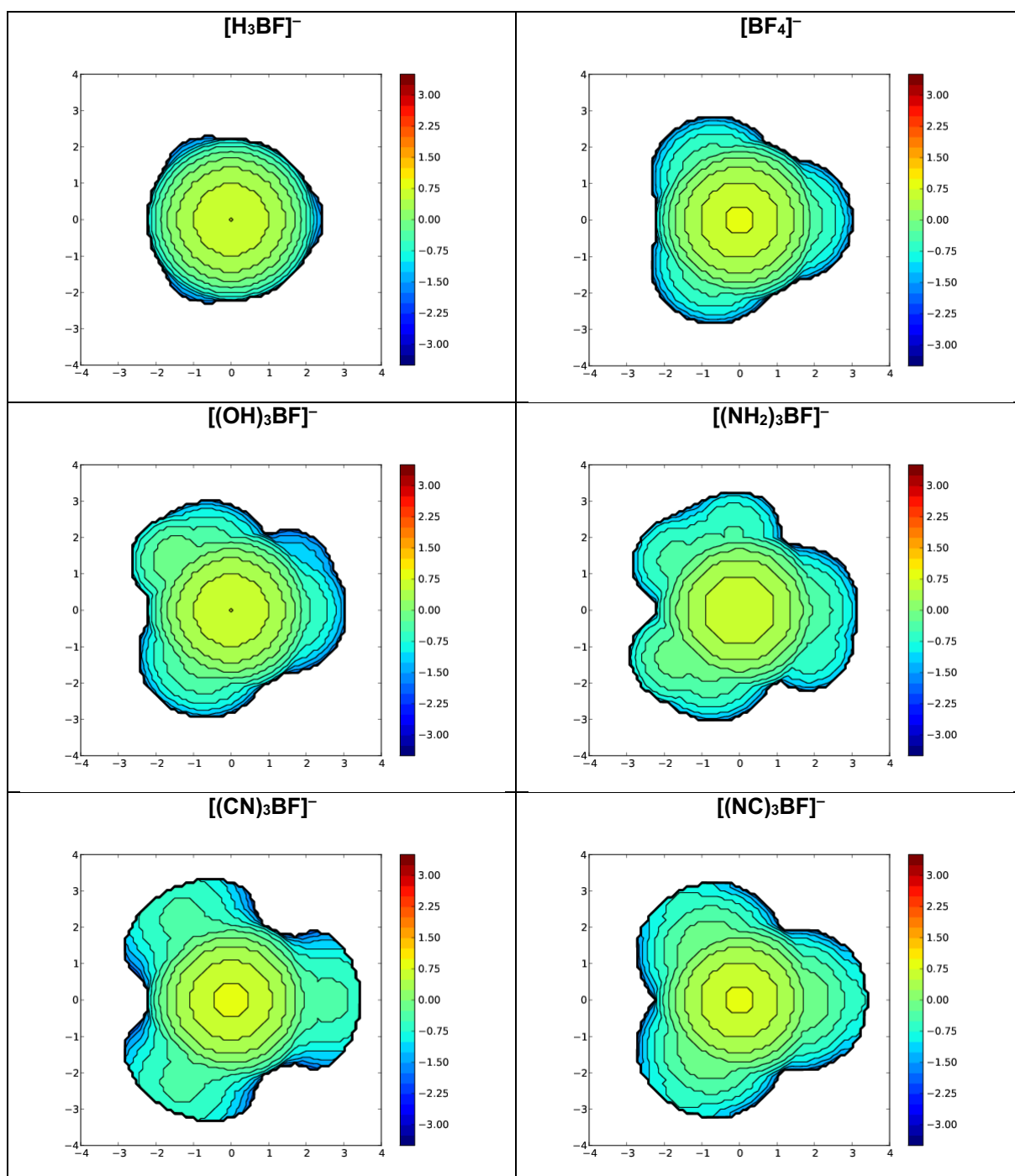
$R = \begin{array}{c} \text{CF}_3 \\ \\ \text{F}_3\text{C}-\text{C}-\text{CF}_3 \\ \\ \text{---} \end{array}$				F 1.69143 -2.17505 -4.07339 F -0.19844 -2.45743 -3.03022 F 0.27046 0.83558 -6.50948 F 0.97314 -1.20889 -6.78112 F 2.03035 0.13407 -5.43876 F -2.34777 -1.52744 -4.33953 F -1.68803 -1.31125 -6.40307 F -2.16195 0.45425 -5.22174 O -1.97364 0.10006 -1.75580 C -2.89521 -0.37415 -0.85747 C -2.81454 -1.93719 -0.68959 C -4.29187 0.00224 -1.50906 C -2.84185 0.30861 0.58369 F -3.58259 -2.38684 0.33384 F -3.22846 -2.56742 -1.80841 F -1.54587 -2.32242 -0.45322 F -4.52534 1.32613 -1.37864 F -5.32607 -0.65966 -0.93122 F -4.31272 -0.28636 -2.81574 F -2.07922 -0.37805 1.45763 F -4.08030 0.38443 1.14545 F -2.36444 1.55497 0.48498 O 2.00636 0.00000 -1.76272 C 2.91478 -0.50680 -0.87072 C 3.36167 0.56670 0.19842 C 4.17583 -0.88522 -1.75562 C 2.44718 -1.81996 -0.10362 F 4.07951 0.00864 1.21050 F 4.15081 1.50738 -0.36987 F 2.30703 1.19072 0.73545 F 3.95060 -2.02929 -2.43689 F 5.29756 -1.06769 -1.01266 F 4.43708 0.07719 -2.65074 F 1.83672 -1.54758 1.06552 F 3.49155 -2.63717 0.18852 F 1.58721 -2.51649 -0.86878 O 0.01825 1.68716 -1.55052 C 0.19453 2.85992 -2.30722 C 1.65670 3.07961 -2.85591 C -0.07748 3.93551 -1.15465 C -0.86531 3.10775 -3.46685 F 1.68424 4.23470 -3.57544 F 2.52284 3.22292 -1.83381 F 2.08388 2.10072 -3.64073 F -1.39281 3.98009 -0.87380 F 0.31781 5.17429 -1.51604 F 0.57599 3.61231 -0.03380 F -0.40437 2.75402 -4.67426 F -1.14434 4.44000 -3.54614 F -2.00400 2.46958 -3.21394		
$\begin{array}{c} \text{SeF}_4 \\ \text{F}-\text{Se}-\text{F} \\ \quad \backslash \\ \text{F} \quad \text{F} \end{array}$	$[\text{SeF}_5]^-$ axial	33.8	1.784 1.876	SE -0.00000 0.00000 -1.87635 F 1.77723 0.00000 -1.72646 F 0.00000 0.00000 0.00000 F 0.15714 1.86972 -1.86310 F 0.31428 0.00000 -3.72620 F 0.15714 -1.86972 -1.86310	292	
$\begin{array}{c} \text{SeF}_4 \\ \text{F}-\text{Se}-\text{F} \\ \quad \backslash \\ \text{F} \quad \text{F} \end{array}$	$[\text{SeF}_5]^-$ equatorial	40.3	1.784 1.876	SE -0.00000 0.00000 -1.78354 F 0.00000 0.00000 0.00000 F 1.86972 0.00000 -1.62585 F 0.00000 -1.86972 -1.62585 F -1.86972 0.00000 -1.62585 F 0.00000 1.86972 -1.62585	292	
$\begin{array}{c} \text{Se}(\text{C}_2\text{F}_5)_4 \\ \text{F}_5\text{C}_2-\text{Se}-\text{C}_2\text{F}_5 \\ \quad \backslash \\ \text{F}_5\text{C}_2 \quad \text{C}_2\text{F}_5 \end{array}$	$[(\text{C}_2\text{F}_5)_4\text{SeF}]^-$	64.2	1.882	SE 0.00000 0.00000 -1.88240 F 0.00000 0.00000 0.00000 C -0.03530 2.26596 -1.57742 C 0.48892 2.92834 -2.87125 C -2.20114 -0.06041 -1.36564 C -3.08310 0.19066 -2.60945 C 2.23472 0.00000 -1.39296 C 3.08958 -0.45885 -2.63087 C 0.10098 -2.28468 -1.59499 C -0.57273 -3.08403 -2.74008 F 2.67498 1.24686 -1.05611 F 2.52992 -0.80200 -0.34106 F 2.30226 -0.86553 -3.65445 F 3.85669 0.55147 -3.10601 F 3.92119 -1.47996 -2.32589 F 0.67956 2.73560 -0.52201 F -1.30849 2.75723 -1.43402 F 0.54585 4.28424 -2.77251 F 1.72465 2.50116 -3.20694 F -0.33749 2.63249 -3.90226 F -2.71229 -0.62775 -3.62244 F -2.98514 1.45853 -3.05210 F -4.39965 -0.04935 -2.35821 F -2.58012 0.81781 -0.40099 F -2.53255 -1.30557 -0.90808 F -1.91283 -3.13557 -2.64261 F -0.13427 -4.37590 -2.76455	166	

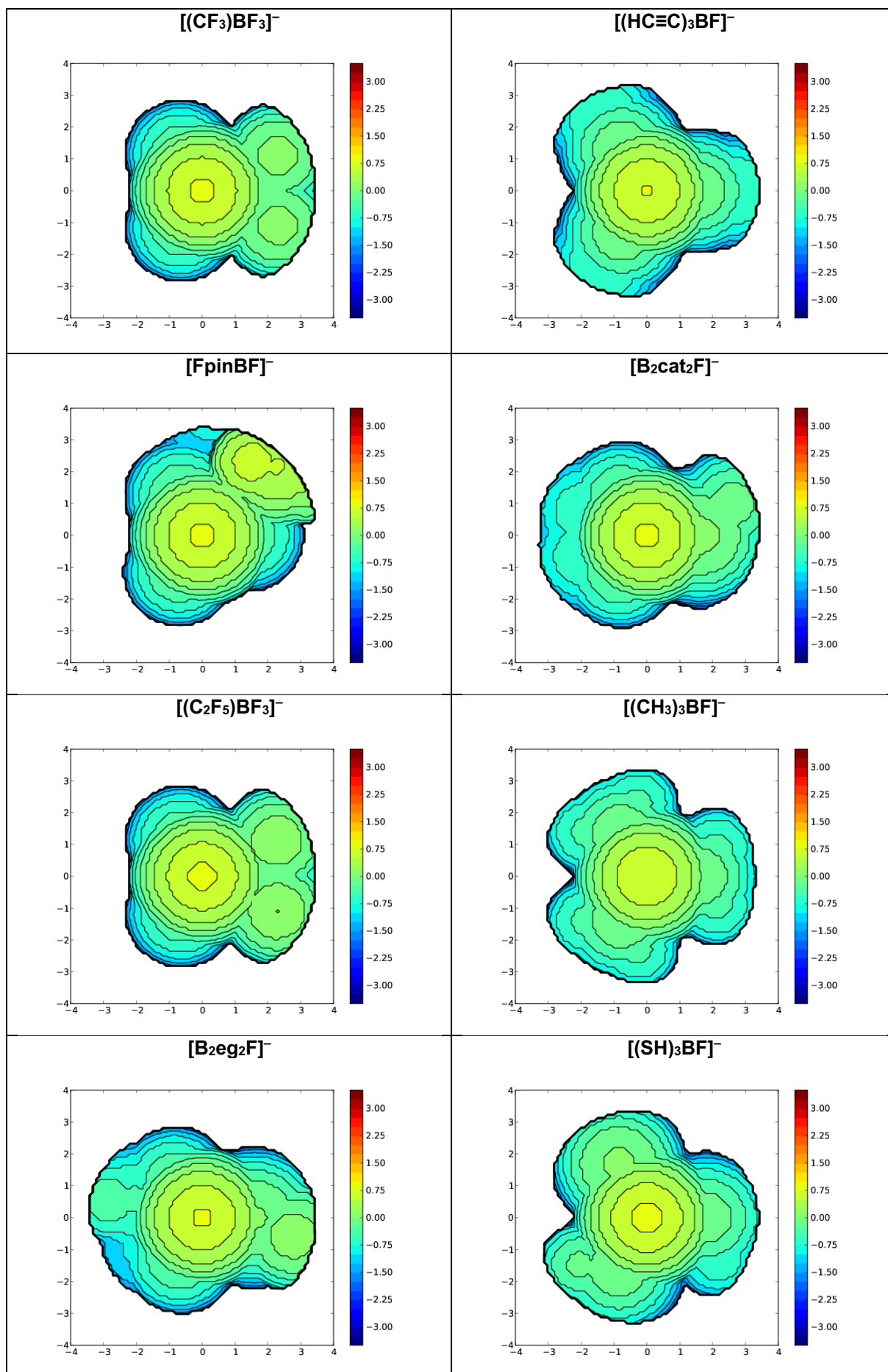
				F -0.34856 -2.77288 -0.41090 F 1.42937 -2.64184 -1.70232 F -0.25592 -2.53589 -3.93650		
$\text{Se}[\text{OC}(\text{CF}_3)_3]_4$  	$\{[\text{OC}(\text{CF}_3)_3]_4\text{SeF}\}^-$	79.2	1.835	F 0.00000 0.00000 0.00000 • -2.02869 -0.27069 -1.72387 C -2.98352 0.71467 -1.70717 C -4.30616 0.05602 -1.13701 C -3.27287 1.24699 -3.16605 C -2.60591 1.93154 -0.77477 F -5.23929 0.98965 -0.81716 F -4.86289 -0.77169 -2.04355 F -4.05023 -0.65452 -0.03054 F -2.27662 2.06015 -3.57676 F -4.42936 1.95921 -3.23679 F -3.37225 0.22606 -4.02185 F -2.62454 1.57907 0.52193 F -3.44012 2.98465 -0.92948 F -1.35645 2.37471 -1.06110 • -0.19908 -0.11630 -3.91262 C 0.53209 -0.01986 -5.05823 C 1.20268 1.40431 -5.19653 C -0.47849 -0.21031 -6.26359 C 1.64104 -1.14061 -5.18144 F 2.18480 1.43713 -6.13075 F 0.28684 2.33875 -5.54627 F 1.73351 1.79262 -4.02552 F -0.85423 -1.50266 -6.37291 F 0.06530 0.15777 -7.45396 F -1.58776 0.52161 -6.08854 F 2.73254 -0.83825 -4.45600 F 2.05369 -1.31560 -6.46661 F 1.16399 -2.31553 -4.74700 O 2.03454 0.00000 -1.82935 C 2.94488 0.51075 -0.93987 C 2.74588 2.05553 -0.68974 C 4.35383 0.29701 -1.63342 C 2.97284 -0.24416 0.46454 F 3.47312 2.50312 0.36160 F 3.11308 2.77968 -1.76787 F 1.44960 2.33504 -0.44527 F 4.68924 -1.00959 -1.61539 F 5.34335 0.98879 -1.01202 F 4.33058 0.69900 -2.91033 F 2.17113 0.33469 1.38023 F 4.22201 -0.25177 1.00603 F 2.59180 -1.51553 0.30508 • 0.20675 -1.84854 -1.86245 C -0.50321 -2.97842 -1.44509 C -0.90172 -3.00862 0.08123 C 0.58363 -4.11996 -1.70016 C -1.77751 -3.29483 -2.34385 F -1.59674 -4.14883 0.34121 F 0.19968 -3.01791 0.85688 F -1.66644 -1.98298 0.44744 F 0.71494 -4.35145 -3.01871 F 0.24310 -5.28681 -1.10836 F 1.77714 -3.75460 -1.22117 F -2.92192 -2.86423 -1.78454 F -1.91945 -4.63878 -2.50708 F -1.64469 -2.74288 -3.54807 SE -0.00000 -0.00000 -1.83494	366	
TeF_4 	$[\text{TeF}_5]^-$ equatorial	34.6	1.950 2.023	TE 0.00000 0.00000 -2.02277 F 1.93919 0.00000 -1.82148 F 0.41545 0.00000 -4.00241 F 0.20773 -2.01196 -2.00120 F 0.00000 0.00000 0.00000 F 0.20773 2.01196 -2.00120	348	
TeF_4 	$[\text{TeF}_5]^-$ axial	40.1	1.950 2.023	TE -0.00000 0.00000 -1.94961 F 0.00000 0.00000 0.00000 F 0.00000 -2.01196 -1.74077 F -2.01196 0.00000 -1.74077 F 0.00000 2.01196 -1.74077 F 2.01196 -0.00000 -1.74077	348	
$\text{Te}(\text{C}_2\text{F}_5)_4$ 	$[(\text{C}_2\text{F}_5)_4\text{TeF}]^-$	62.9	2.018	TE 0.00000 0.00000 -2.01830 F 0.00000 0.00000 0.00000 C 0.00004 -2.38532 -1.51582 C -0.46408 -3.21153 -2.73295 C 2.38283 0.00000 -1.50975 C 3.21100 -0.44978 -2.73075 C -0.00073 2.38515 -1.51556 C 0.46357 3.21117 -2.73265 C -2.38317 -0.00044 -1.51065 C -3.21077 0.44851 -2.73235 F -0.77591 -2.73253 -0.45291	360	

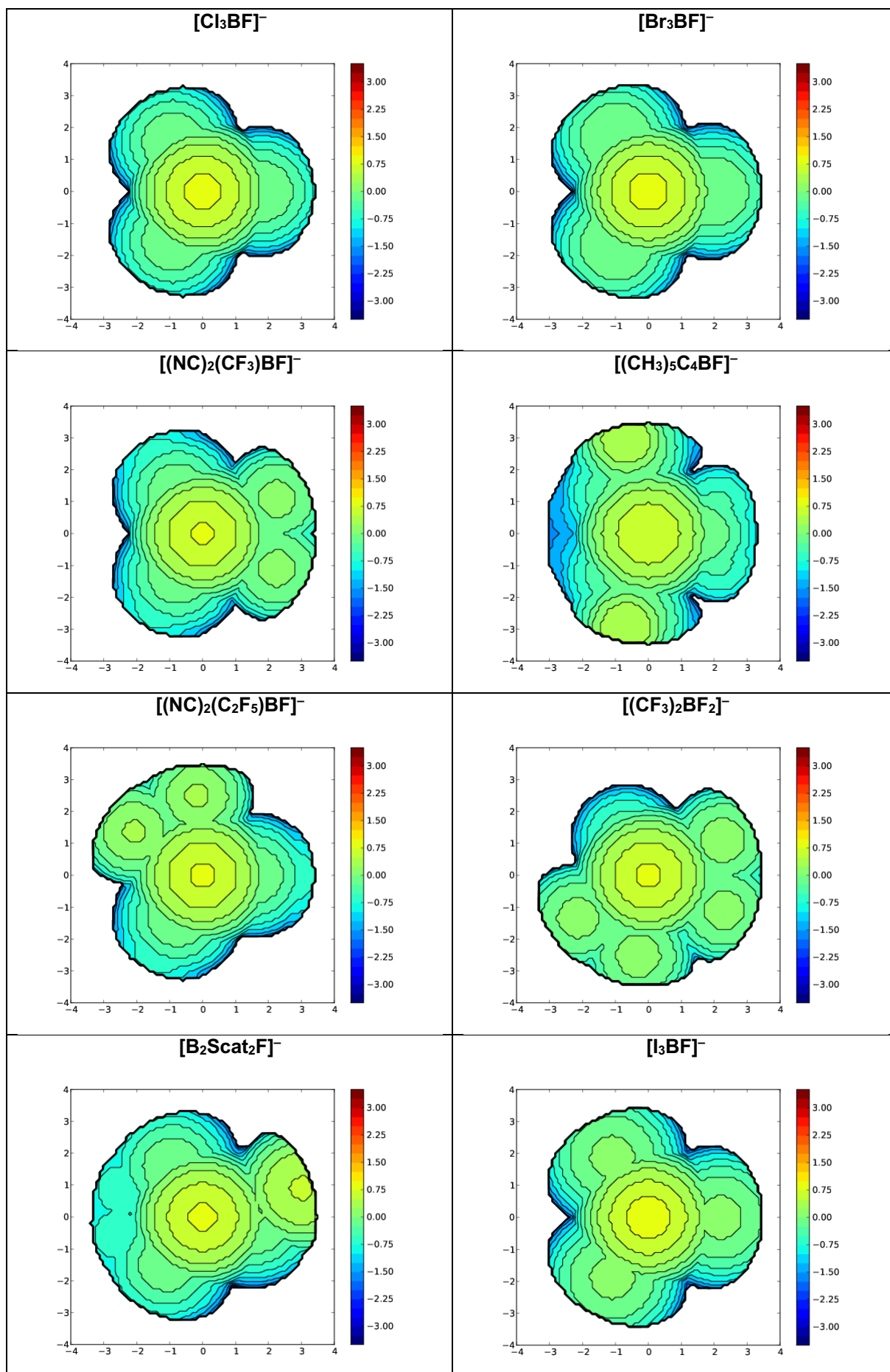
				F 1.27044 -2.83038 -1.24390 F -0.38143 -4.55141 -2.51428 F 0.31561 -2.93065 -3.80672 F -2.94512 -0.35543 -3.79172 F -4.55029 0.38740 -2.50534 F -2.82624 -1.26725 -1.22061 F -2.72887 0.78892 -0.45721 F -2.92226 1.71406 -3.09786 F 2.91672 -1.71278 -3.10064 F 4.55027 -0.39643 -2.50038 F 2.95199 0.35848 -3.78840 F 2.82659 1.26643 -1.21930 F 2.72702 -0.78971 -0.45604 F 0.77512 2.73235 -0.45259 F -1.27112 2.83005 -1.24371 F 0.38227 4.55110 -2.51389 F 1.73899 2.93616 -3.07186 F -0.31686 2.93105 -3.80609 F -1.73991 -2.93770 -3.07160		
$\text{Te}[\text{OC}(\text{CF}_3)_3]_4$  $\text{R} = \text{F}_3\text{C}-\text{C}(\text{CF}_3)_2-\text{C}(\text{CF}_3)_2-\text{F}_3$	$\{[\text{OC}(\text{CF}_3)_3]_4\text{TeF}\}^-$	75.3	1.990	TE -0.00000 -0.00000 -1.99012 F 0.00000 0.00000 0.00000 • 2.18221 -0.00000 -1.89439 C 3.05649 -1.04979 -1.91036 C 4.46125 -0.49065 -1.45027 C 3.19134 -1.64408 -3.36704 C 2.63296 -2.20143 -0.91681 F 5.33825 -1.49113 -1.17156 F 5.01523 0.27221 -2.41375 F 4.33822 0.26105 -0.34815 F 2.07719 -2.34811 -3.68242 F 4.25015 -2.48324 -3.49814 F 3.33202 -0.66345 -4.26366 F 2.78631 -1.82675 0.36403 F 3.32853 -3.34552 -1.10084 F 1.31828 -2.50655 -1.09369 O 0.12784 0.15862 -4.15956 C -0.52002 0.39984 -5.33424 C -1.56577 -0.74972 -5.62210 C 0.56425 0.39294 -6.48482 C -1.25910 1.79365 -5.34914 F -2.45503 -0.43083 -6.59248 F -0.93854 -1.88591 -6.00872 F -2.25769 -1.03983 -4.50739 F 1.30391 1.52073 -6.45833 F 0.00080 0.30379 -7.71859 F 1.40105 -0.64687 -6.34813 F -2.37976 1.75046 -4.60353 F -1.62166 2.16385 -6.60658 F -0.46766 2.75493 -4.85663 O -2.11883 0.45443 -1.92773 C -3.16825 0.00714 -1.17769 C -3.26875 -1.56706 -1.17742 C -4.47145 0.59504 -1.85559 C -3.12110 0.51562 0.32829 F -4.08027 -2.04494 -0.20801 F -3.72724 -2.03636 -2.35513 F -2.03891 -2.10933 -0.98747 F -4.57930 1.91567 -1.60038 F -5.60216 -0.00702 -1.40217 F -4.43632 0.43506 -3.18464 F -2.40462 -0.31207 1.11531 F -4.36522 0.59052 0.87542 F -2.57532 1.73487 0.38553 O 0.18097 2.02401 -2.02227 C 0.86228 3.06437 -1.41198 C 1.21927 2.87190 0.11192 C -0.15092 4.28175 -1.54432 C 2.18560 3.40939 -2.21759 F 1.96778 3.92177 0.54542 F 0.10296 2.83214 0.86268 F 1.92532 1.76254 0.33448 F -0.21878 4.69446 -2.82582 F 0.21539 5.34608 -0.79240 F -1.37816 3.91329 -1.16075 F 3.24369 2.70337 -1.77796 F 2.50523 4.72408 -2.08461 F 2.02145 3.15347 -3.51814	430	

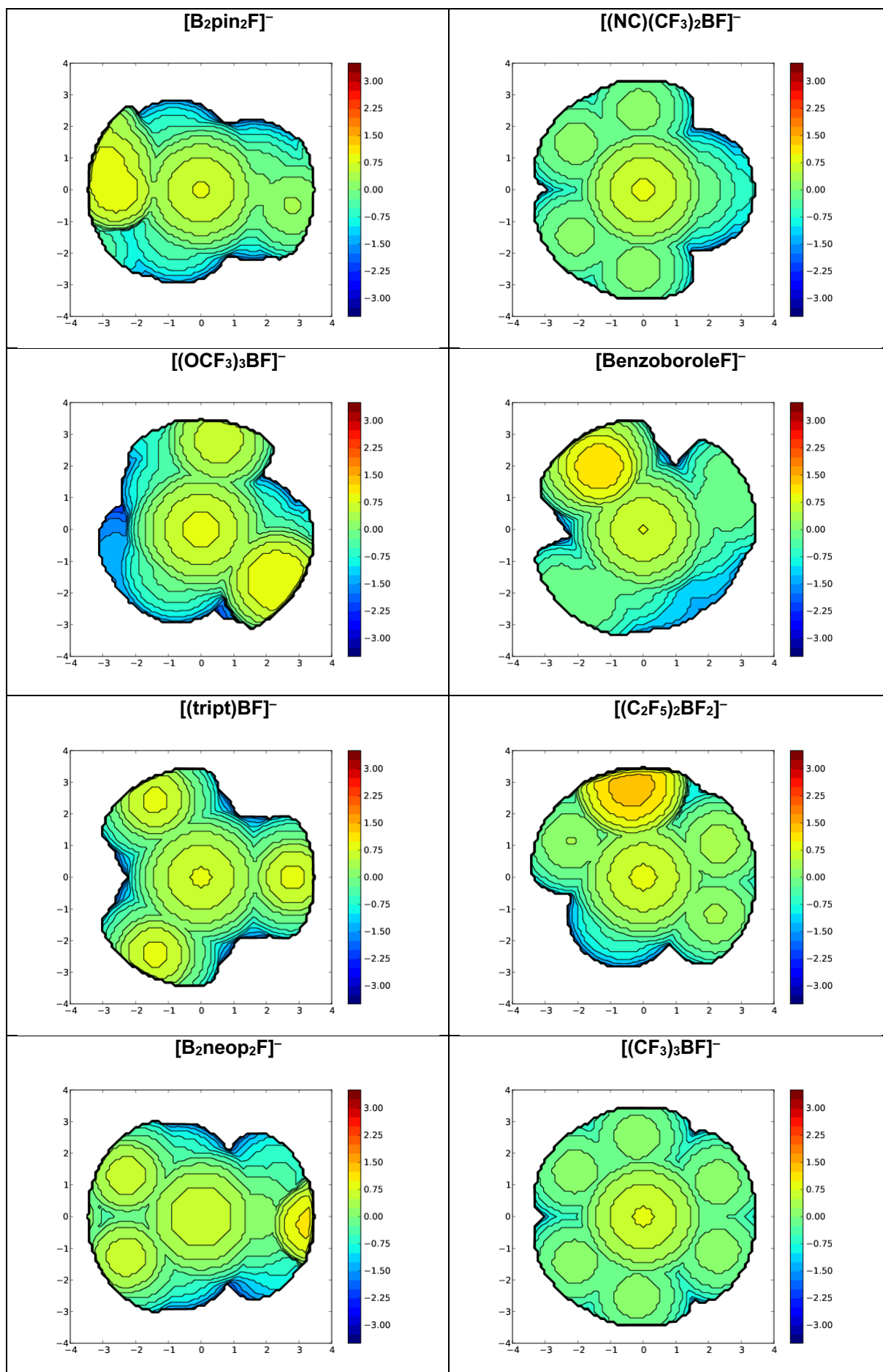
2. Topographic steric maps of selected Lewis Acids

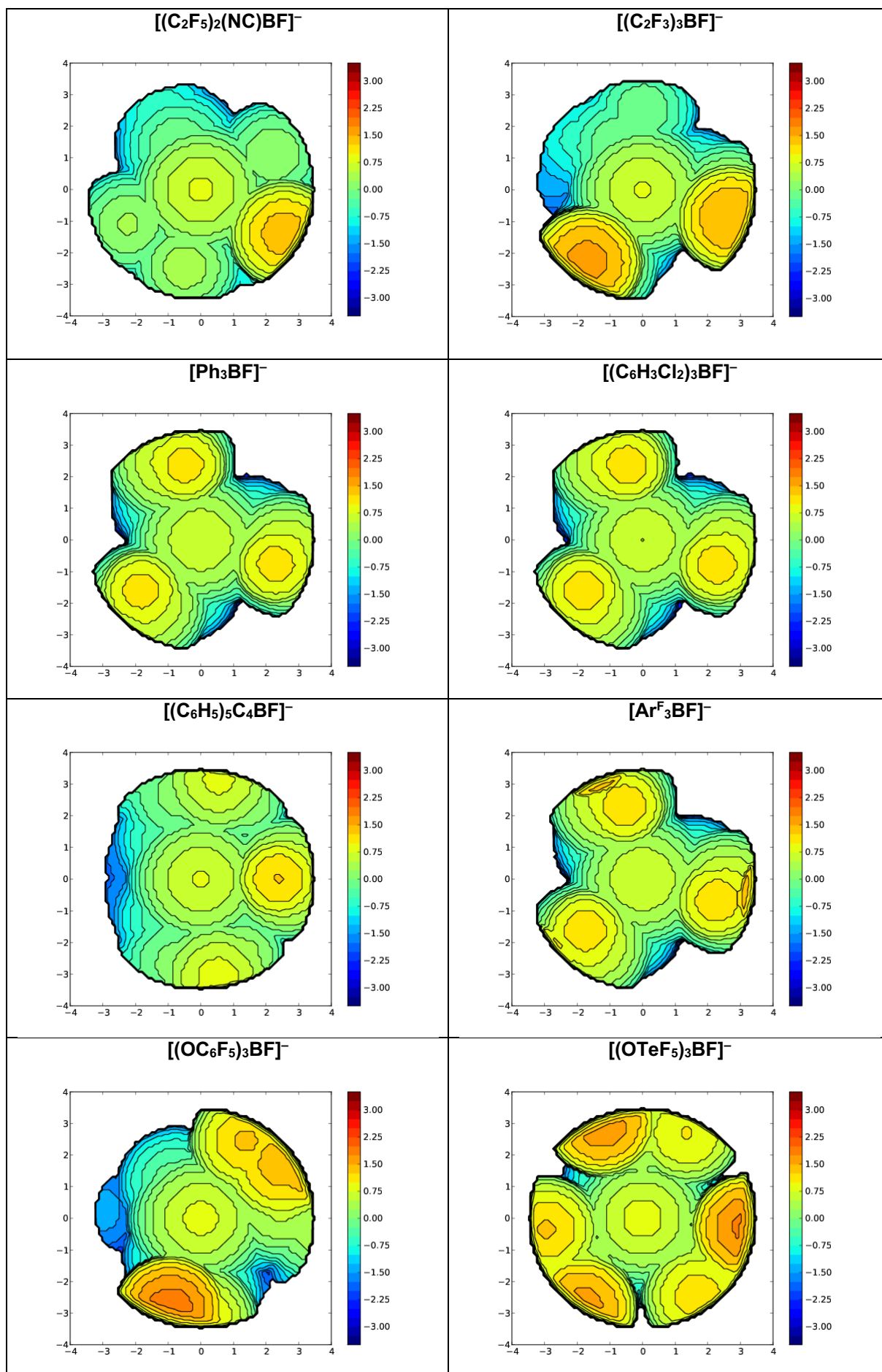
Figure S1. Topographic steric maps of the Lewis acids *LA* under consideration (see Table S1) in their fluoride adducts $[LA-F]^-$ ($R = 3.50$ Å). The isocontour scheme is given in Å, red and blue zones indicate the more- and less-hindered zones with respect of the origin. The steric maps allow to differentiate shapes of the Lewis acids/bases. Topographic steric maps have been obtained from the SambVca 2.1 web application: <https://www.molnac.unisa.it/OMtools/sambvca2.1/index.html>.

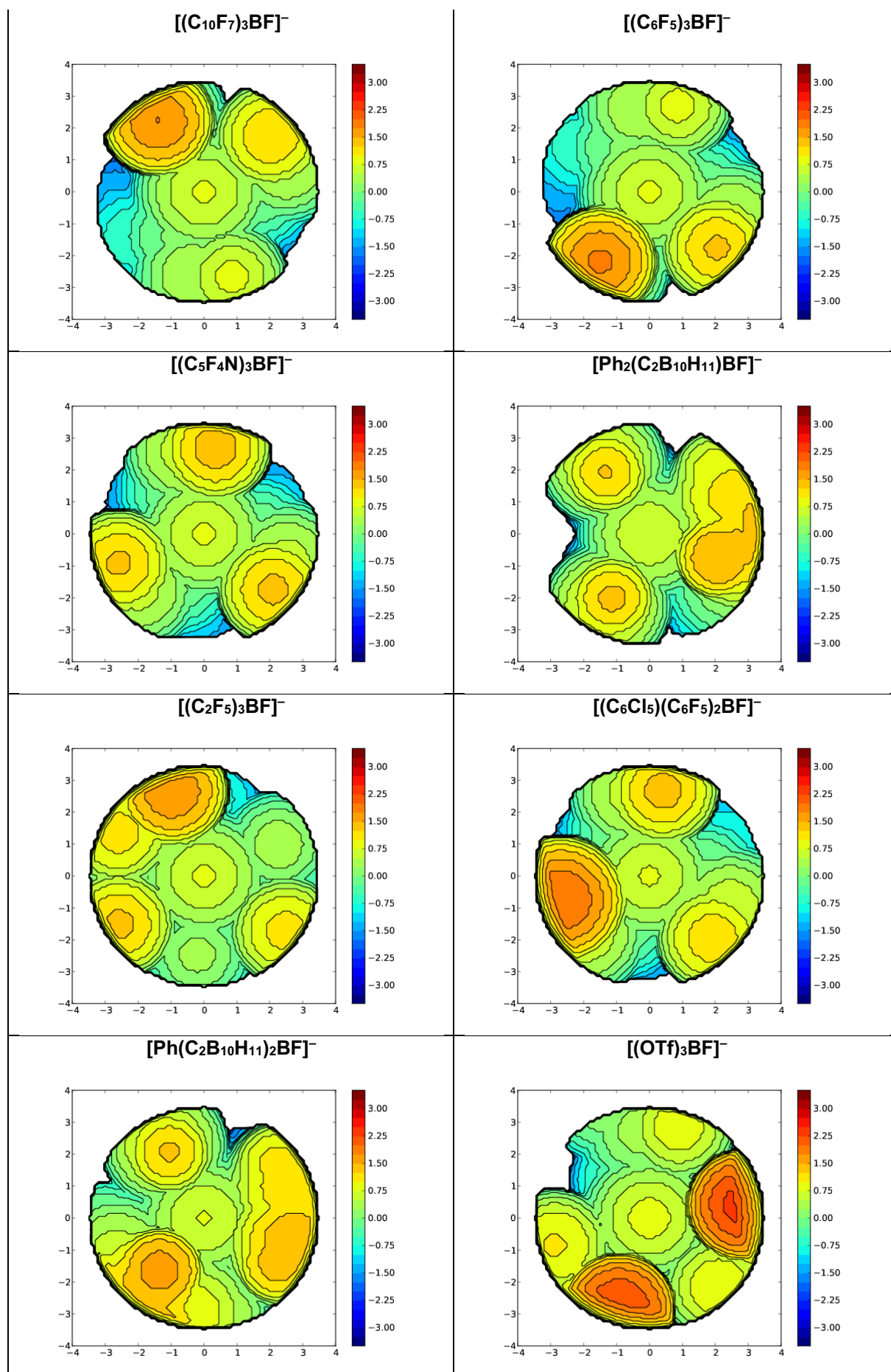


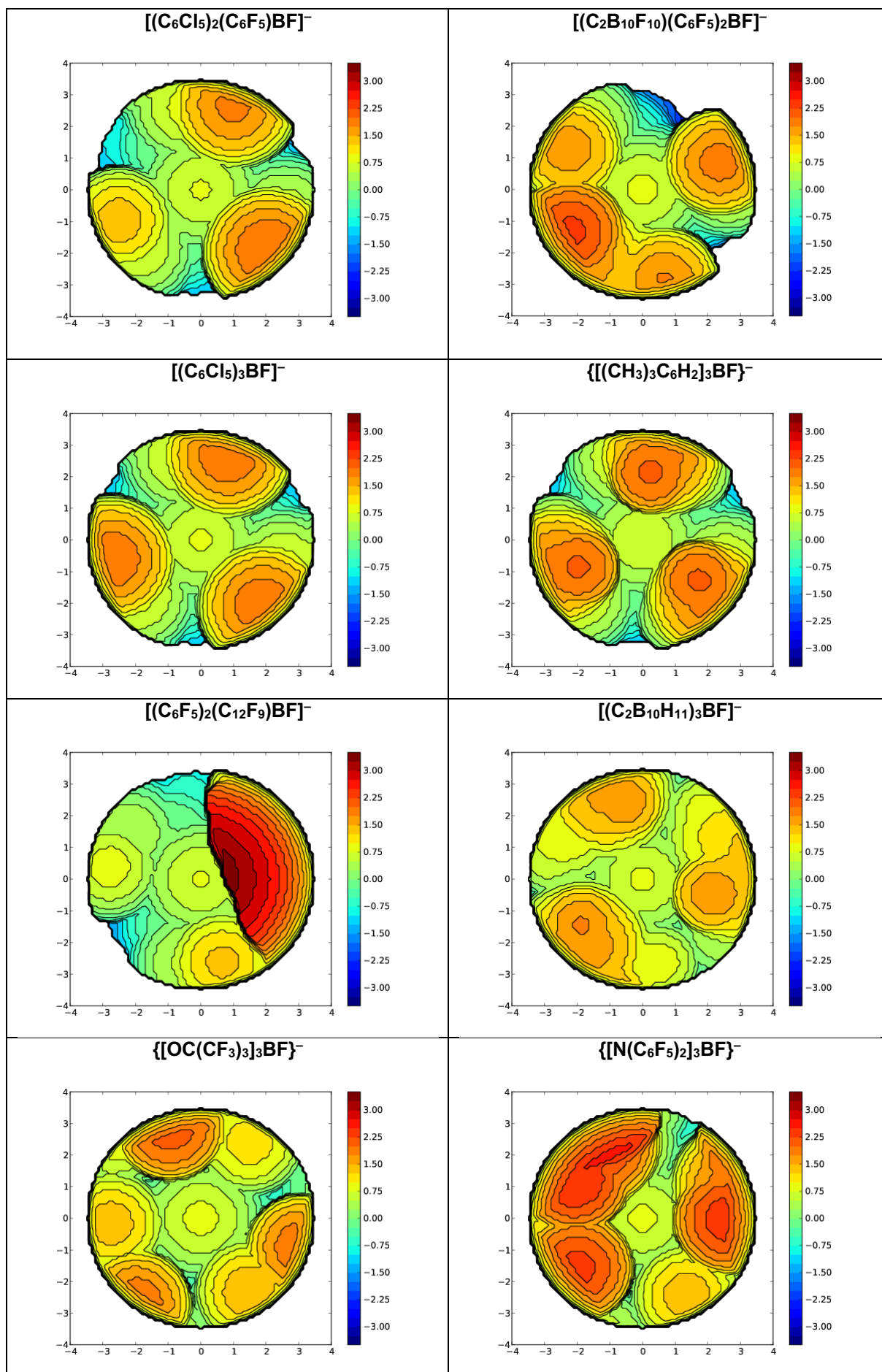


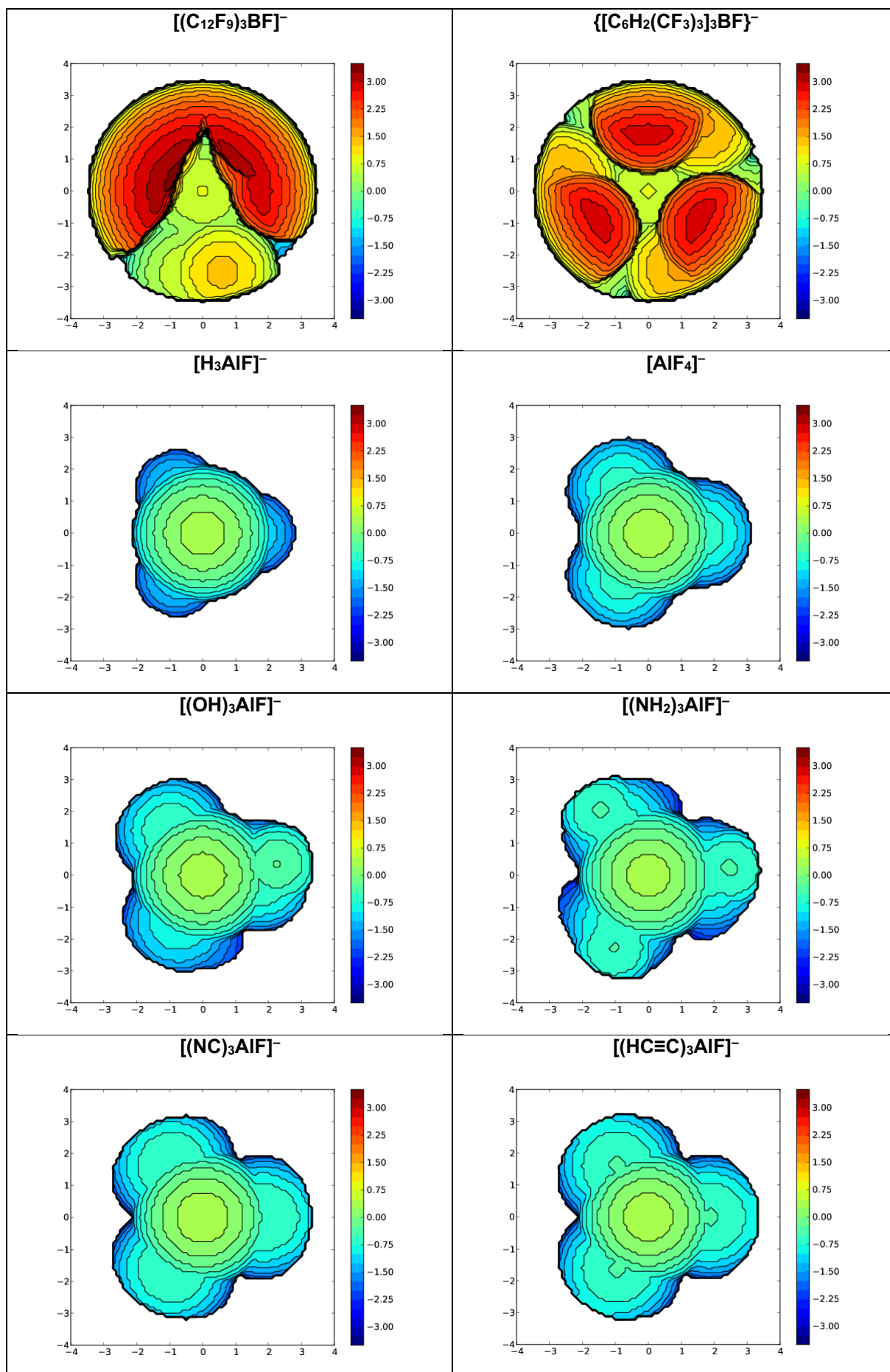


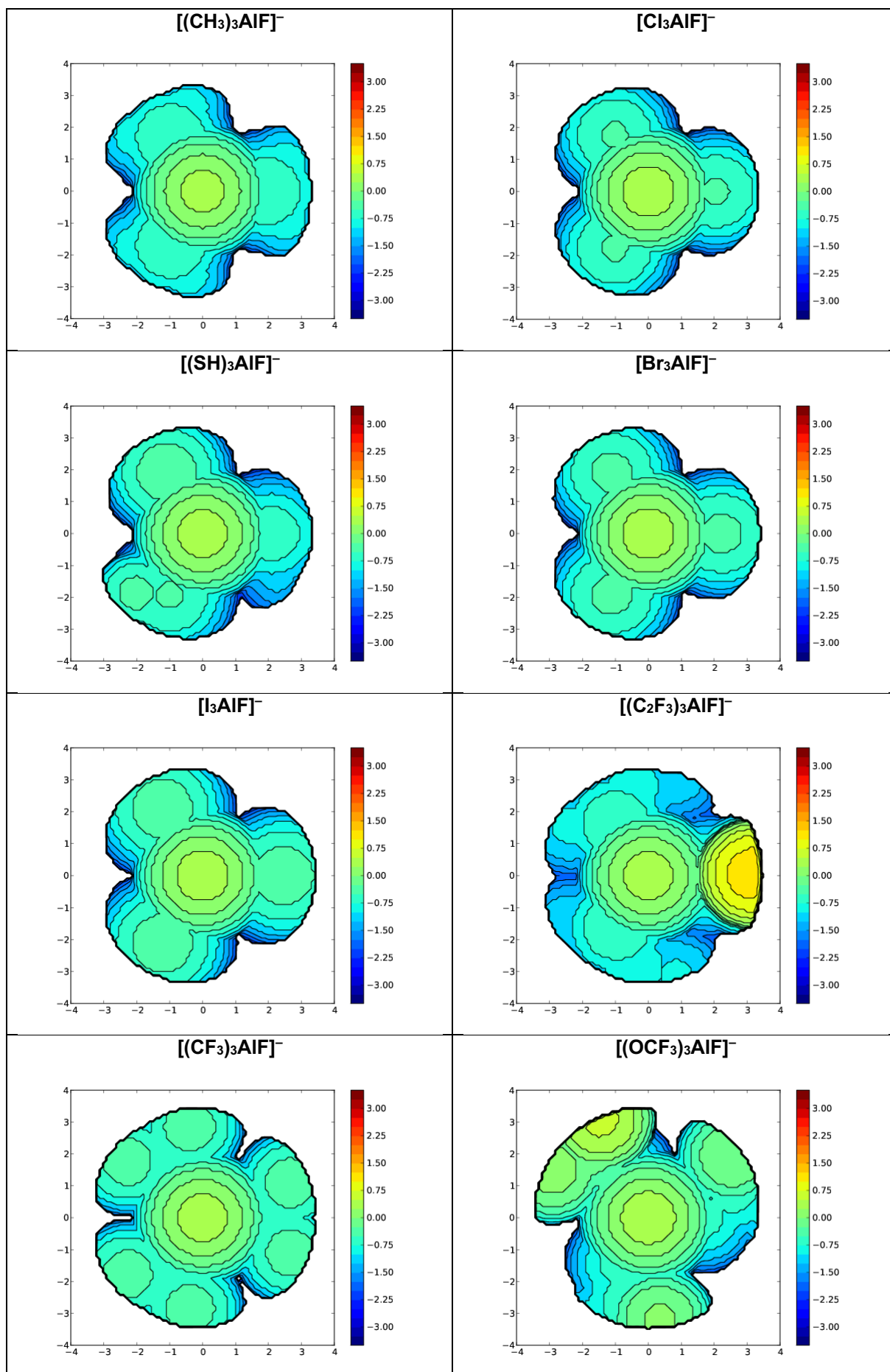


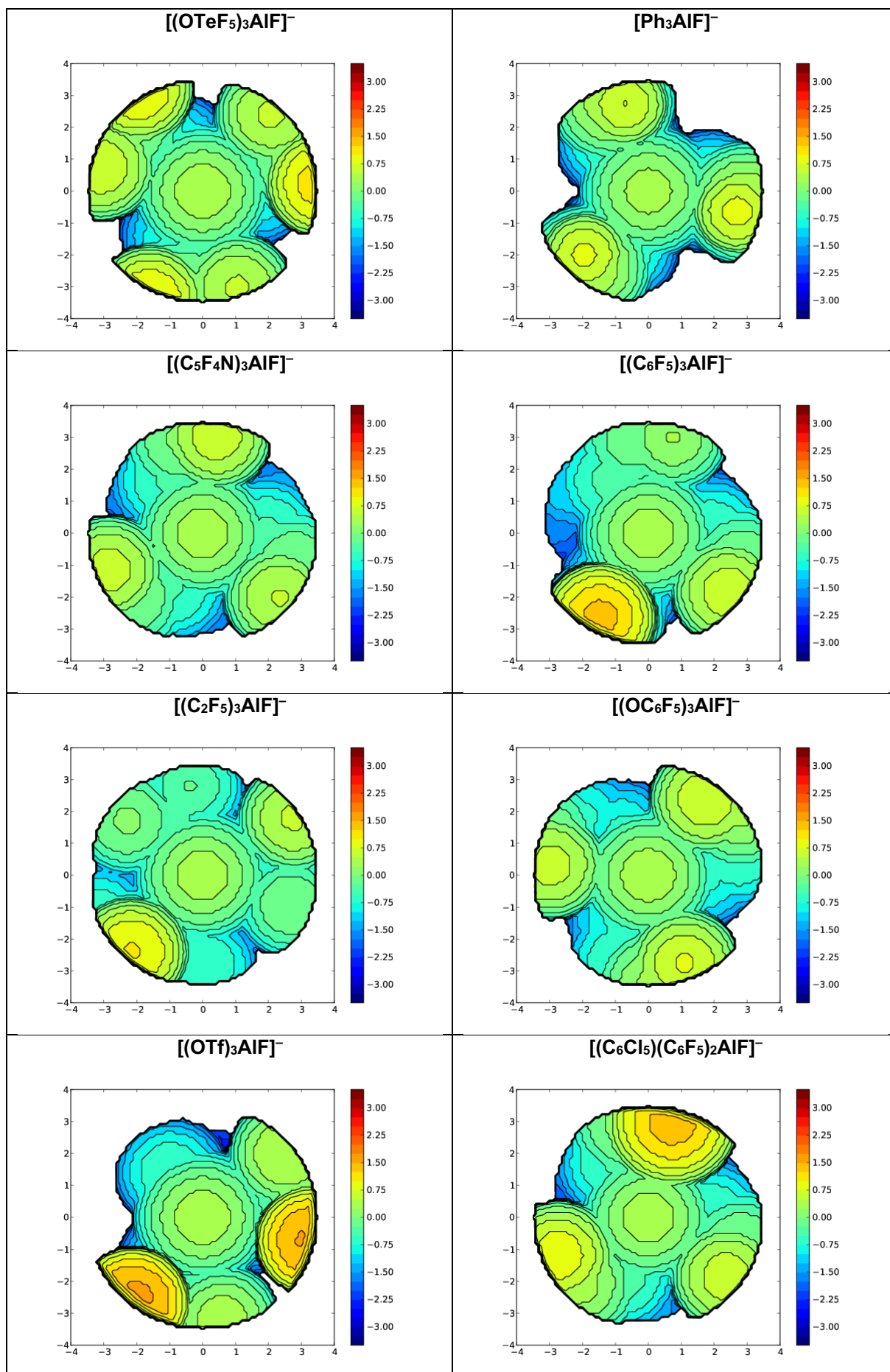


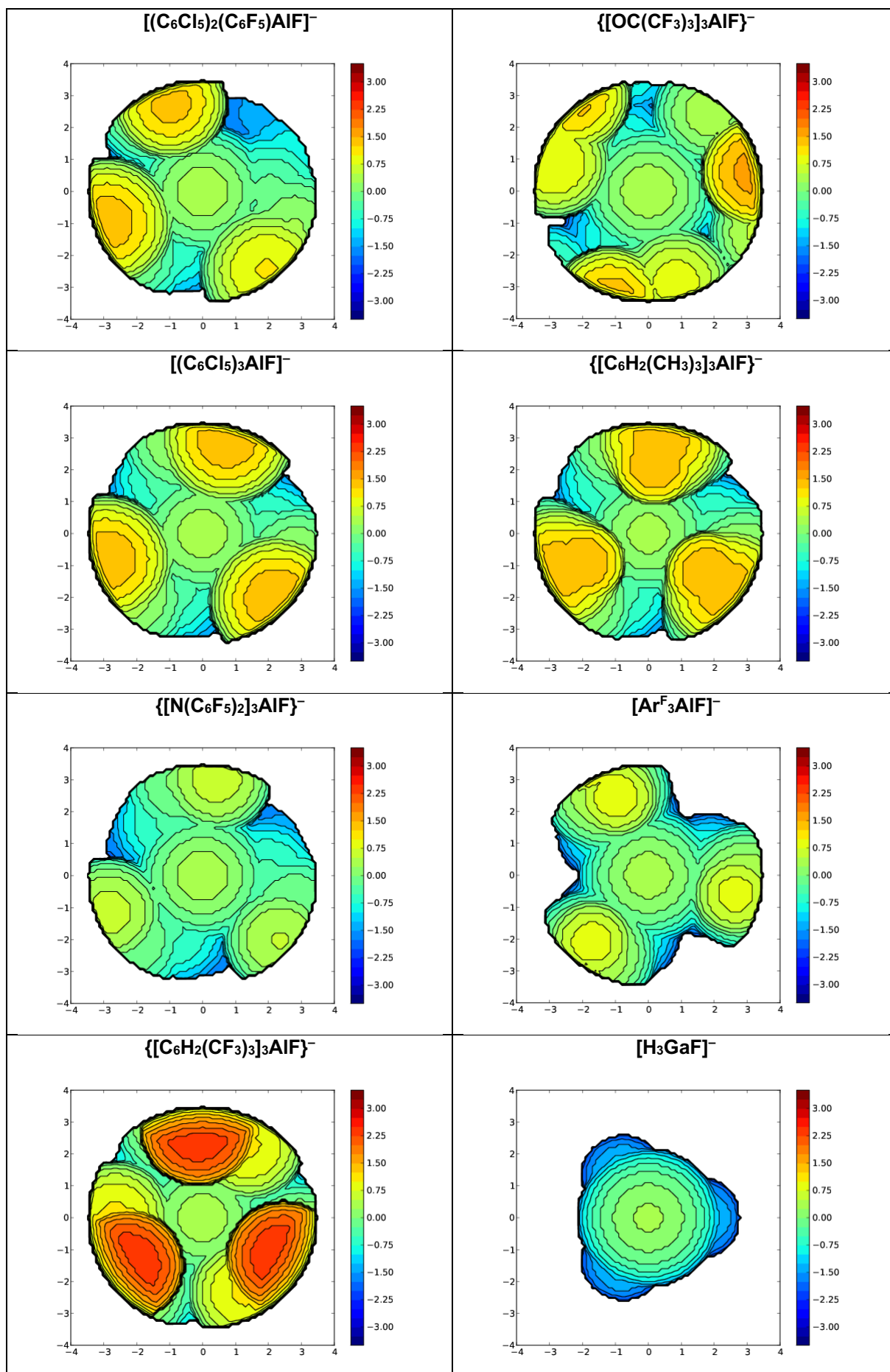


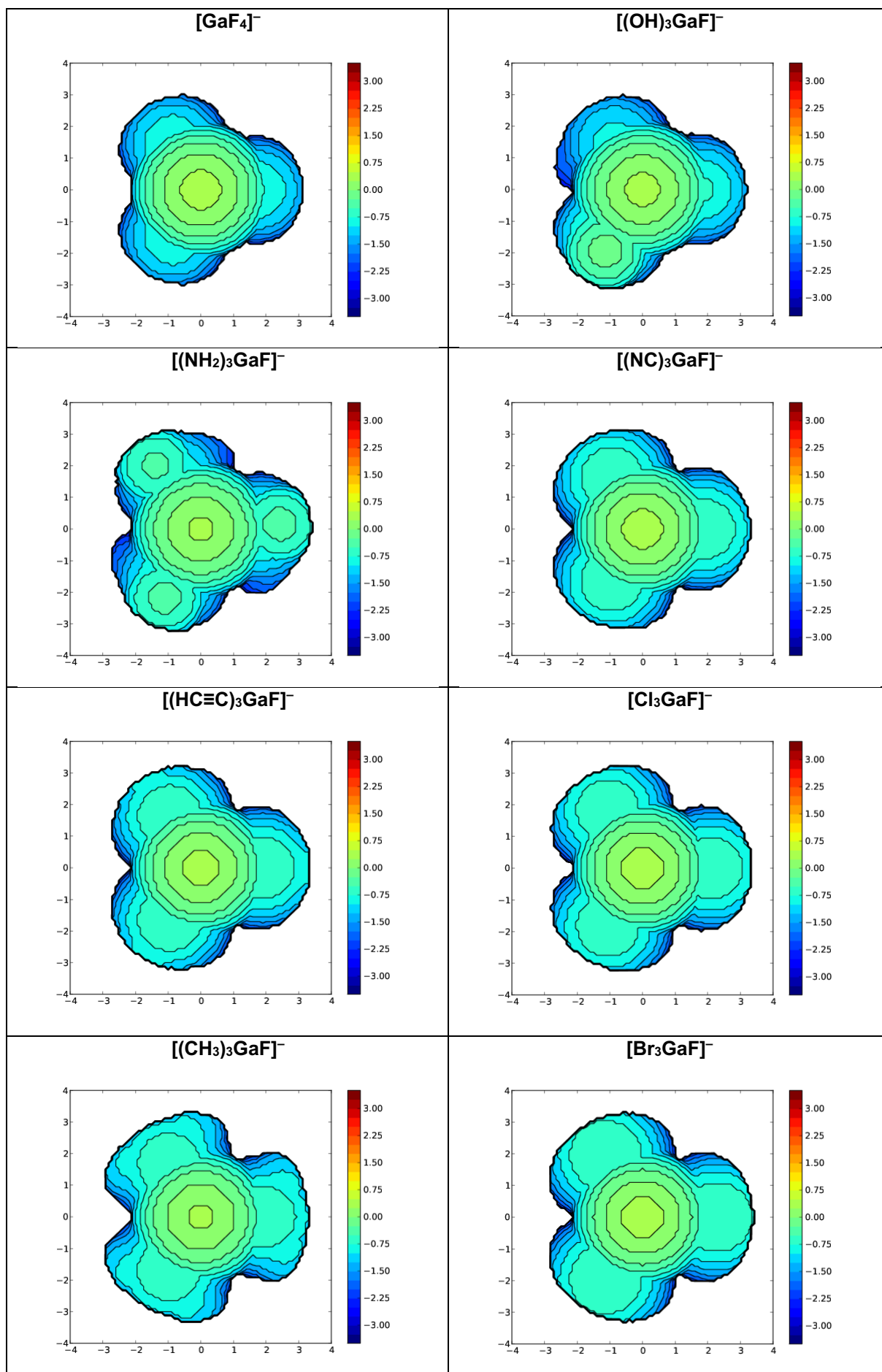


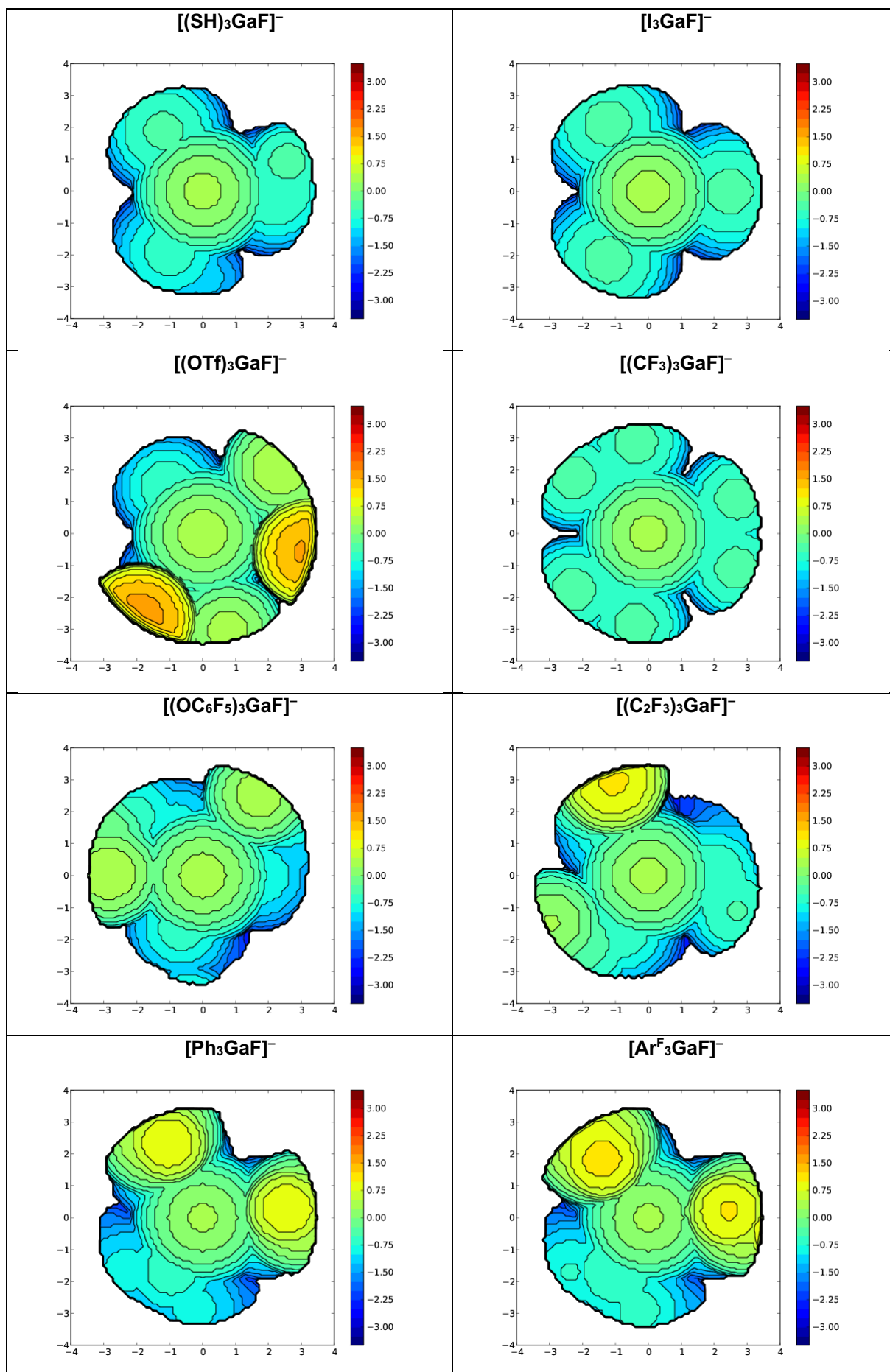


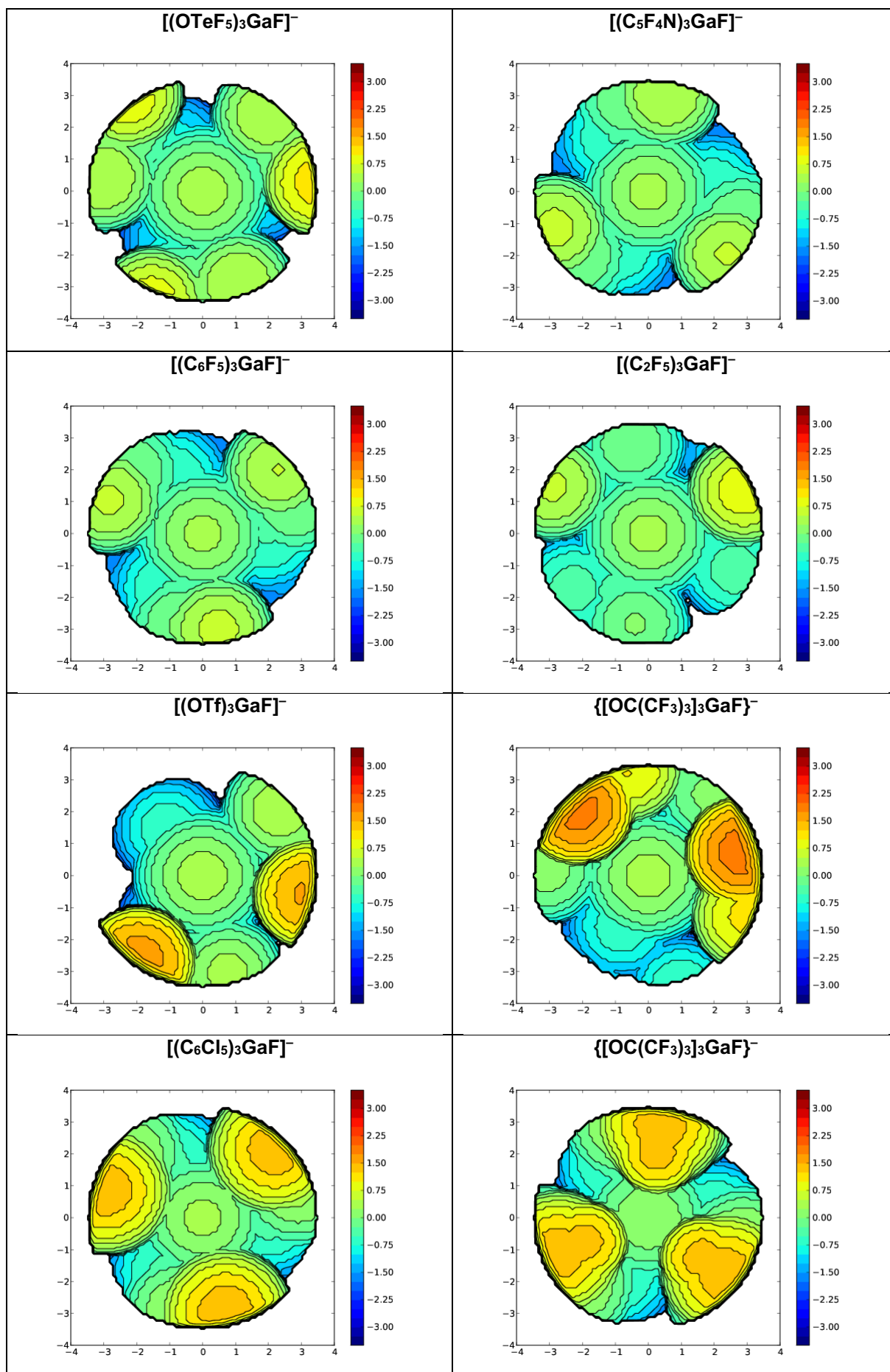


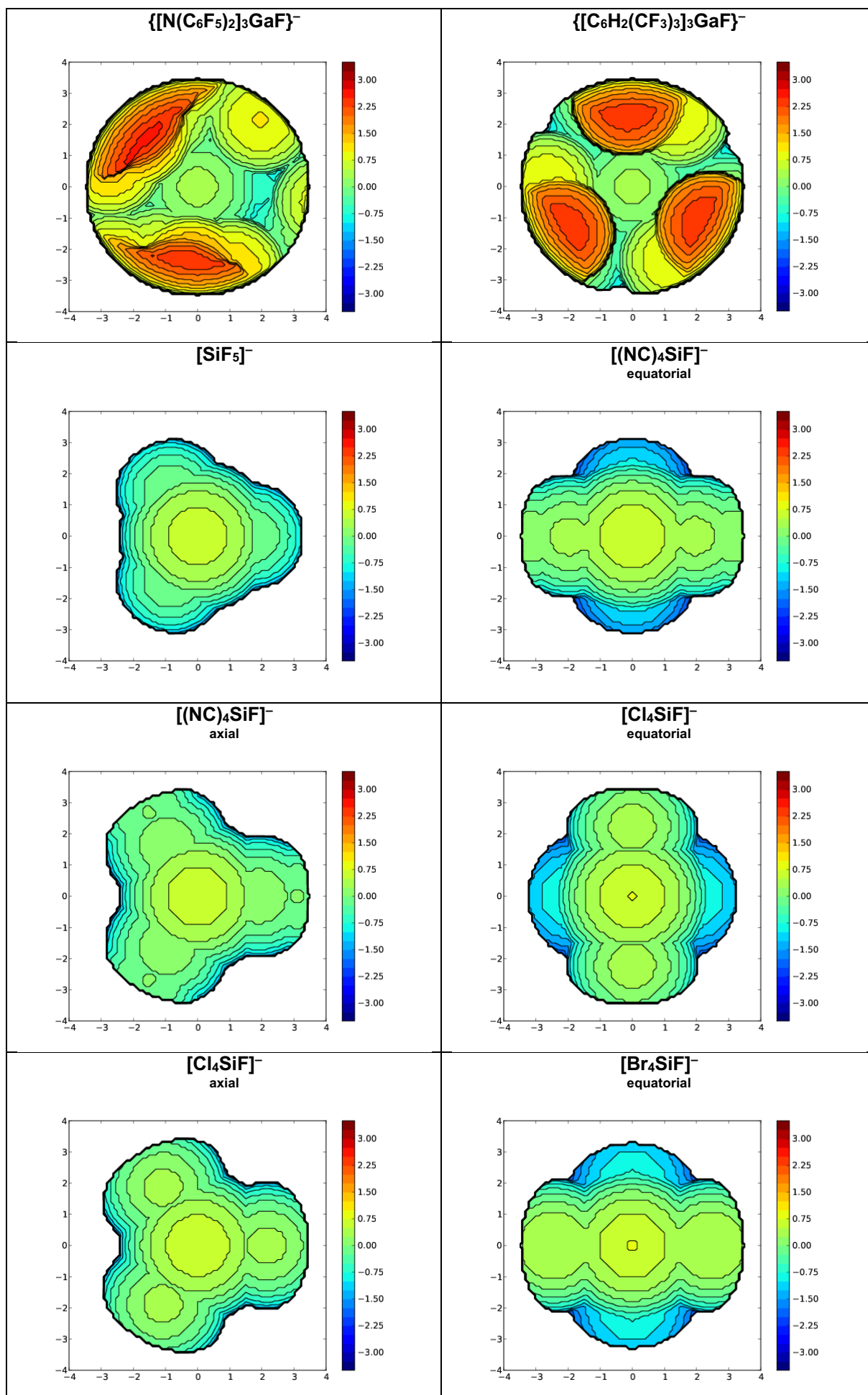


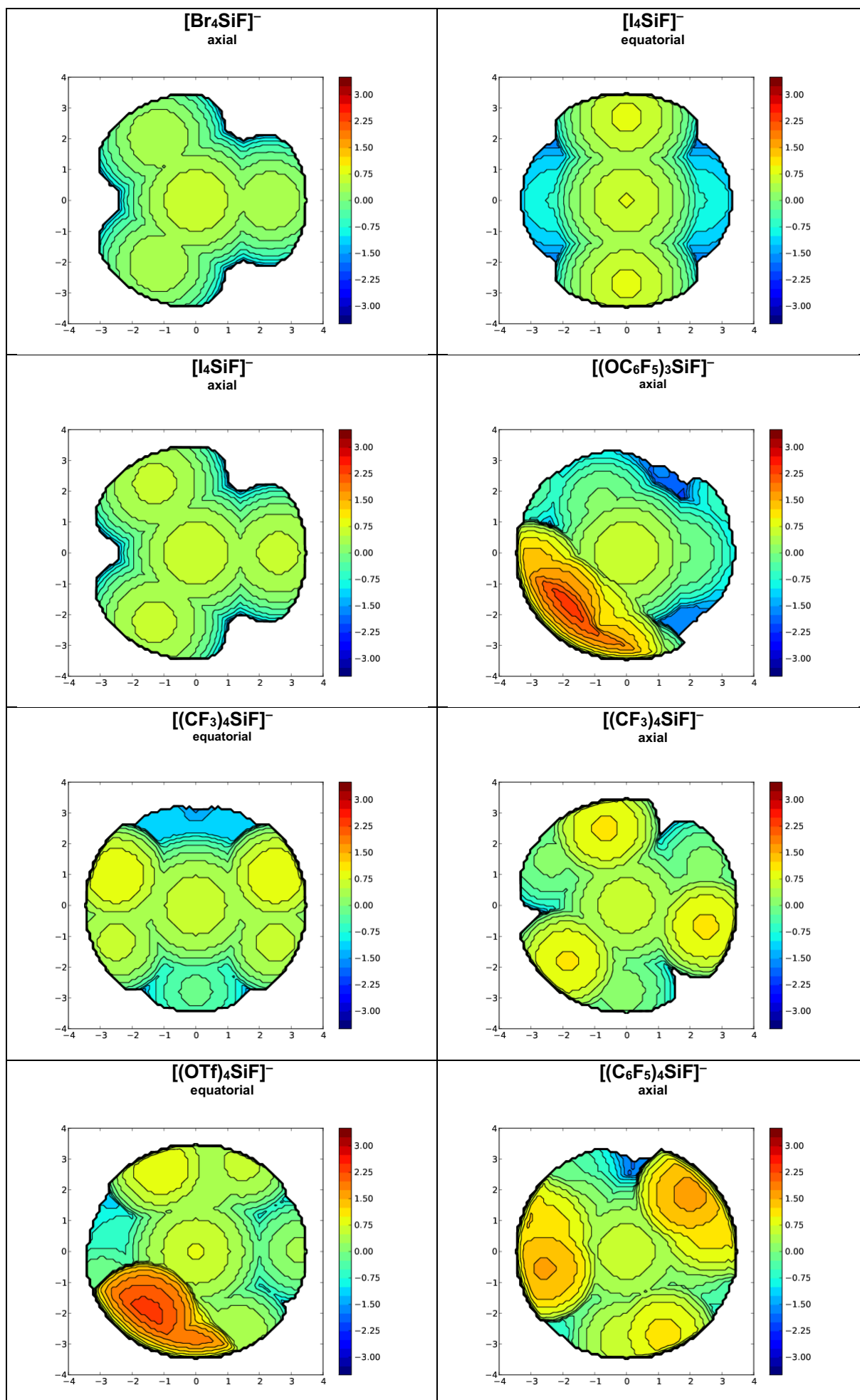


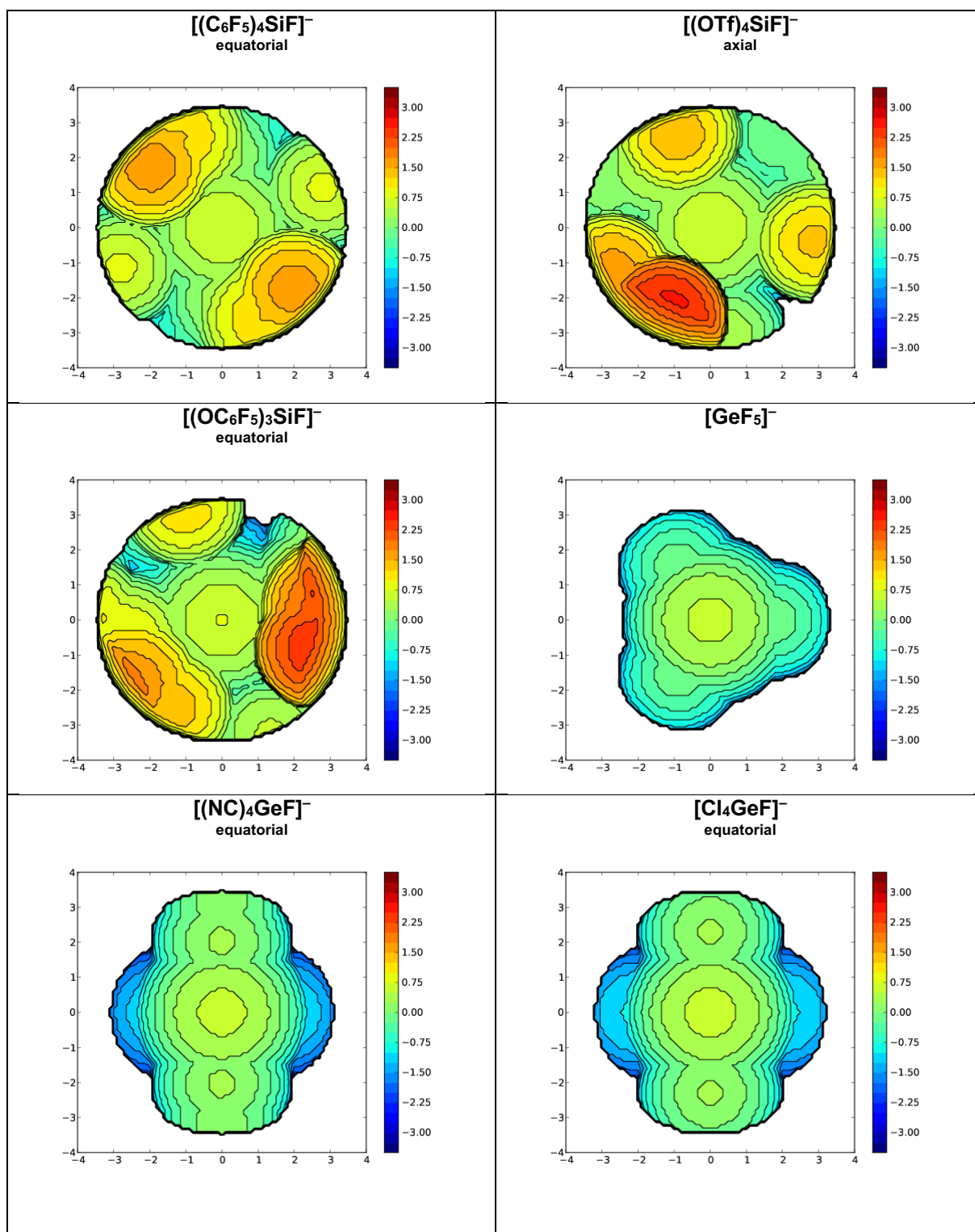


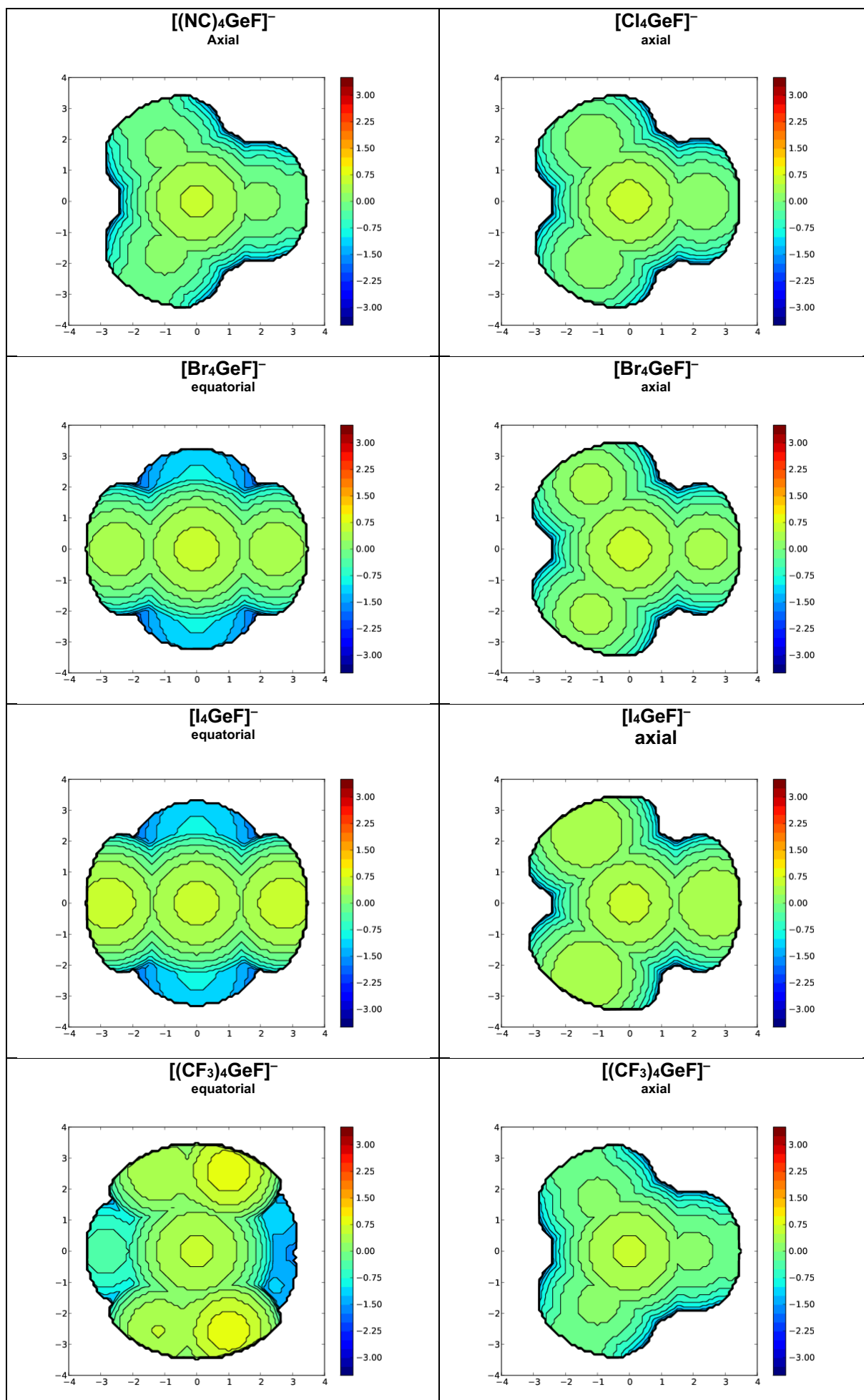


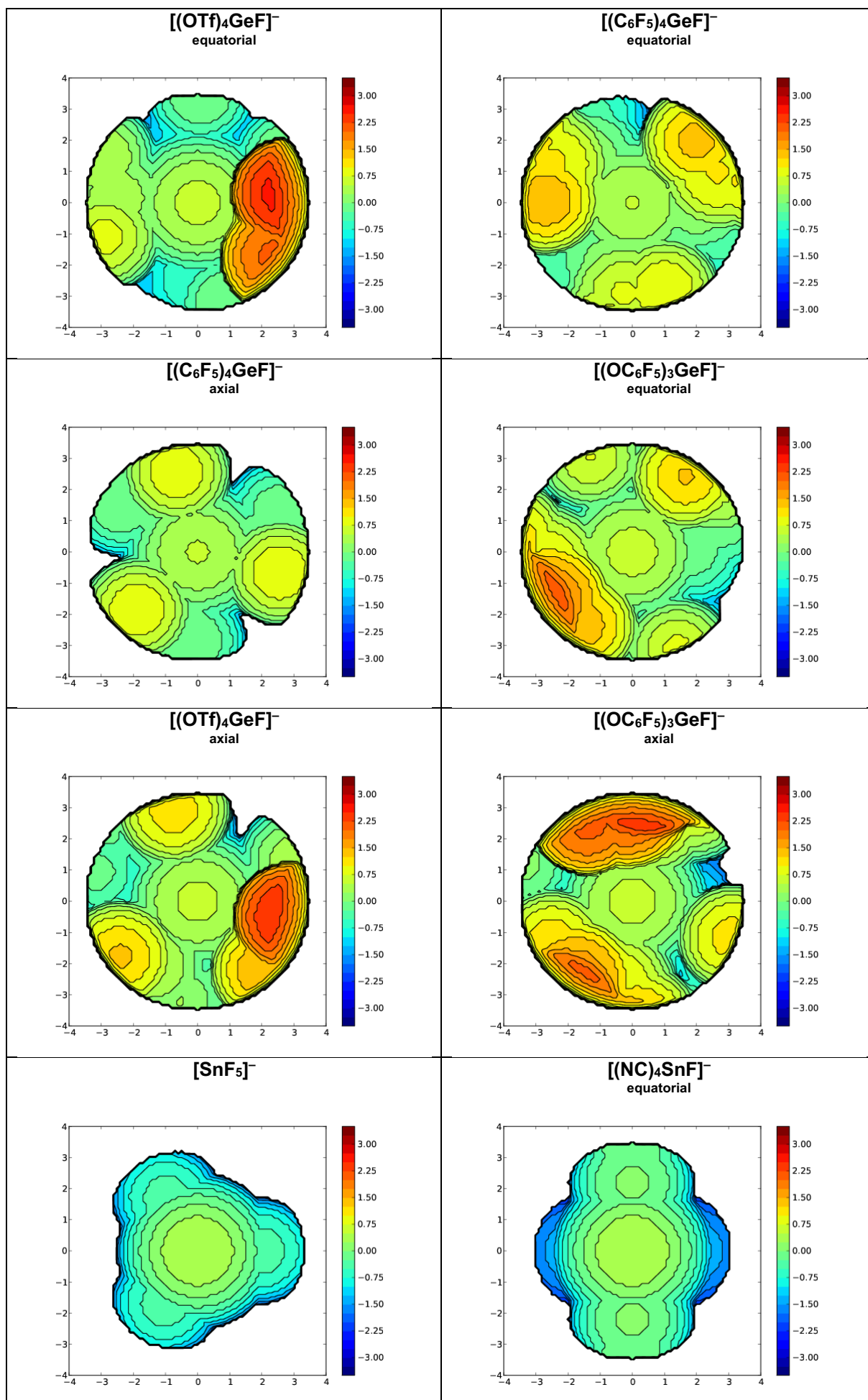


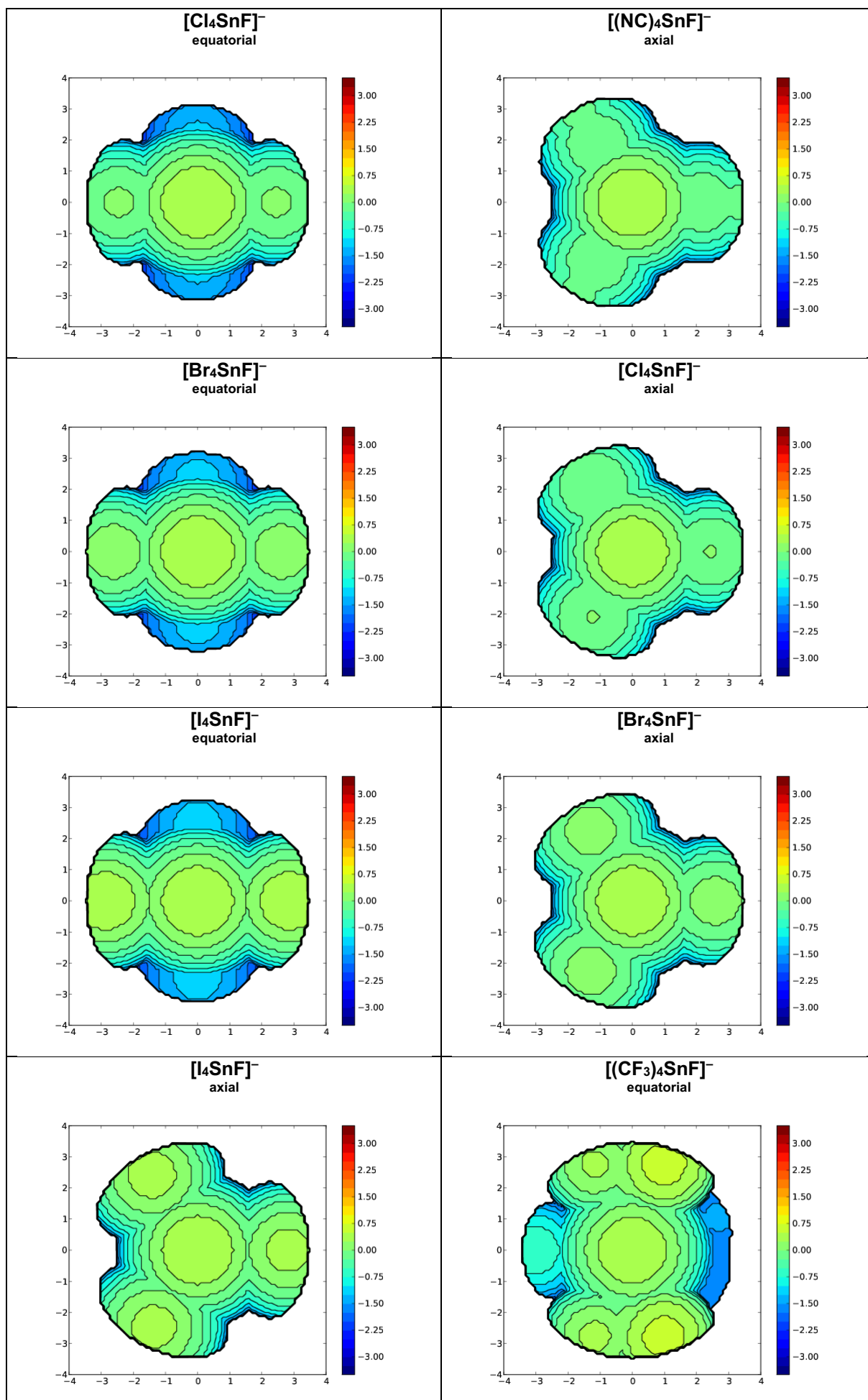


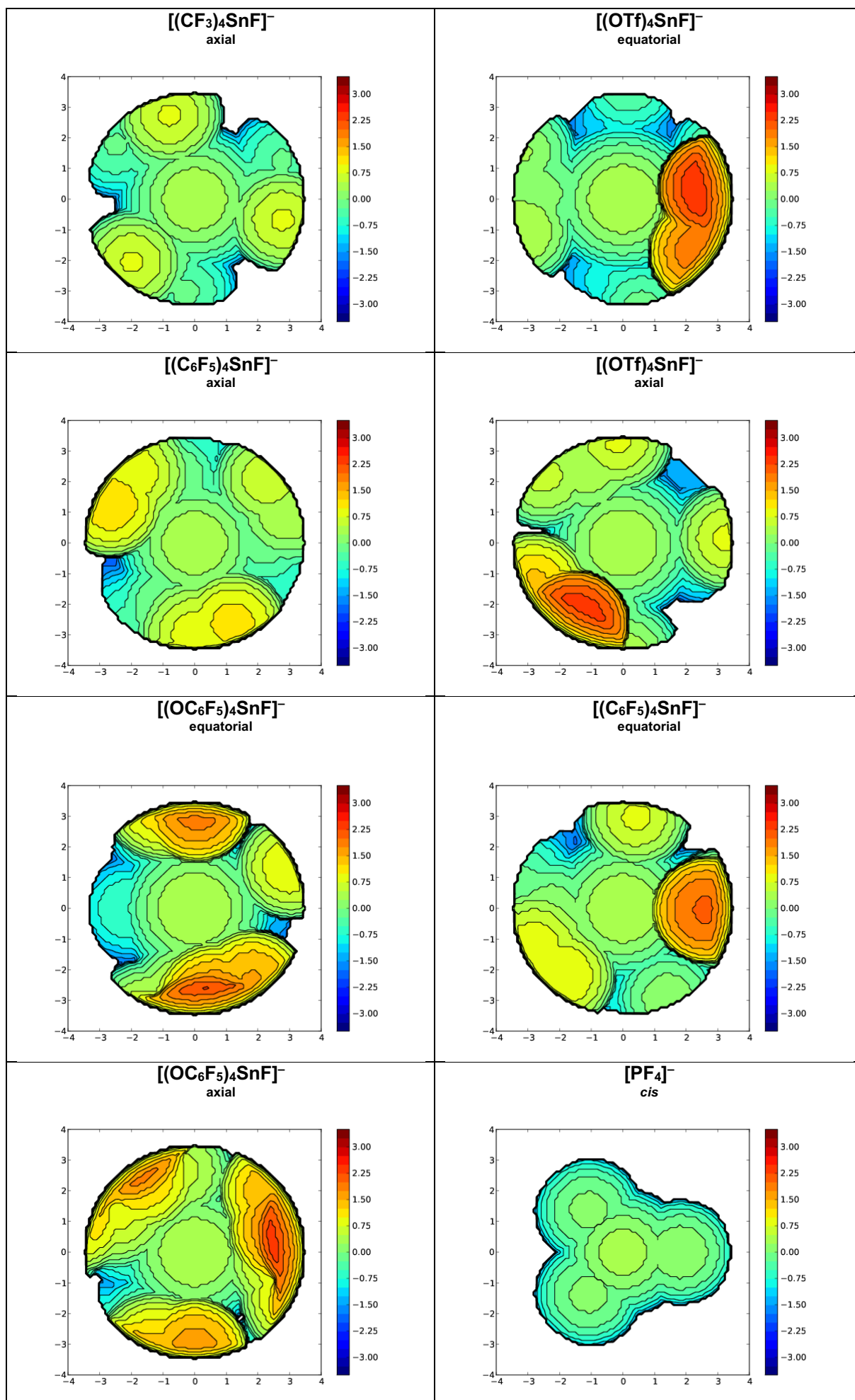


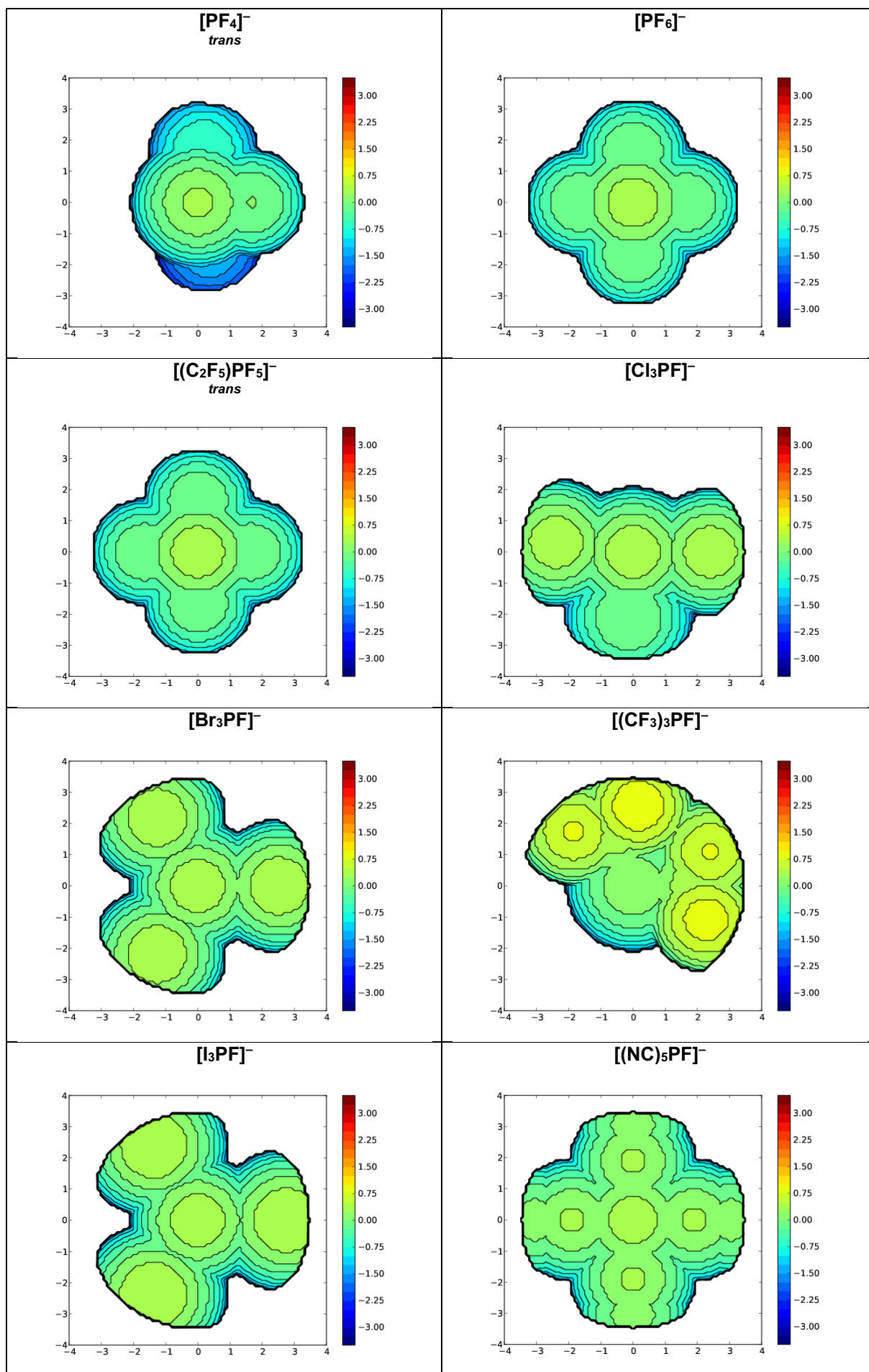


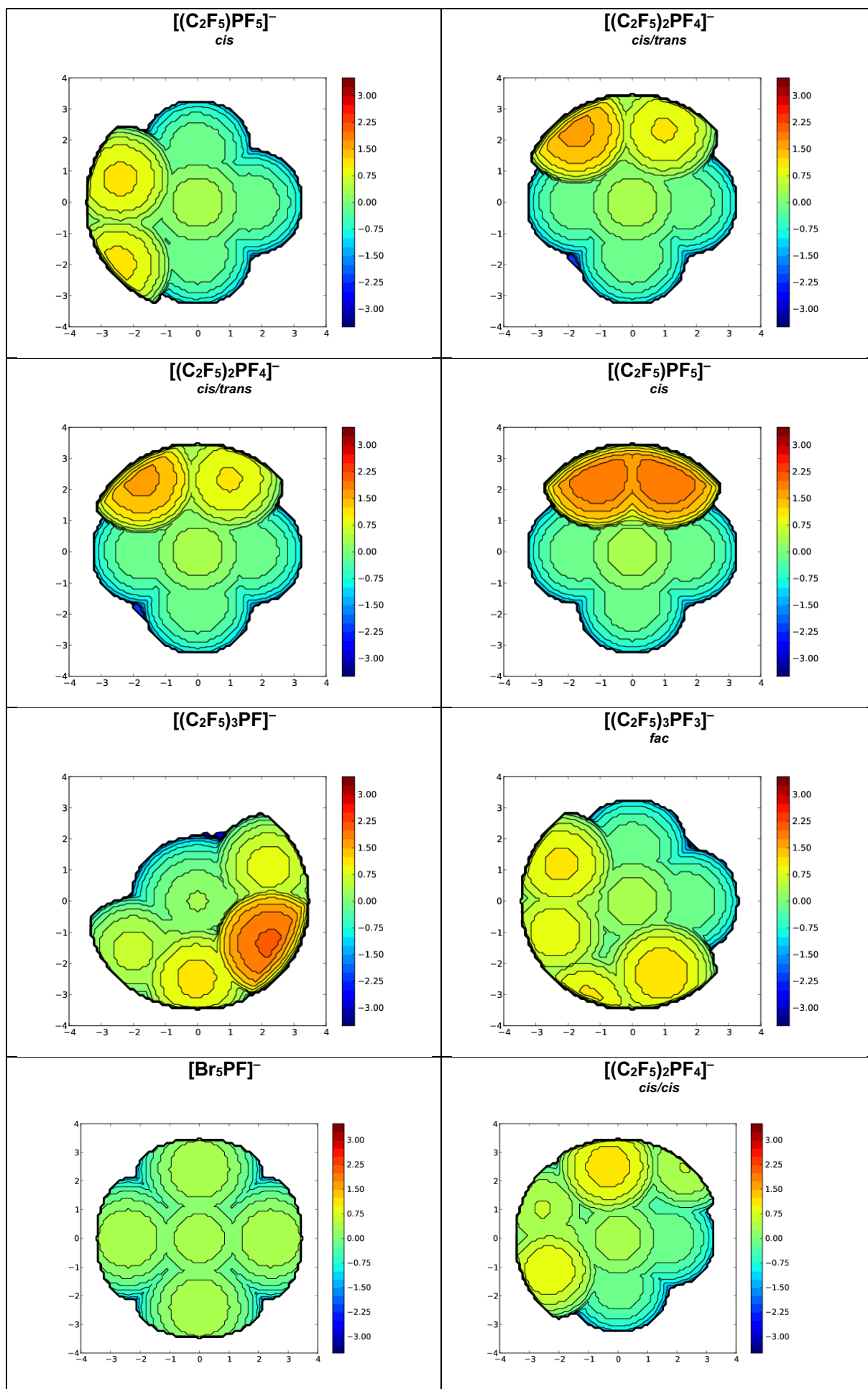


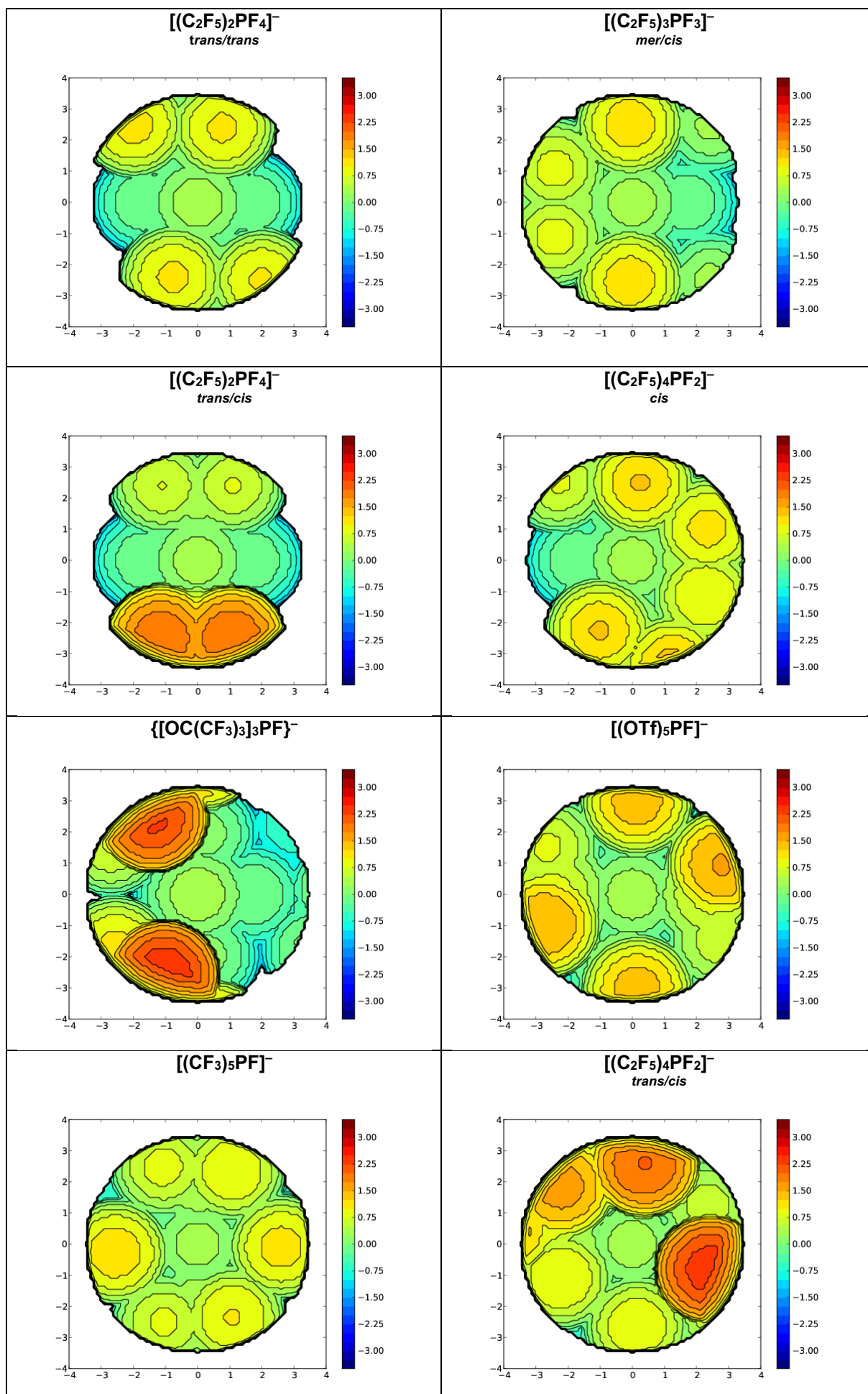


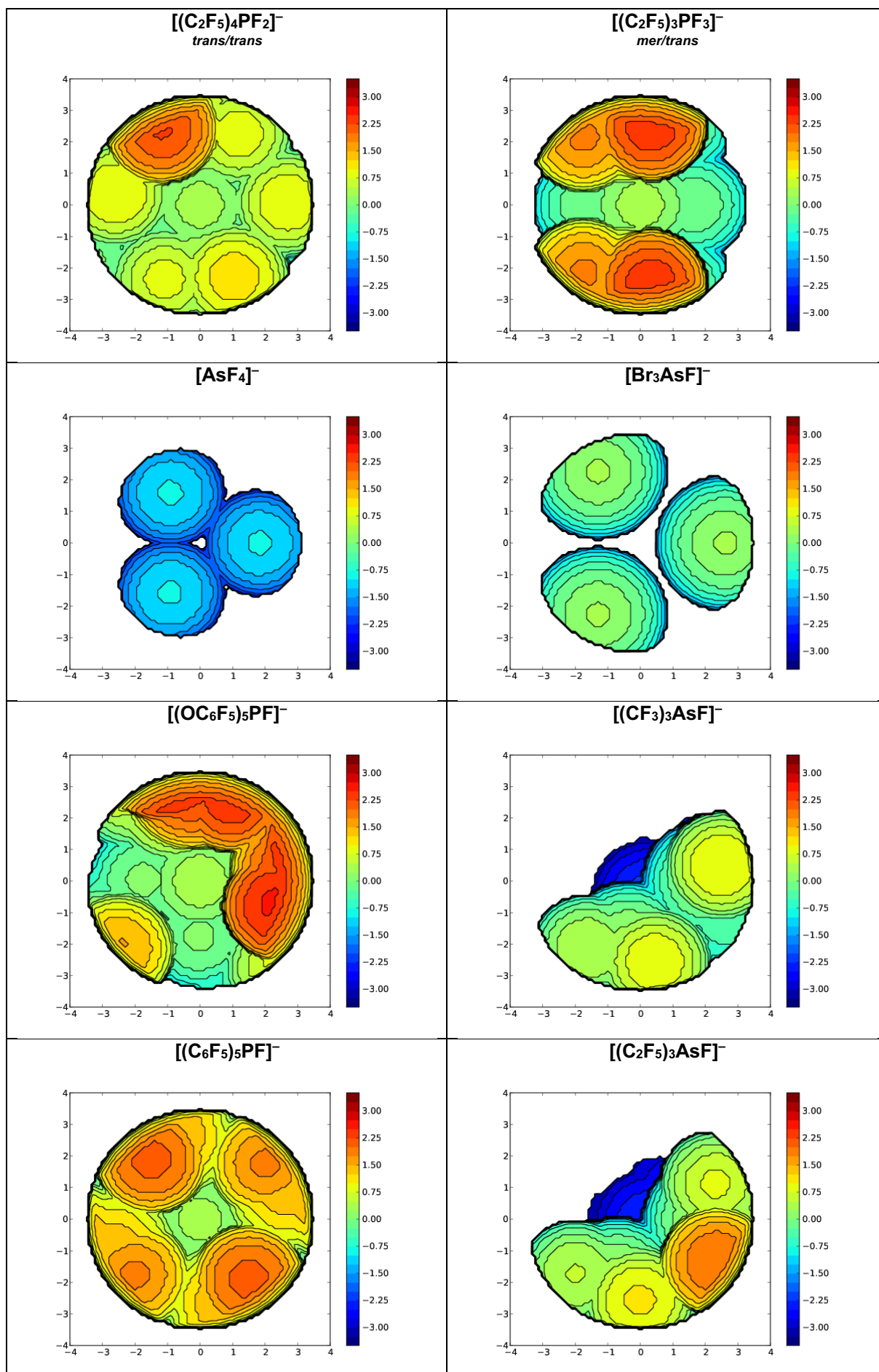


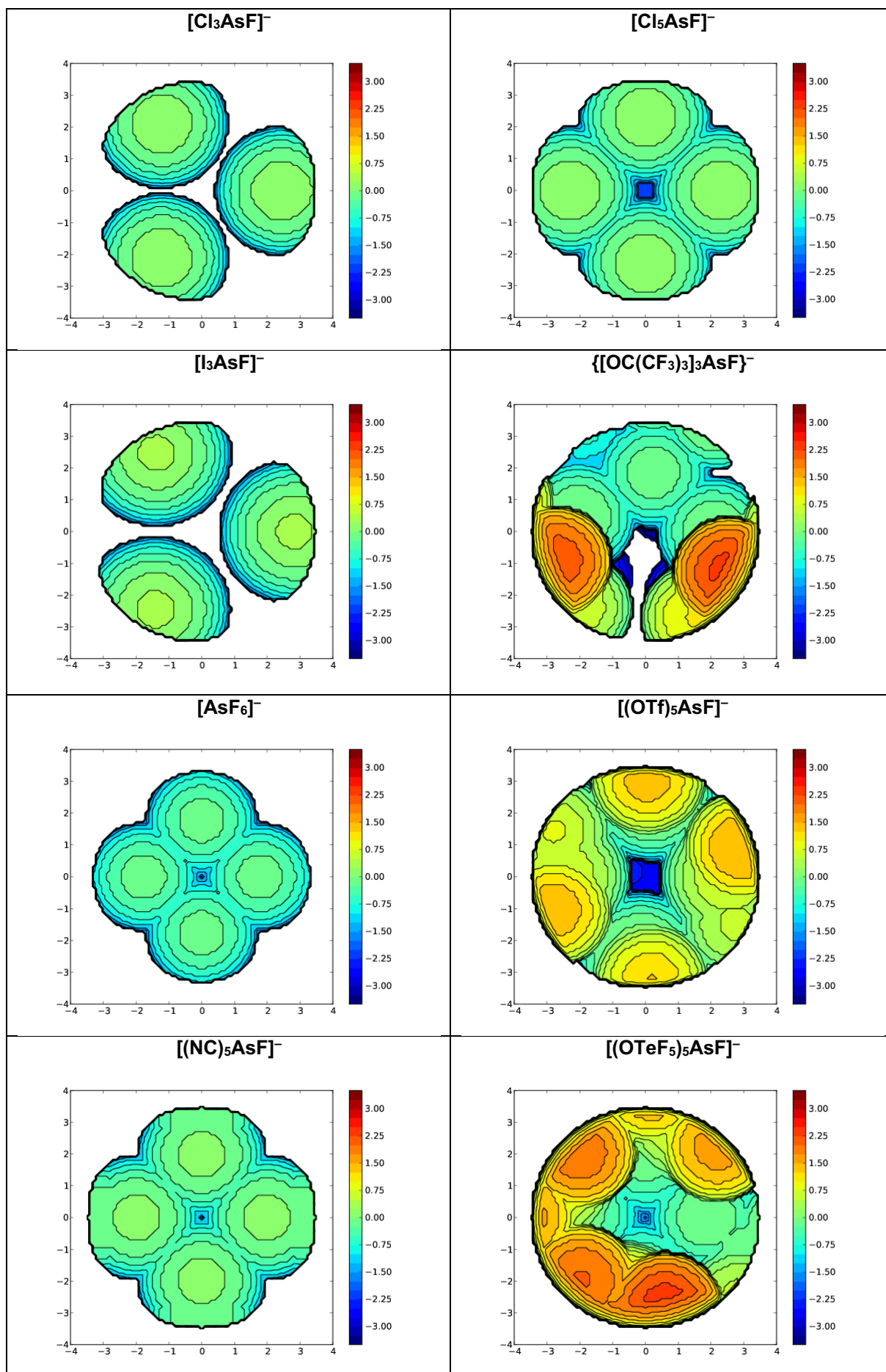


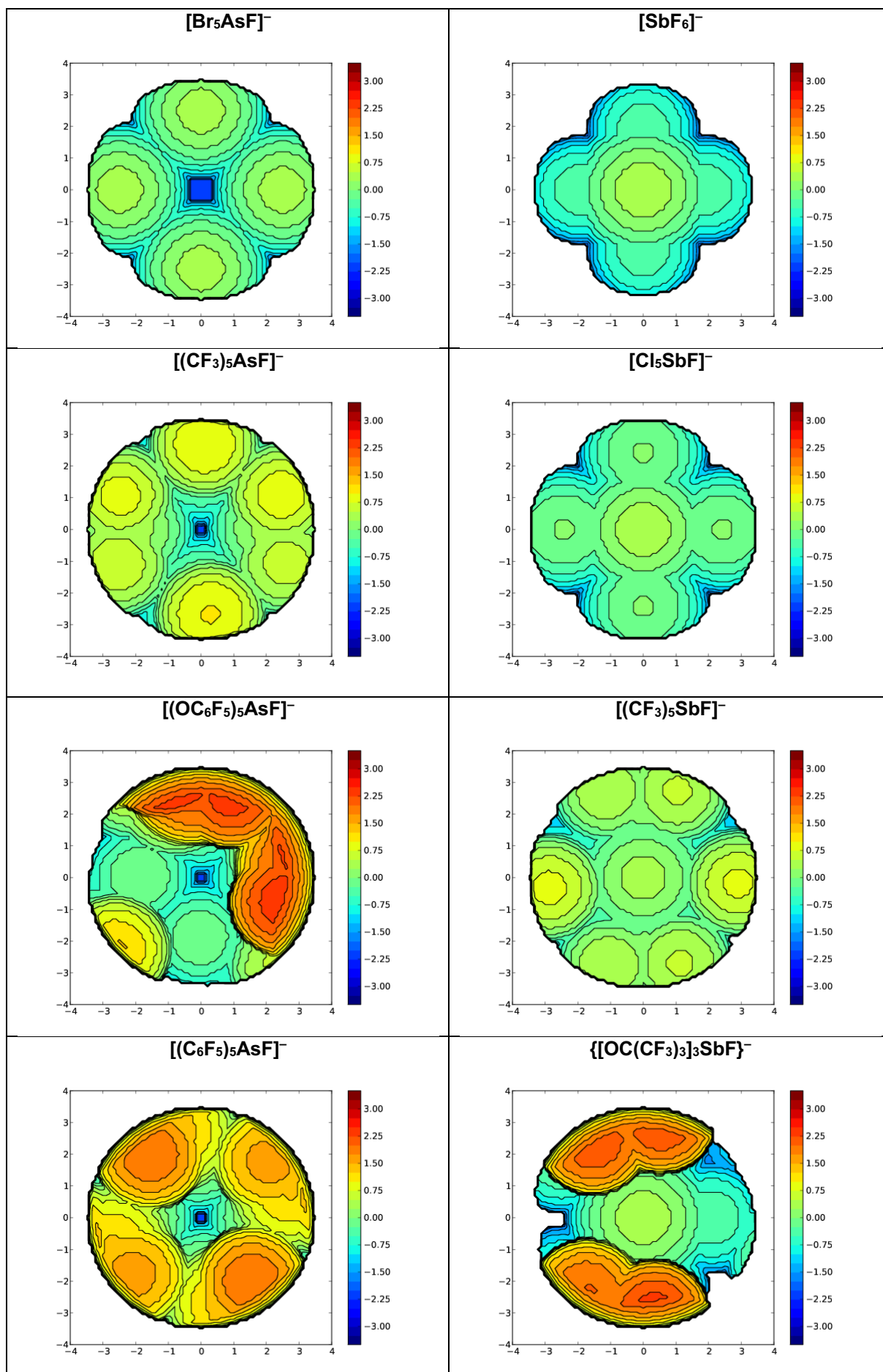


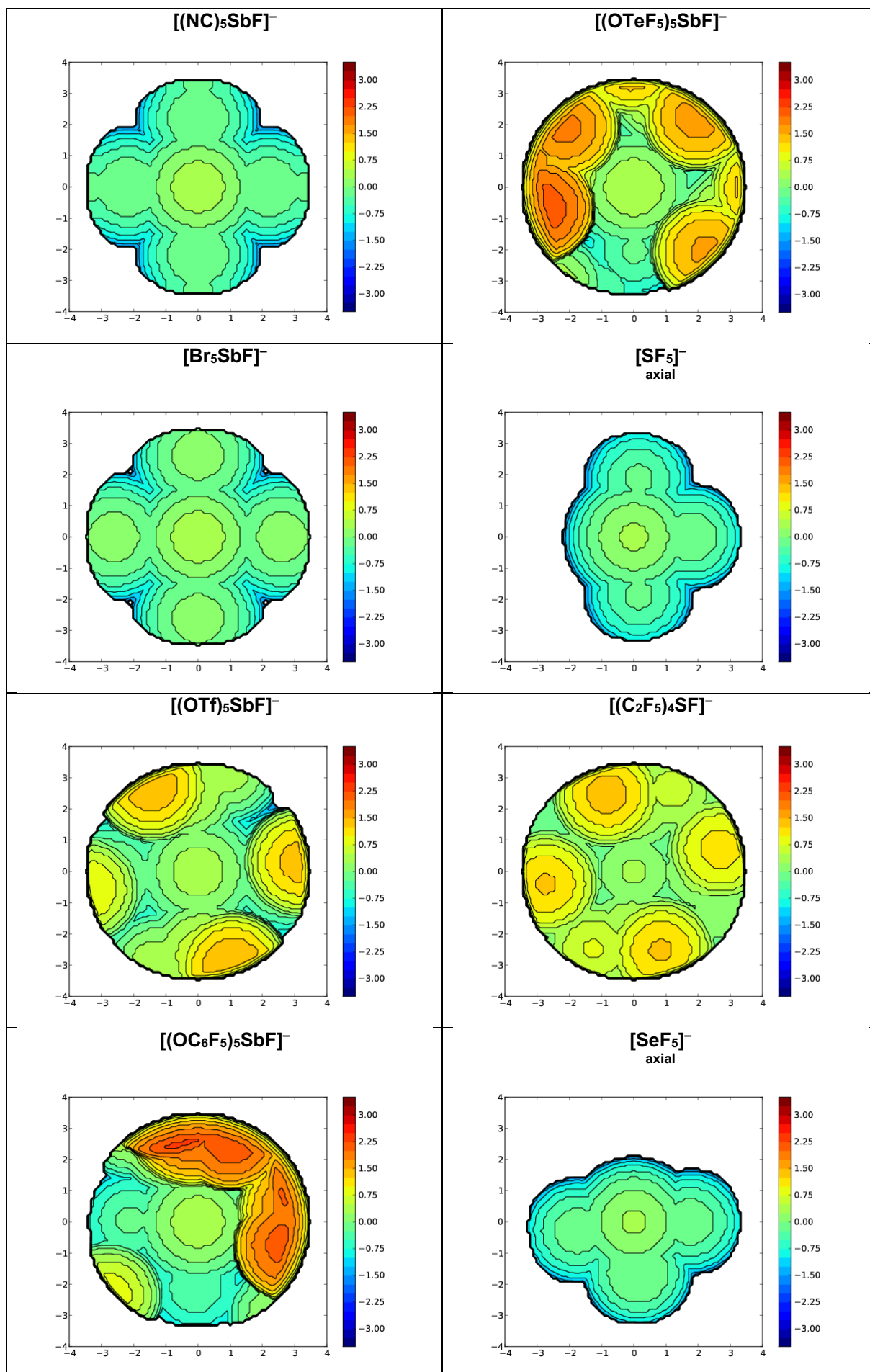


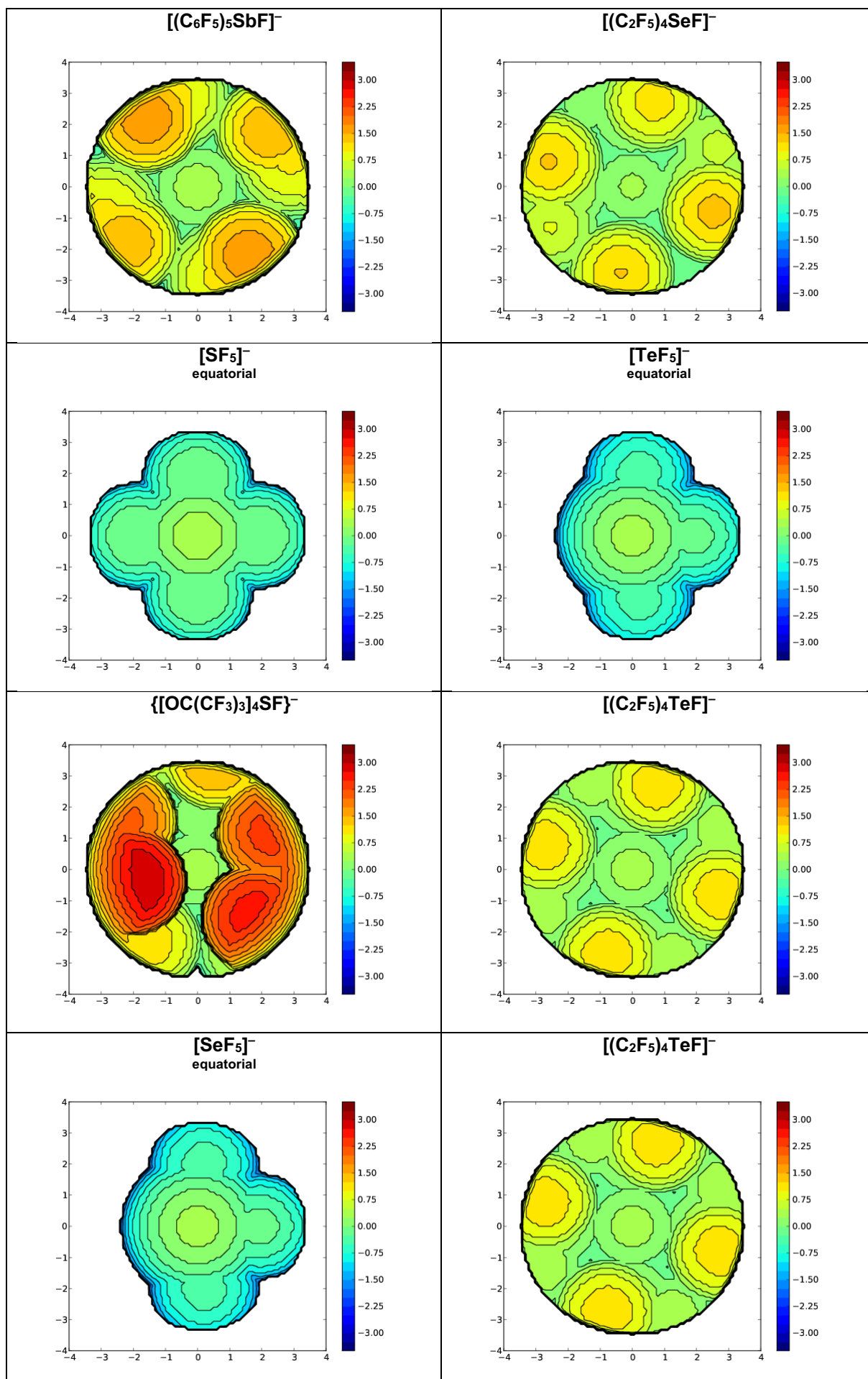


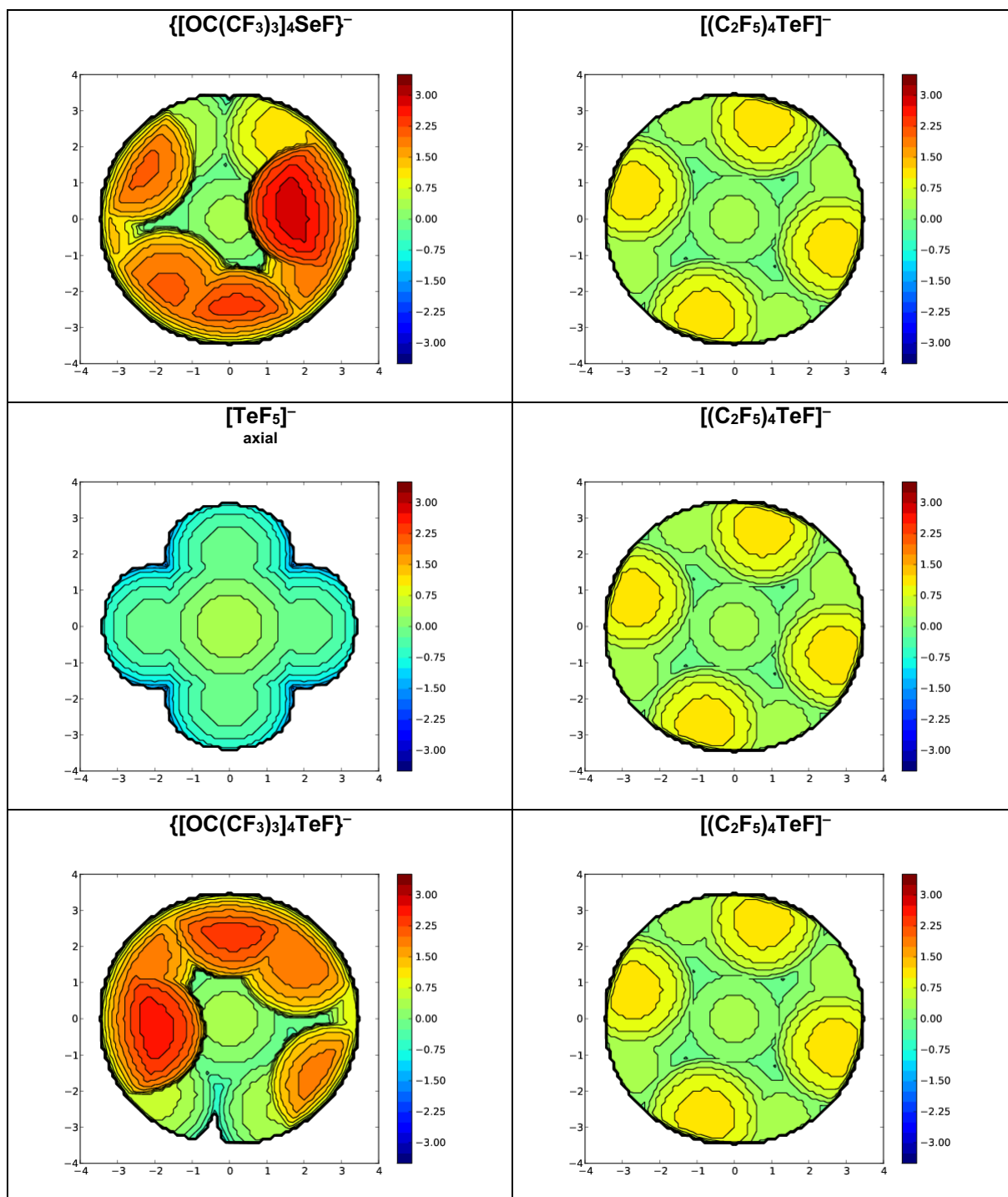












3. Correlation plots of % V_{Bur} versus FIA

Figure S2. Correlation % V_{Bur} vs. Lewis-acidic center E in ER_x .

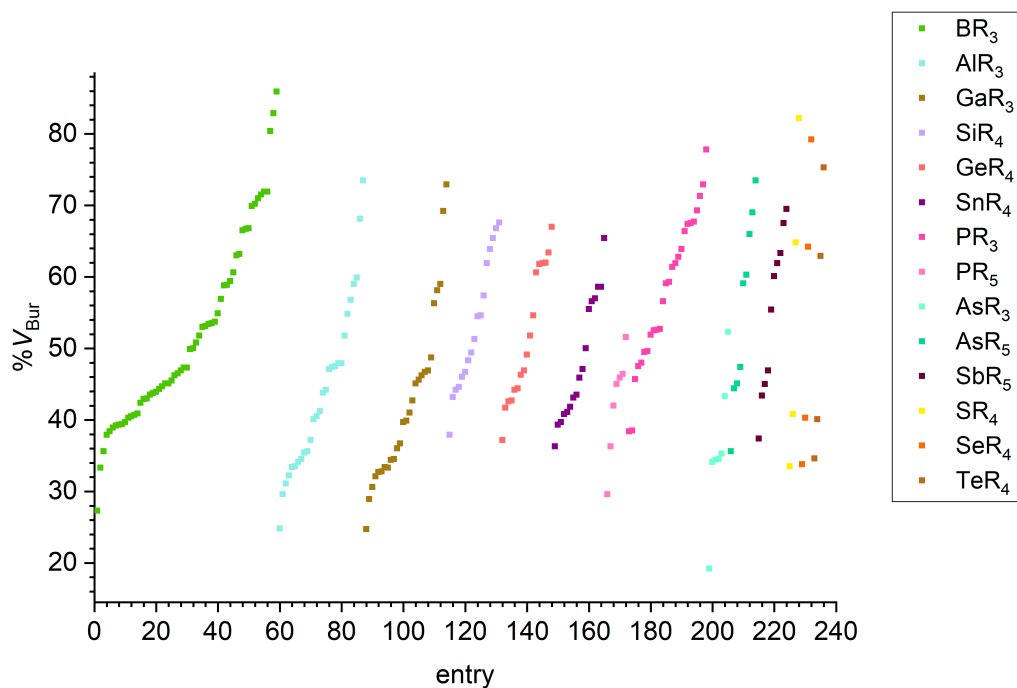


Figure S3. Correlation % V_{Bur} vs. FIA.

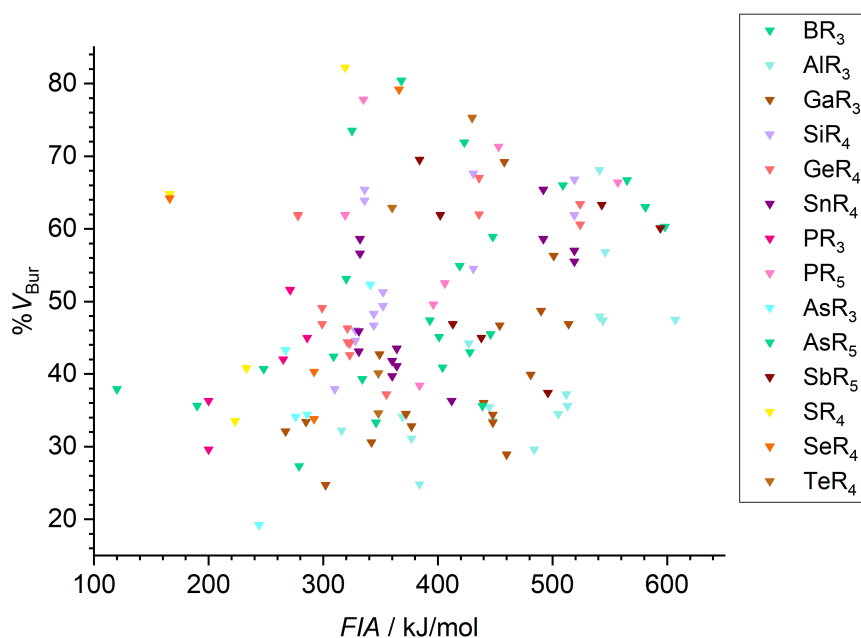


Figure S4. Correlation % V_{Bur} of selected boron Lewis acids vs. FIA reported.

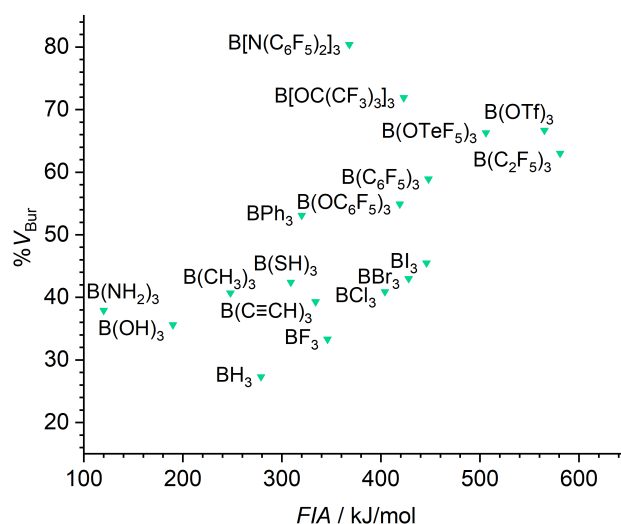


Figure S5. Correlation % V_{Bur} of selected aluminum Lewis acids vs. FIA reported.

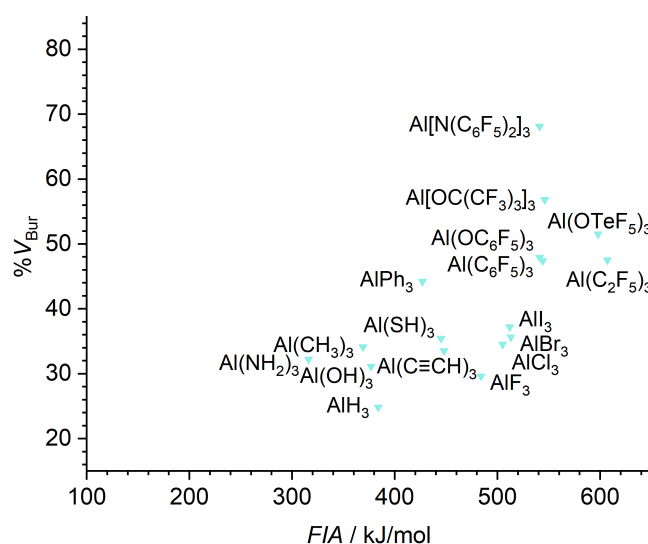


Figure S6. Correlation % V_{Bur} of selected gallium Lewis acids vs. FIA reported.

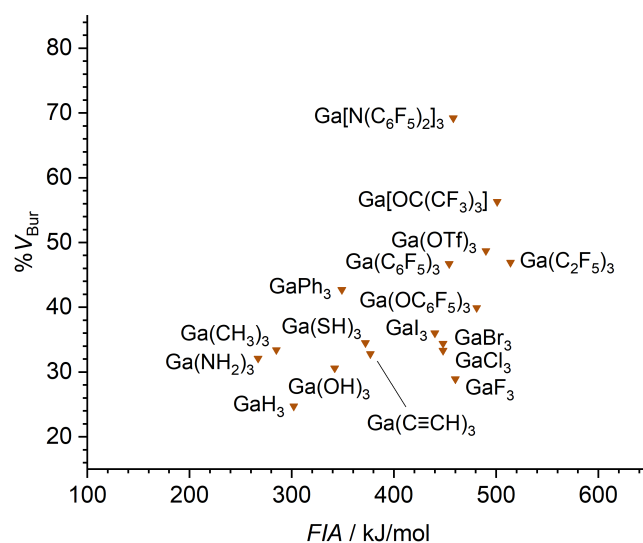


Figure S7. Correlation % V_{Bur} of selected silicon Lewis acids vs. FIA reported.

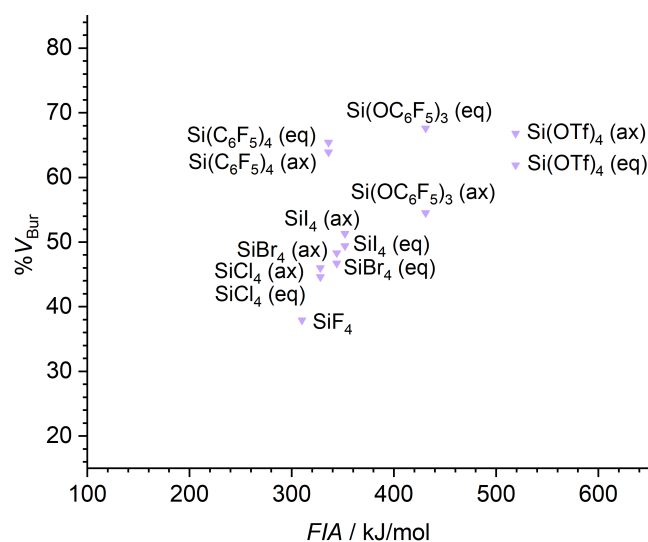


Figure S8. Correlation % V_{Bur} of selected germanium Lewis acids vs. FIA reported.

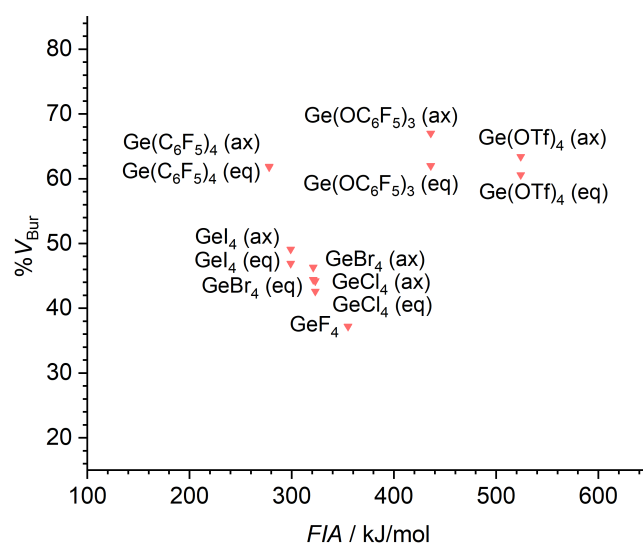


Figure S9. Correlation % V_{Bur} of selected tin Lewis acids vs. FIA reported.

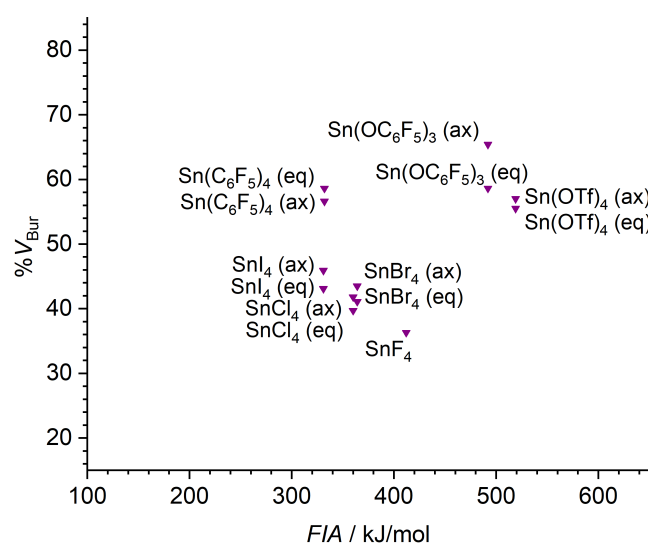


Figure S10. Correlation % V_{Bur} of selected phosphorous Lewis acids vs. FIA reported.

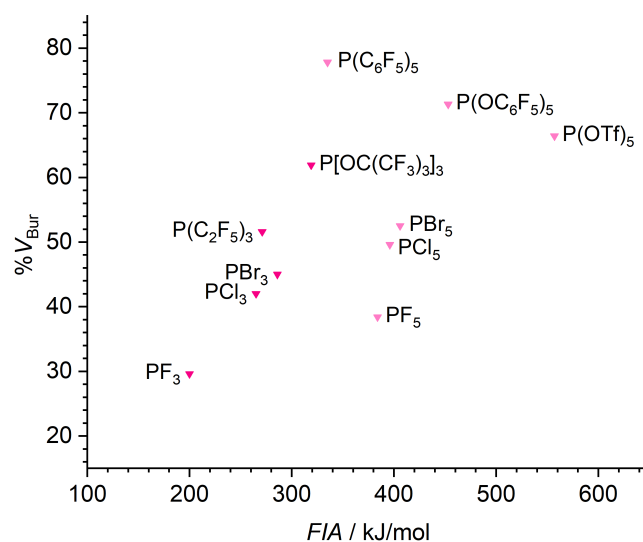


Figure S11. Correlation % V_{Bur} of selected arsenic Lewis acids vs. FIA reported.

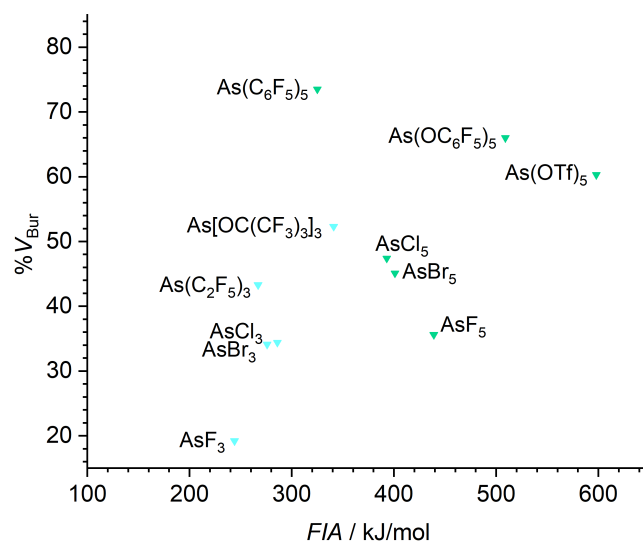


Figure S12. Correlation % V_{Bur} of selected antimony Lewis acids vs. FIA reported.

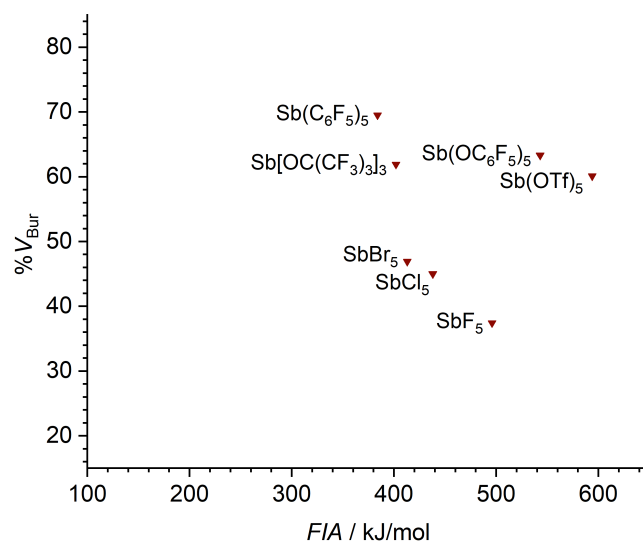


Figure S13. Correlation % V_{Bur} of selected group 16 Lewis acids vs. FIA reported.

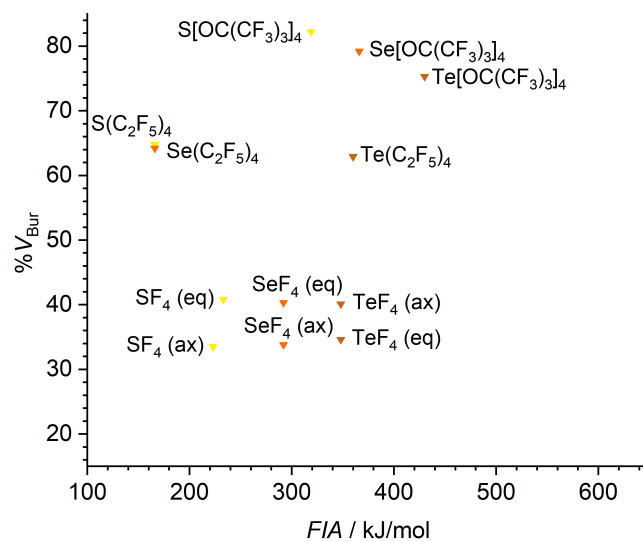
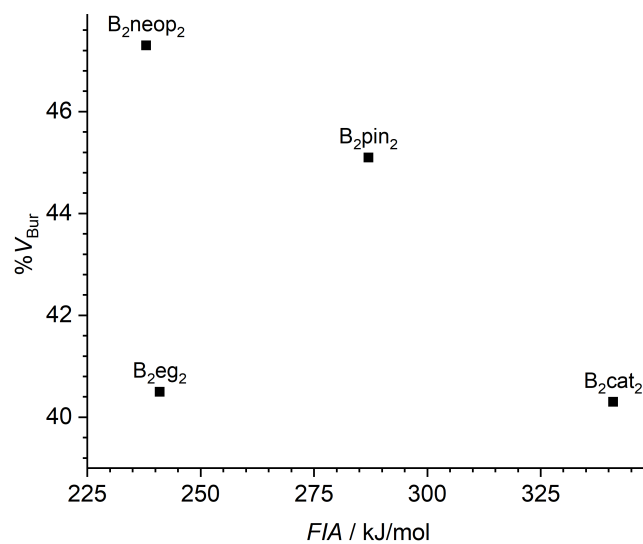


Figure S14. Correlation % V_{Bur} vs. FIA reported for selected diboron(4) compounds.



4. Steric aspects of the pentafluoroethyl(fluoro)phosphoranes $P(C_2F_5)_nF_{5-n}$ and their buried volumes

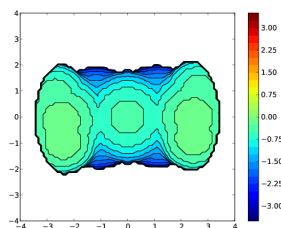
Fluoride addition to the mono- C_2F_5 substituted phosphorane $(C_2F_5)PF_4$ leads to the $[(C_2F_5)PF_5]^-$ anion, which shows two distinct fluoride positions, *trans* and *cis* to the C_2F_5 substituent (Figure 5 top left). Since four fluorine substituents are neighbors next to the fluorine substituent in *trans*-position, the % V_{Bur} value (38.5%) is close to the value obtained for PF_5 (38.4%). For the optimized structure of $[(C_2F_5)PF_4]^-$ four different % V_{Bur} values for the four *cis*-fluoride substituents ranging from 45.7% to 51.9% were calculated, depending on the relative orientation of the C_2F_5 substituent. Since the C_2F_5 group can freely rotate around the P–C bond, we typically consider the lowest value determined as the substituents would adopt the sterically most favored position if steric factors were decisive. The bis(pentafluoroethyl)phosphorane $(C_2F_5)_2PF_3$ reveals a significantly increased % V_{Bur} compared to the sterically most favored position of $P(C_2F_5)F_4$ because at least one pentafluoroethyl group interferes with the Lewis base. Two isomers can be expected for $(C_2F_5)_2PF_3/[(C_2F_5)_2PF_4]^-$ that have the C_2F_5 substituents in *cis* or *trans* alignment. % V_{Bur} values of 49.5% and 52.7% were obtained for the *cis*-isomer, depending on whether the fluoride is located *trans* (49.5%) or *cis* (52.7%) to the second C_2F_5 substituent. In case of *trans*- $[(C_2F_5)_2PF_4]^-$, % V_{Bur} amounts to 56.5%. We and others demonstrated earlier that $[(C_2F_5)_3PF_3]^-$ typically adopts the *mer*-configuration (Figure 5, bottom left). The two different fluorine positions in the *mer*-conformer result in % V_{Bur} of 59.3% (*trans* to fluorine) and 67.7% (*trans* to C_2F_5). Even the lowest % V_{Bur} for a fluorine substituent in *mer*- $[(C_2F_5)_3PF_3]^-$ (59.3%) is approximately 20% higher than % V_{Bur} of the parent $[PF_6]^-$ ion (38.4%), which nicely demonstrates the greater steric demand of C_2F_5 groups compared to fluorine substituents. The lowest % V_{Bur} obtained for *fac*- $[(C_2F_5)_3PF_3]^-$ is 54.8%. All fluorine positions of the experimentally unknown isomers *cis*- and *trans*- $[(C_2F_5)_4PF_2]^-$ are crowded with % V_{Bur} of 62.8 and 67.4% for the *cis*- and *trans*-isomer, respectively. In case of the even more hypothetical $[(C_2F_5)_5PF]^-$ anion we were not able to find a reasonable minimum structure. In summary, the known series of P(V) Lewis acids with fluorine and C_2F_5 substituents, $(C_2F_5)_nPF_{5-n}$ ($n = 0-3$), allows a delicate tuning of the steric effects in conjunction with the Lewis acidity of the phosphorane.

5. % V_{Bur} of selected Lewis Bases

Evaluation of % V_{Bur} of selected Lewis bases as their DFT geometry optimized (def2-SV(P)/BP86) [L–Ni(CO) $_3$] complexes

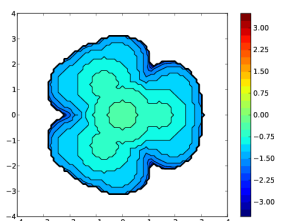
2,6-lutidine:

$$\%V_{\text{Bur}} (d = 2.11 \text{ \AA}; R = 3.5 \text{ \AA}) = 28.6$$



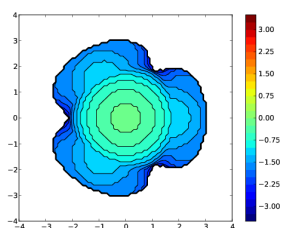
NMe $_3$:

$$\%V_{\text{Bur}} (d = 2.14 \text{ \AA}; R = 3.5 \text{ \AA}) = 26.9$$



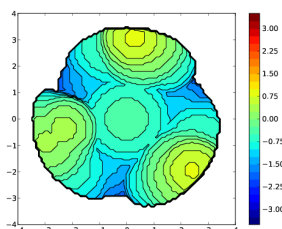
PMe $_3$:

$$\%V_{\text{Bur}} (d = 2.23 \text{ \AA}; R = 3.5 \text{ \AA}) = 24.1$$



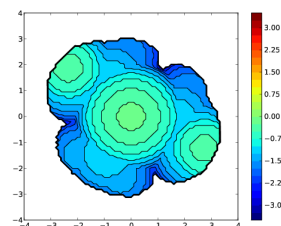
PEt $_3$:

$$\%V_{\text{Bur}} (d = 2.24 \text{ \AA}; R = 3.5 \text{ \AA}) = 28.0$$



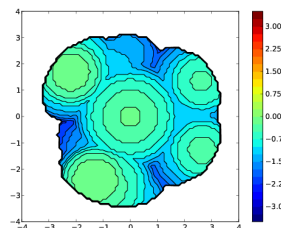
PCy $_3$:

$$\%V_{\text{Bur}} (d = 2.27 \text{ \AA}; R = 3.5 \text{ \AA}) = 33.7$$



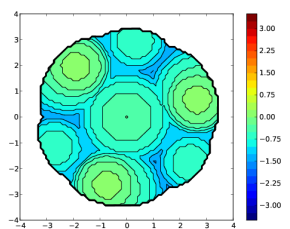
PtBu $_3$:

$$\%V_{\text{Bur}} (d = 2.21 \text{ \AA}; R = 3.5 \text{ \AA}) = 38.3$$



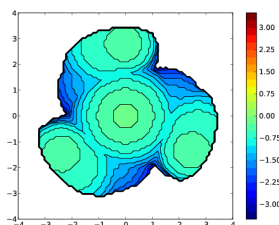
PPh₃:

$$\%V_{\text{Bur}} (d = 2.25 \text{ \AA}; R = 3.5 \text{ \AA}) = 31.1$$



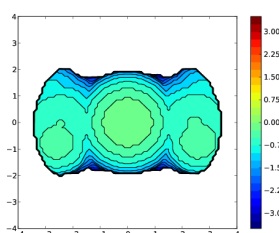
PMes₃:

$$\%V_{\text{Bur}} (d = 2.38 \text{ \AA}; R = 3.5 \text{ \AA}) = 41.6$$



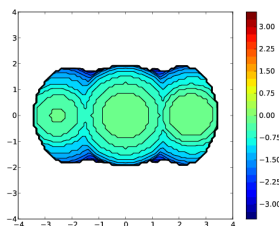
IMe:

$$\%V_{\text{Bur}} (d = 2.01 \text{ \AA}; R = 3.5 \text{ \AA}) = 27.4$$



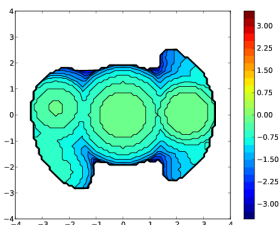
IMe^{Me}:

$$\%V_{\text{Bur}} (d = 1.99 \text{ \AA}; R = 3.5 \text{ \AA}) = 27.1$$



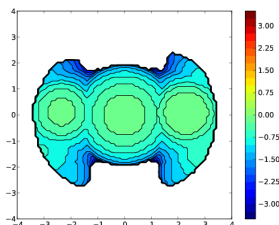
I/Pr:

$$\%V_{\text{Bur}} (d = 1.99 \text{ \AA}; R = 3.5 \text{ \AA}) = 28.8$$



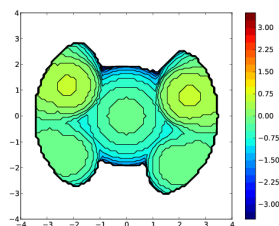
I/Pr^{Me}:

$$\%V_{\text{Bur}} (d = 2.00 \text{ \AA}; R = 3.5 \text{ \AA}) = 29.1$$



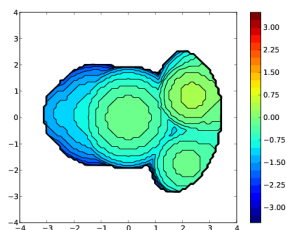
I*t*Bu:

$$\%V_{\text{Bur}} (d = 2.06 \text{ \AA}; R = 3.5 \text{ \AA}) = 37.9$$



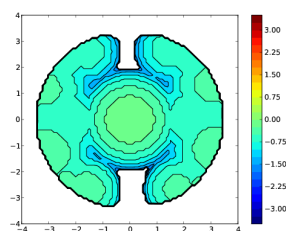
altBu:

$$\%V_{\text{Bur}} (d = 2.01 \text{ \AA}; R = 3.5 \text{ \AA}) = 28.8$$



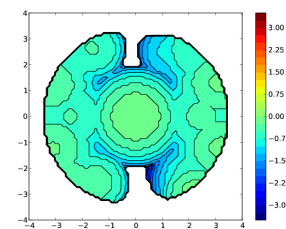
IMes:

$$\%V_{\text{Bur}} (d = 1.97 \text{ \AA}; R = 3.5 \text{ \AA}) = 35.9$$



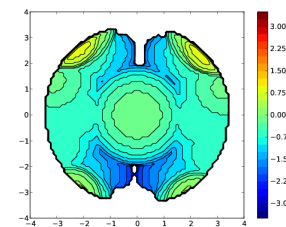
SIMes:

$$\%V_{\text{Bur}} (d = 1.96 \text{ \AA}; R = 3.5 \text{ \AA}) = 36.5$$



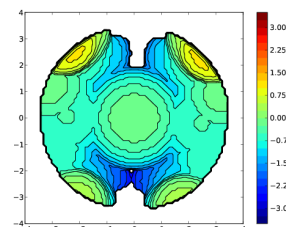
IDipp:

$$\%V_{\text{Bur}} (d = 1.96 \text{ \AA}; R = 3.5 \text{ \AA}) = 36.8$$



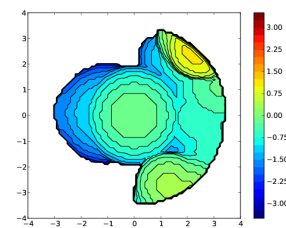
SIDipp:

$$\%V_{\text{Bur}} (d = 1.96 \text{ \AA}; R = 3.5 \text{ \AA}) = 38.6$$



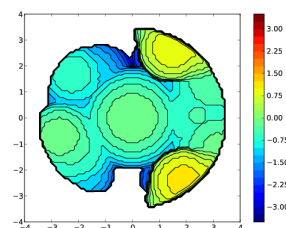
aIDipp:

$$\%V_{\text{Bur}} (d = 1.98 \text{ \AA}; R = 3.5 \text{ \AA}) = 31.8$$



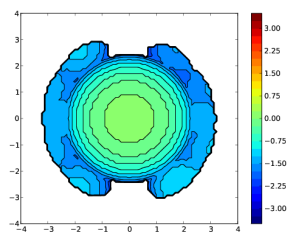
cAAC^{Me}:

$$\%V_{\text{Bur}} (d = 1.95 \text{ \AA}; R = 3.5 \text{ \AA}) = 40.5$$



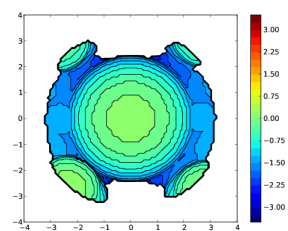
Mes₂NHSi:

$$\%V_{\text{Bur}} (d = 2.20 \text{ \AA}; R = 3.5 \text{ \AA}) = 30.1$$



Dipp₂NHSi:

$$\%V_{\text{Bur}} (d = 2.21 \text{ \AA}; R = 3.5 \text{ \AA}) = 31.1$$

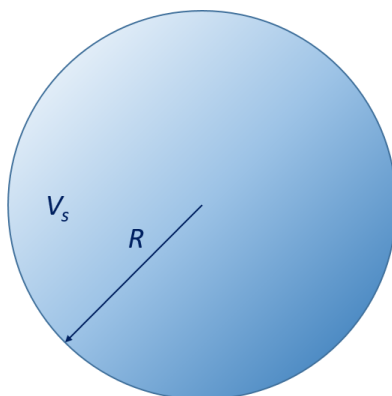


6. Mathematical description of the LAB-Rep model

General equations

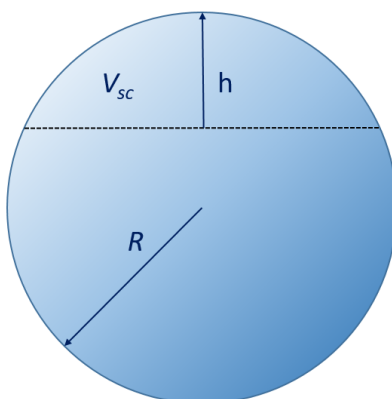
$$V_{sphere} = \frac{4\pi}{3}R^3 = V_s \quad \text{Equation S1}$$

Figure S15. Sphere S with radius R and volume V_s .



$$V_{spherical\ cap} = \frac{\pi}{3}h^2(3R - h) = V_{sc} \quad \text{Equation S2}$$

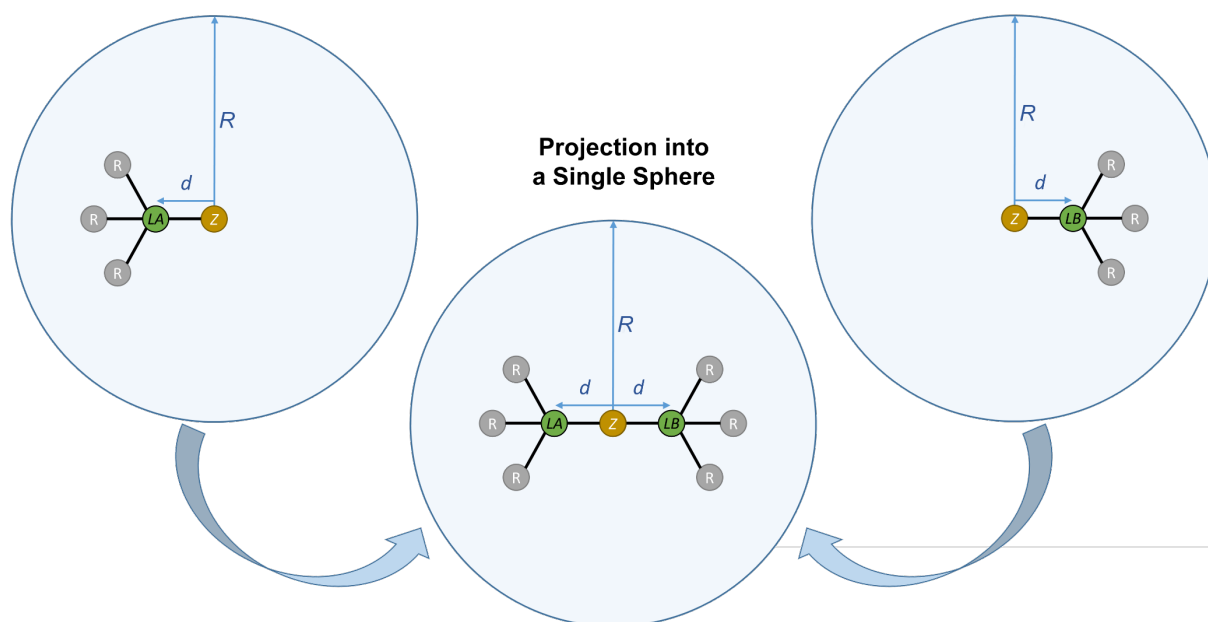
Figure S16. Sphere S with radius R and volume of its spherical cap V_{sc} with height h .



Definition of the buried volume

- Lewis acid (LA) or Lewis base (LB) coordinated in a certain distance d to a coordinating center Z (e.g. fluoride or metal)
- Sphere S with radius R , which is centered at the coordinating center Z (this work $R = 3.5 \text{ \AA}$)
- Percentage share of the volume covered by the Lewis acid or base is assigned to the buried volume $\%V_{Bur}$
- For the evaluation of steric properties of Lewis acid-base adducts projection of both in one sphere S with radius R (this work $R = 3.5 \text{ \AA}$) with center Z

Figure S17. Illustration of $\%V_{\text{Bur}}$ exemplified for a Lewis acid (left) and a Lewis base (right) and projection of the compounds into a single sphere (middle); $R = 3.5 \text{ \AA}$.

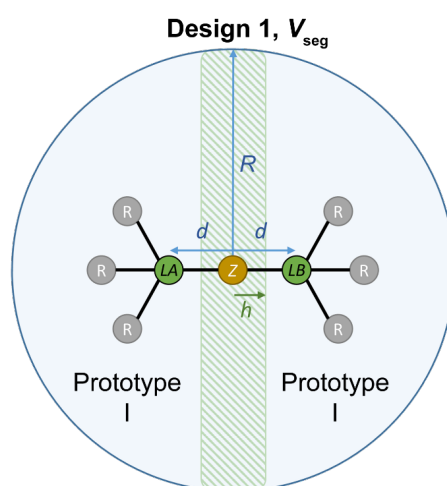


- Since the actual distance D of the $LA-LB$ bond is shorter than $2d$ ($D < 2d$) a correction volume V_{corr} has to be applied
- Adding up its percentage share $\%V_{\text{corr}}$ of the sphere S with $\%V_{\text{Bur_LA}}$ and $\%V_{\text{Bur_LB}}$ provides an assessment if, a stable Lewis acid-base adduct can be formed
- To take into account that the Lewis acids and bases feature different shapes, five different designs were modeled for the correction volume V_{corr}

Design 1 – Segment

- For a Lewis acid-base pair with two cone-shaped (Prototype I) molecules (e.g. BMe₃ and PMe₃) the correction volume V_{corr} can be approximated with the volume of a segment V_{seg} of the sphere S

Figure S18. Sphere S with radius R and coordinating center Z bonded to a LA and a LB within distance d and segment seg with height h and volume V_{seg} .



$$\begin{aligned}
 V_{\text{segment}} &= 2 \cdot \frac{\pi h}{6} (3R_{\text{seg}}^2 + 3R^2 + h^2) \\
 &= \frac{\pi h}{3} (3(R^2 - h^2) + 3R^2 + h^2) \\
 &= \frac{\pi h}{3} (6R^2 - 2h^2) = V_{\text{seg}}
 \end{aligned}$$

Equation S3

- h can be approximated to be $d/2$
- if $d_{LA} \neq d_{LB}$ h can be approximated to be $(d_{LA} + d_{LB})/4$

$$h = \frac{d}{2} = \frac{(d_{LA} + d_{LB})}{4}$$

Equation S4

$$\%V_{\text{seg}} = V_{\text{seg}}/V_s$$

Equation S5

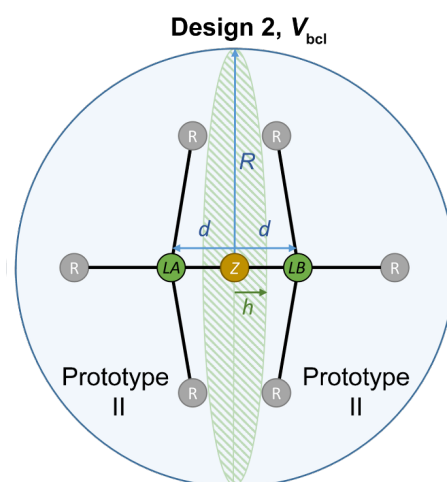
$$\%V_{\text{Bur_all_seg}} = \%V_{\text{Bur_LA}} + \%V_{\text{Bur_LB}} + \%V_{\text{seg}}$$

Equation S6

Design 2 – Biconvex lens

- For a Lewis acid-base pair with two bulky or fan-like (Prototype II) molecules (e.g. $\text{PF}_2(\text{C}_2\text{F}_5)_3$ and IDipp) the correction volume V_{corr} can be approximated with the volume of a biconvex lens V_{bcl}

Figure S19. Sphere S with radius R and coordinating center Z bonded to a LA and a LB within distance d and biconvex lens bcl with height h and volume V_{bcl} .



$$\begin{aligned}
 V_{\text{biconvex_lens}} &= 2 \cdot V_{\text{sc}} = 2 \cdot \frac{\pi}{3} h^2 (3R_{\text{lens}} - h) \\
 &= 2 \cdot \frac{\pi}{3} h^2 \left(3 \left(\frac{R^2 - h^2}{2h} + h \right) - h \right) \\
 &= \frac{\pi}{3} h^2 \left(\frac{3(R^2 - h^2)}{h} + 4h \right) \\
 &= \pi h (R^2 - h^2) + \frac{4\pi h^3}{3} = V_{\text{bcl}}
 \end{aligned}$$

Equation S7

- h can be approximated to be $d/2$
- if $d_{\text{LA}} \neq d_{\text{LB}}$ h can be approximated to be $(d_{\text{LA}} + d_{\text{LB}})/4$ (Equation S4)

$$\%V_{\text{bcl}} = V_{\text{bcl}}/V_{\text{s}}$$

Equation S8

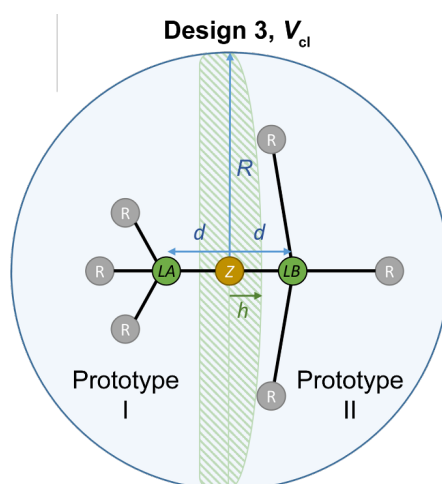
$$\%V_{\text{Bur_all_bcl}} = \%V_{\text{Bur_LA}} + \%V_{\text{Bur_LB}} + \%V_{\text{bcl}}$$

Equation S9

Design 3 – Convex lens

- For a Lewis acid-base pair with one bulky or fan-like (Prototype II) and one cone-shaped (Prototype I) molecule (e.g. BMe₃ and IDipp) the correction volume V_{corr} can be approximated with the volume of a convex lens V_{cl}

Figure S20. Sphere S with radius R and coordinating center Z bonded to a LA and a LB within distance d and convex lens cl with height h and volume V_{cl} .



$$\begin{aligned}
 V_{\text{convex_lens}} &= 0.5 \cdot V_{\text{seg}} + V_{\text{sc}} \\
 &= 0.5 \cdot \frac{\pi h}{3} (6R^2 - 2h^2) + \frac{\pi}{3} h^2 \left(\frac{3(R^2 - h^2)}{2h} + 2h \right) \\
 &= \frac{\pi h}{6} (6R^2 - 2h^2) + \frac{\pi(R^2 - h^2)h}{2} + \frac{2\pi h^3}{3} \\
 &= \pi h \left(\frac{(3R^2 - h^2)}{3} + \frac{(R^2 - h^2)}{2} + \frac{2h^2}{3} \right) = V_{\text{cl}}
 \end{aligned}$$

Equation S10

- h can be approximated to be $d/2$
- if $d_{\text{LA}} \neq d_{\text{LB}}$ h can be approximated to be $(d_{\text{LA}} + d_{\text{LB}})/4$ (Equation S4)

$$\%V_{\text{cl}} = V_{\text{cl}}/V_{\text{s}}$$

Equation S11

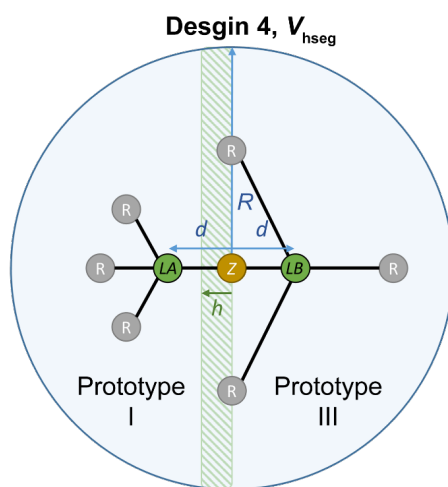
$$\%V_{\text{Bur_all_cl}} = \%V_{\text{Bur_LA}} + \%V_{\text{Bur_LB}} + \%V_{\text{cl}}$$

Equation S12

Design 4 – Half segment

- For a Lewis acid-base pair with one cone-shaped (Prototype I) molecule (e.g. BMe₃) and one sterically overcrowded (%V_{Bur} ≥ 50%, Prototype III) molecule the correction volume V_{corr} can be approximated with the volume of a half segment V_{hseg}
- To take into account that sterically overcrowded (%V_{Bur} ≥ 50%, Prototype III) molecules may also extend into the hemisphere of the potential adduct partner, the portion of %V_{Bur} exceeding 50% is scaled by the empirical factor of 0.5 and subtracted from 0.5 · V_{seg}.

Figure S21. Sphere S with radius R and coordinating center Z bonded to a LA and a LB within distance d and half segment hseg with hight h and volume V_{hseg}.



$$\begin{aligned}
 V_{half_segment} &= 0.5 \cdot V_{seg} - 0.5 \cdot (\%V_{Bur>50\%} - 50\%) \cdot V_s \\
 &= 0.5 \cdot \frac{\pi h}{3} (6R^2 - 2h^2) - 0.5 \cdot (\%V_{Bur>50\%} - 50\%) \cdot V_s \\
 &= \frac{\pi h}{6} (6R^2 - 2h^2) - 0.5 \cdot (\%V_{Bur>50\%} - 50\%) \cdot V_s \\
 &= \frac{\pi h}{3} (3R^2 - h^2) - 0.5 \cdot (\%V_{Bur>50\%} - 50\%) \cdot V_s = V_{hseg}
 \end{aligned}
 \tag{Equation S13}$$

- h can be approximated to be $d_{conshaped_molecule}/2$

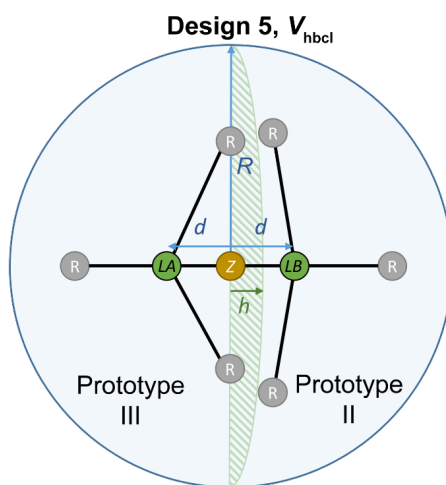
$$\%V_{hseg} = V_{hseg}/V_s \tag{Equation S14}$$

$$\%V_{Bur_all_hseg} = \%V_{Bur_LA} + \%V_{Bur_LB} + \%V_{hseg} \tag{Equation S15}$$

Design 5 – Half biconvex lens

- For a Lewis acid-base pair with one bulky or fan-like (Prototype II) molecule (e.g. IDipp) and one sterically overcrowded ($\%V_{Bur} \geq 50\%$, Prototype III) molecule the correction volume V_{corr} can be approximated with the volume of a half biconvex lens V_{hbcl}
- To take into account that sterically overcrowded ($\%V_{Bur} \geq 50\%$, Prototype III) molecules may also extend into the hemisphere of the potential adduct partner, the portion of $\%V_{Bur}$ exceeding 50% is scaled by the empirical factor of 0.5 and subtracted from $0.5 \cdot V_{bcl}$

Figure S22. Sphere S with radius R and coordinating center Z bonded to a LA and a LB within distance d and half biconvex lens $hbcl$ with height h and volume V_{hbcl} .



$$\begin{aligned}
 V_{half\,biconvex\,lens} &= 0.5 \cdot V_{bcl} - 0.5 \cdot (\%V_{Bur>50\%} - 50\%) \cdot V_s \\
 &= 0.5 \cdot \left(\pi h(R^2 - h^2) + \frac{4\pi h^3}{3} \right) - 0.5 \cdot (\%V_{Bur>50\%} - 50\%) \cdot V_s \\
 &= \frac{\pi h}{2} (R^2 - h^2) + \frac{4\pi h^3}{6} - 0.5 \cdot (\%V_{Bur>50\%} - 50\%) \cdot V_s = V_{hbcl} \quad \text{Equation S16}
 \end{aligned}$$

- h can be approximated to be $d_{bulky_molecule}/2$

$$\%V_{hbcl} = V_{hbcl}/V_s \quad \text{Equation S17}$$

$$\%V_{Bur_all_hbcl} = \%V_{Bur_LA} + \%V_{Bur_LB} + \%V_{hbcl} \quad \text{Equation S18}$$

Case studies

Example 1: Historic example H. C. Brown

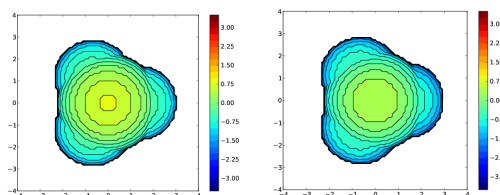
BF₃/2,6-lutidine vs. BMe₃/2,6-lutidine

- since BF₃ and BMe₃ are cone-shaped but 2,6-lutidine is quite bulky with the methyl groups in *ortho*-position to the Lewis basic nitrogen, Design **3** (convex lens) was considered to fit best
- using equation S10 and S11 gives the procentage share %V_{corr} of the „correction volume“
- equation S4 has to be applied to calculate *h*

BF₃:

$$\%V_{\text{Bur}}(d = 1.42 \text{ \AA}; R = 3.5 \text{ \AA}) = 33.3$$

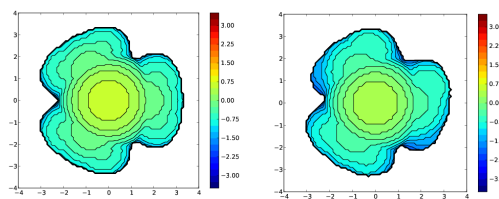
$$\%V_{\text{Bur}}(d = 1.72 \text{ \AA}; R = 3.5 \text{ \AA}) = 30.2$$



BMe₃:

$$\%V_{\text{Bur}}(d = 1.47 \text{ \AA}; R = 3.5 \text{ \AA}) = 40.7$$

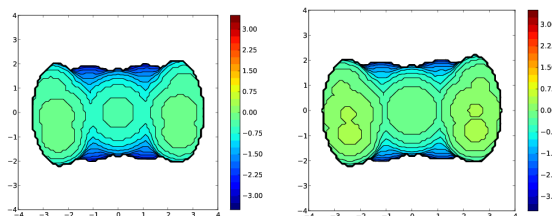
$$\%V_{\text{Bur}}(d = 1.72 \text{ \AA}; R = 3.5 \text{ \AA}) = 36.1$$



2,6-lutidine:

$$\%V_{\text{Bur}}(d = 2.11 \text{ \AA}; R = 3.5 \text{ \AA}) = 28.6$$

$$\%V_{\text{Bur}}(d = 1.72 \text{ \AA}; R = 3.5 \text{ \AA}) = 34.1$$



Calculation:

BF₃/2,6-lutidine

- $d(2,6\text{-lutidine}) = 2.11 \text{ \AA}$ and $d(\text{BF}_3) = 1.42 \text{ \AA}$: mean value $1.765 \text{ \AA} \rightarrow h = 0.8825 \text{ \AA}$

$$V_{cl}(R = 3.5 \text{ \AA}, h = 0.8825 \text{ \AA}) = 50.584 \text{ \AA}^3$$

$$\%V_{cl}(R = 3.5 \text{ \AA}, h = 0.8825 \text{ \AA}) = 28.2\%$$

$$\%V_{\text{Bur_all_cl}}(\%V_{\text{Bur_LA}} = 33.3\%, \%V_{\text{Bur_LB}} = 28.6\%, \%V_{cl} = 28.2\%) = 89.7\%$$

→ **sterically allowed**, right prediction

BMe₃/2,6-lutidine

- $d(2,6\text{-lutidine}) = 2.11 \text{ \AA}$ and $d(\text{BMe}_3) = 1.47 \text{ \AA}$: mean value $1.790 \text{ \AA} \rightarrow h = 0.8950 \text{ \AA}$

$$V_{cl}(R = 3.5 \text{ \AA}, h = 0.8950 \text{ \AA}) = 51.290 \text{ \AA}^3$$

$$\%V_{cl}(R = 3.5 \text{ \AA}, h = 0.8950 \text{ \AA}) = 28.6\%$$

$$\%V_{Bur_all_cl}(\%V_{Bur_LA} = 40.7\%, \%V_{Bur_LB} = 28.6\%, \%V_{cl} = 28.6\%) = 97.9\%$$

→ limit

Calculation with $\%V_{Bur}$ values for an equilibrium distance of $d = 1.72 \text{ \AA}$:

- DFT calculations have shown that the equilibrium B–N distance in the BF₃/2,6-lutidine adduct is $1.72 \text{ \AA}$
- h corresponds to half of the B–N distance $\rightarrow h = 0.86 \text{ \AA}$

$$V_{cl}(R = 3.5 \text{ \AA}, h = 0.86 \text{ \AA}) = 49.312 \text{ \AA}^3$$

$$\%V_{cl}(R = 3.5 \text{ \AA}, h = 0.86 \text{ \AA}) = 27.5\%$$

BF₃/2,6-lutidine

$$\%V_{Bur_all_cl}(\%V_{Bur_LA} = 30.2\%, \%V_{Bur_LB} = 34.1\%, \%V_{cl} = 27.5\%) = 91.8\%$$

BMe₃/2,6-lutidine

$$\%V_{Bur_all_cl}(\%V_{Bur_LA} = 36.1\%, \%V_{Bur_LB} = 34.1\%, \%V_{cl} = 27.5\%) = 97.7\%$$

Example 2: FLP's

BPh₃/PPh₃ and B(C₆F₅)₃/PPh₃

- the buried volumes of BPh₃ and B(C₆F₅) exceed 50%, so Design **5** (half segment) has to be applied with $h = (2.25 \text{ Å})/2 = 1.125 \text{ Å}$

BPh₃:

$$\%V_{\text{Bur}}(d = 1.46 \text{ Å}; R = 3.5 \text{ Å}) = 53.1$$

B(C₆F₅)₃:

$$\%V_{\text{Bur}}(d = 1.46 \text{ Å}; R = 3.5 \text{ Å}) = 58.9$$

PPh₃:

$$\%V_{\text{Bur}}(d = 2.25 \text{ Å}; R = 3.5 \text{ Å}) = 31.1$$

Calculation:

- $d(\text{PPh}_3) = 2.25 \text{ Å} \rightarrow h = 1.125 \text{ Å}$

BPh₃/PPh₃

$$V_{\text{hseg}}(R = 3.5 \text{ Å}, h = 1.125 \text{ Å}) = 39.020 \text{ Å}^3$$

$$\%V_{\text{hseg}}(R = 3.5 \text{ Å}, h = 1.125 \text{ Å}) = 21.7\%$$

$$\%V_{\text{bur_all_hseg}}(\%V_{\text{bur_LA}} = 53.1\%, \%V_{\text{bur_LB}} = 31.1\%, \%V_{\text{hseg}} = 21.7\%) = 105.9\%$$

→ **limit**

B(C₆F₅)₃/PPh₃

$$V_{\text{hseg}}(R = 3.5 \text{ Å}, h = 1.125 \text{ Å}) = 33.812 \text{ Å}^3$$

$$\%V_{\text{hseg}}(R = 3.5 \text{ Å}, h = 1.125 \text{ Å}) = 18.8\%$$

$$\%V_{\text{bur_all_hseg}}(\%V_{\text{bur_LA}} = 58.9\%, \%V_{\text{bur_LB}} = 31.1\%, \%V_{\text{hseg}} = 18.8\%) = 108.8\%$$

→ **limit**

Example 3: NHC and phosphane adducts of phosphoranes

<i>LA</i>	<i>LB</i>	isomer	V_{corr}	$d(LA) / \text{\AA}$	$d(LB) / \text{\AA}$	% V_{corr}	% $V_{\text{Bur_LA}}$	% $V_{\text{Bur_LB}}$	% $V_{\text{Bur_all}}$
PF ₅	IMe	-	bcl	1.65	2.01	20.1	38.4	27.4	85.9
PF ₅	IPr	-	bcl	1.65	1.99	21.0	38.4	28.8	89.7
PF ₅	ItBu	-	bcl	1.65	2.06	20.3	38.4	37.9	96.6
PF ₅	altBu	-	bcl	1.65	2.01	20.1	38.4	28.8	87.3
PF ₅	IDipp	-	bcl	1.65	1.96	19.8	38.4	36.5	94.7
PF ₅	alDipp	-	bcl	1.65	1.98	19.9	38.4	31.8	90.1
PF ₂ (C ₂ F ₅) ₃	IMe	<i>mer-trans</i>	hbcl	1.69	2.01	16.0	67.7	27.4	102.3
PF ₂ (C ₂ F ₅) ₃	IPr	<i>mer-trans</i>	hbcl	1.69	1.99	15.8	67.7	28.8	103.5
PF ₂ (C ₂ F ₅) ₃	ItBu	<i>mer-trans</i>	hbcl	1.69	2.06	16.4	67.7	37.9	113.1
PF ₂ (C ₂ F ₅) ₃	altBu	<i>mer-trans</i>	hbcl	1.69	2.01	16.0	67.7	28.8	103.7
PF ₂ (C ₂ F ₅) ₃	IDipp	<i>mer-trans</i>	hbcl	1.69	1.96	15.6	67.7	36.5	111.0
PF ₂ (C ₂ F ₅) ₃	alDipp	<i>mer-trans</i>	hbcl	1.69	1.98	15.8	67.7	31.8	106.4
PF ₅	PMe ₃	-	cl	1.65	2.21	30.8	38.4	24.1	93.3
PF ₂ (C ₂ F ₅) ₃	PMe ₃	<i>mer-cis fac</i>	hseg	1.67	2.21	18.2	59.3	24.1	101.6
				1.67		20.5	54.8		99.4
PF ₅	PPh ₃	-	cl	1.65	2.25	31.1	38.4	31.1	100.6
PF ₂ (C ₂ F ₅) ₃	PPh ₃	<i>mer-cis fac</i>	hseg	1.67	2.25	18.7	59.3	31.1	109.1
				1.67		20.9	54.8		106.8

Synthesis and Characterization of 1

Analytical Instruments and Details

^1H , ^{11}B , ^{13}C , and ^{31}P NMR spectra were recorded in $[\text{D}_8]\text{toluene}$ on a Bruker Avance Neo I 600 spectrometer. NMR signals were referenced against TMS (^1H and ^{13}C with $\Delta(^{13}\text{C}) = 25.145020$ MHz), $\text{BF}_3 \cdot \text{OEt}_2$ in CDCl_3 ($\Delta(^{11}\text{B}) = 32.083974$ MHz), and H_3PO_4 ($\Delta(^{31}\text{P}) = 40.480742$ MHz).^[6] Chemical shifts were calibrated against the residual solvent signal, respectively ($\delta(^1\text{H})$: $[\text{D}_7]\text{toluene}$ 2.08, 6.97, 7.01 and 7.09 ppm, $\delta(^{13}\text{C})$: $[\text{D}_8]\text{toluene}$ 137.48, 128.87, 127.96, 125.13, and 20.43 ppm.^[7] Solid-state NMR spectra were recorded on a Bruker Avance Neo 400 NMR spectrometer (^1H , 400.13 MHz; ^{13}C , 100.6 MHz; ^{11}B , 128.4 MHz, ^{31}P 162.0 MHz) at 293 K with a 4 mm (o.d.) bottom-layer rotor of ZrO_2 containing ca. 100 mg of sample. The spectra were conducted with MAS spinning rates between of 15 kHz using a Bruker 4 mm WB CP/MAS probe. All chemical shifts were calibrated by setting the ^{13}C lowfield signal of adamantane to $\delta = 38.48$ ppm according to the IUPAC recommendations^[6] with $\Delta(^{13}\text{C}) = 25.145020$ MHz, $\Delta(^{11}\text{B}) = 32.083974$ MHz, $\Delta(^{31}\text{P}) = 40.480742$ MHz. IR spectra were recorded at room temperature with a Bruker Alpha-FT-IR spectrometer with an apodized resolution of 2 cm^{-1} in the attenuated total reflection (ATR) mode in the region of $4000\text{--}400\text{ cm}^{-1}$ using a setup with a diamond crystal. Raman spectra were measured at room temperature on a Bruker MultiRAM FT spectrometer with an apodized resolution of 2 cm^{-1} in the region of $4000\text{--}400\text{ cm}^{-1}$. The sample contained in melting point capillaries was excited with 1064 nm line of a Nd/YAG laser. Thermal analyses were performed with a DSC 204 F1 Phoenix (Netzsch) in the temperature range of -150 to $500\text{ }^\circ\text{C}$ with a heating rate of 10 K min^{-1} .

Chemicals

PPh_3 and BPh_3 were obtained from commercial sources and used without further purification. Solvents were dried according to standard protocols^[8] and stored under argon atmosphere.

Synthesis

Triphenylphosphine-triphenylborane

Triphenylborane (484 mg, 2.00 mmol) was dissolved in THF (3 mL) and added to a solution of triphenylphosphine (525 mg, 2.00 mmol) in THF (3 mL). Immediately after addition the product precipitates. The suspension was stirred for five minutes at room temperature and the precipitate was filtered off, washed with THF ($3 \times 2\text{ mL}$) and dried under vacuum. Yield: 968 mg (1.92 mmol, 96% calculated with respect to triphenylborane) of a white powder.

Melting point: $213\text{--}216\text{ }^\circ\text{C}$.

Crystals of $\text{PPh}_3\text{--BPh}_3$ suitable for an X-ray diffraction study were obtained by recrystallization from hot THF.

In solution at room temperature, only BPh_3 and PPh_3 can be observed via NMR spectroscopy, but not $\text{PPh}_3\text{-BPh}_3$. Adduct formation in solution takes place at temperatures below approximately -20°C (see Figure S25).

$^{11}\text{B}\{^1\text{H}\}$ NMR (192.6 MHz, 298 K, $[\text{D}_8]\text{toluene}$): $\delta = 65.8$ ppm (s, 1B, BPh_3).

$^{31}\text{P}\{^1\text{H}\}$ NMR (243.0 MHz, 298 K, $[\text{D}_8]\text{toluene}$): $\delta = -5.0$ ppm (s, 1P, PPh_3).

$^{11}\text{B}\{^1\text{H}\}$ NMR (192.6 MHz, 183 K, $[\text{D}_8]\text{toluene}$): $\delta = -4.3$ ppm (s, 1B, BPh_3).

$^{31}\text{P}\{^1\text{H}\}$ NMR (243.0 MHz, 183 K, $[\text{D}_8]\text{toluene}$): $\delta = -1.7$ ppm (s, 1P, PPh_3).

$^{11}\text{B}\{^1\text{H}\}$ RSHE/MAS NMR (128.4 MHz, $\nu_{\text{rot}} = 15$ kHz): $\delta = -1.7$ ppm (m, 1B).

$^{31}\text{P}\{^1\text{H}\}$ CP/MAS NMR (162.0 MHz, $\nu_{\text{rot}} = 15$ kHz): $\delta = 4.6$ ppm (s, 1P).

IR ($[\text{cm}^{-1}]$): 3051, 1587, 1483, 1431, 1189, 1154, 1094, 1072, 998, 846, 743, 701, 691, 634, 605, 526, 507, 485, 448.

Raman ($[\text{cm}^{-1}]$): 3060, 1587, 1572, 1188, 1158, 1110, 1099, 1031, 1002, 636, 617.

Figure S23. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of a solution of $\text{PPh}_3\text{-BPh}_3$ in $[\text{D}_8]\text{toluene}$; the signal is assigned to BPh_3 .

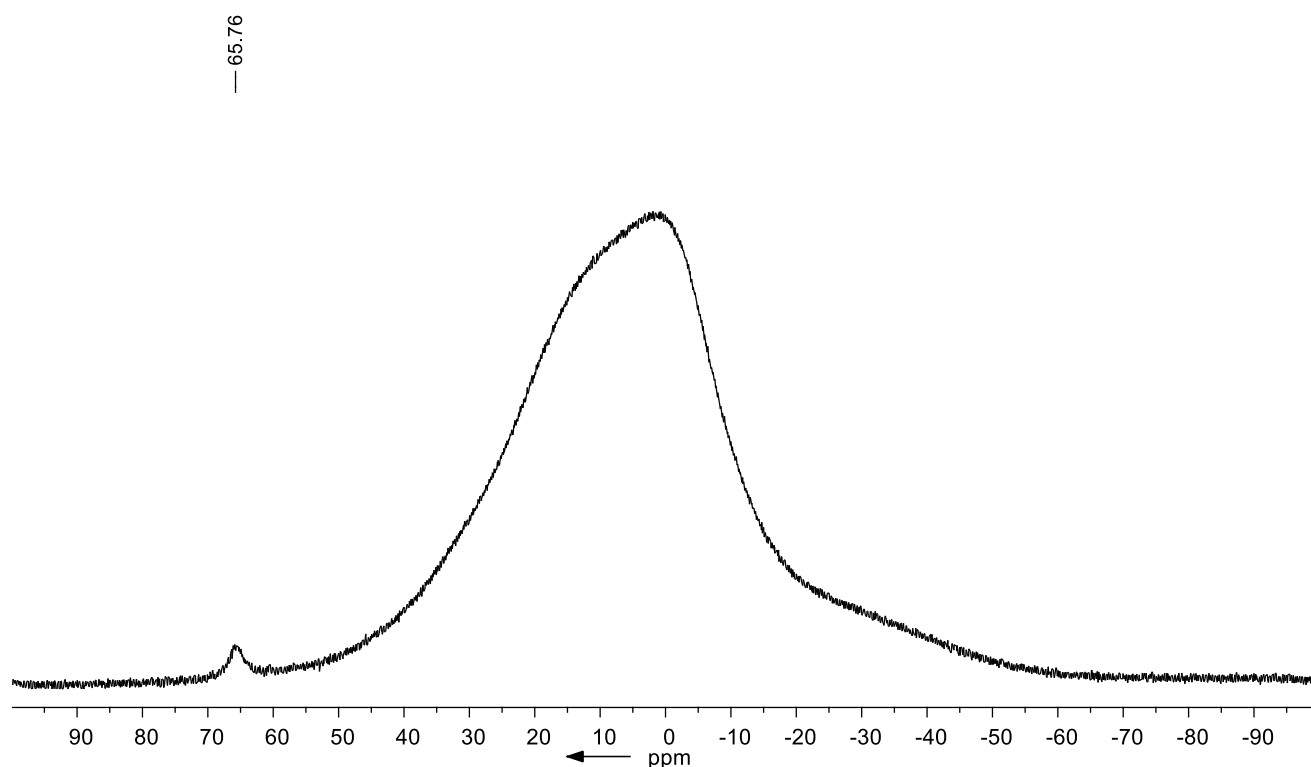


Figure S24. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of a solution of $\text{PPh}_3\text{-BPh}_3$ in $[\text{D}_8]\text{toluene}$; the signal is assigned to PPh_3 .

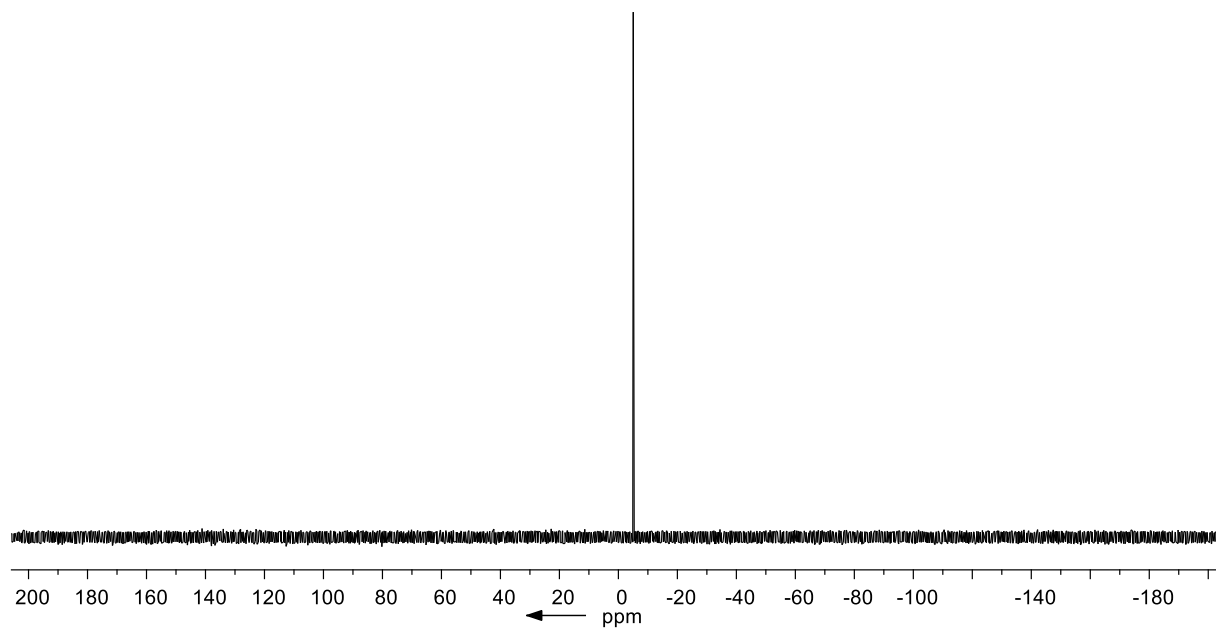


Figure S25. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of a solution of PPh_3 and BPh_3 in $[\text{D}_8]\text{toluene}$ at different temperatures.

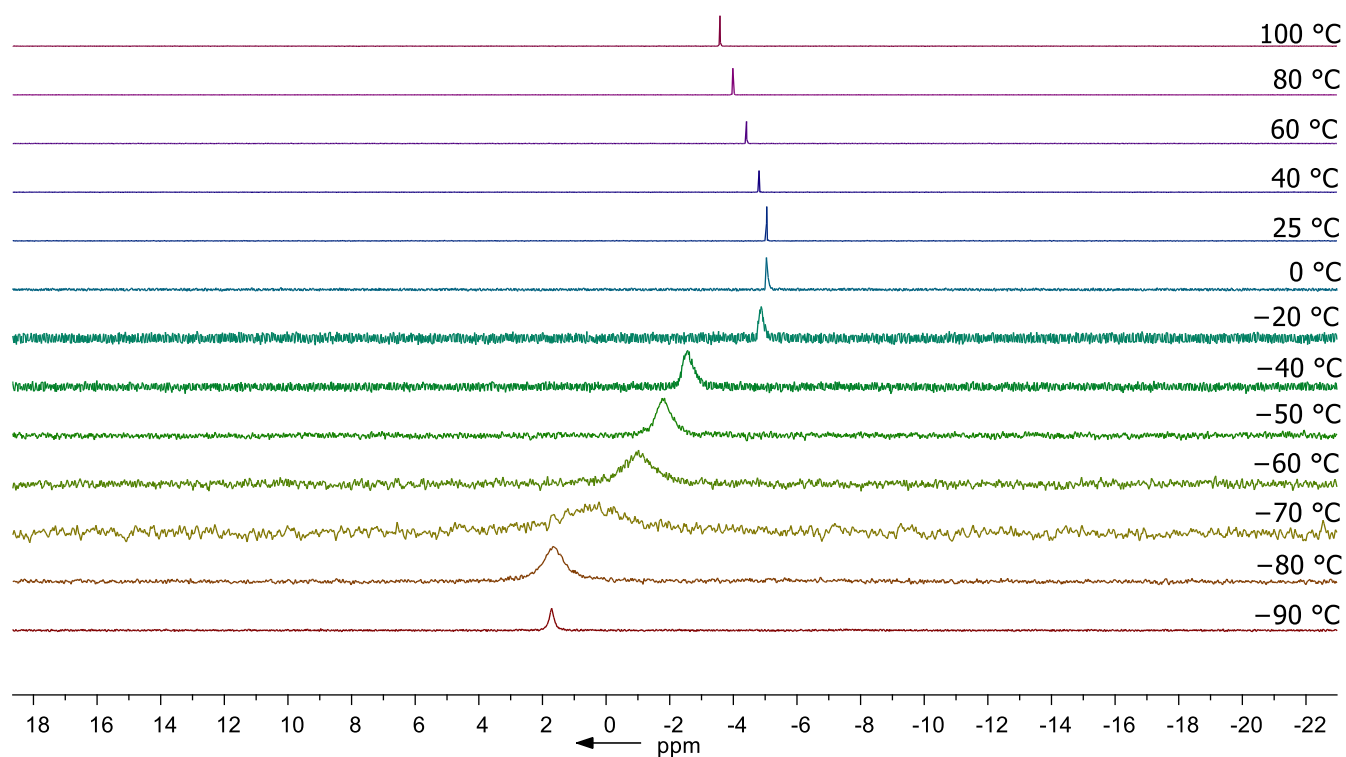


Figure S26. $^{31}\text{P}\{^1\text{H}\}$ and $^{31}\text{P}\{^{11}\text{B}, ^1\text{H}\}$ NMR spectra of $\text{PPh}_3\text{-BPh}_3$ in $[\text{D}_8]\text{toluene}$ at $-90\text{ }^\circ\text{C}$.

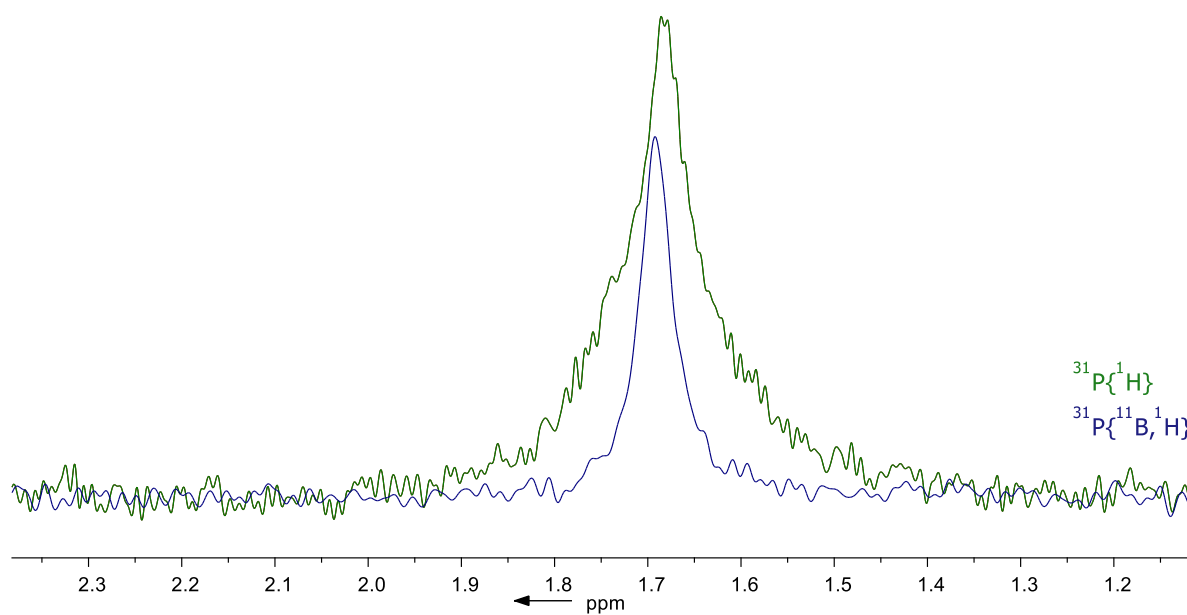


Figure S27. $^{11}\text{B}\{^1\text{H}\}$ RSHE/MAS NMR spectrum of $\text{PPh}_3\text{-BPh}_3$.

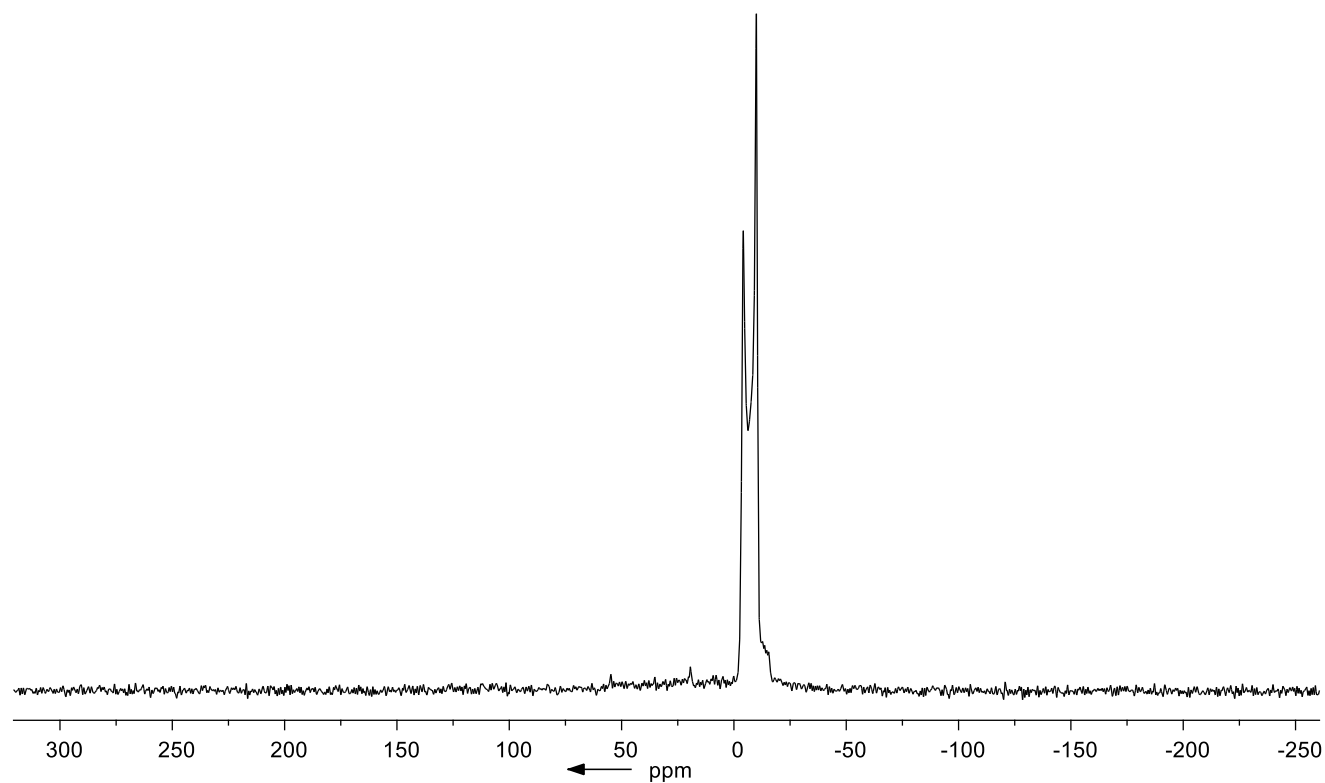


Figure S28. $^{31}\text{P}\{^1\text{H}\}$ CP/MAS NMR spectrum of $\text{PPh}_3\text{-BPh}_3$.

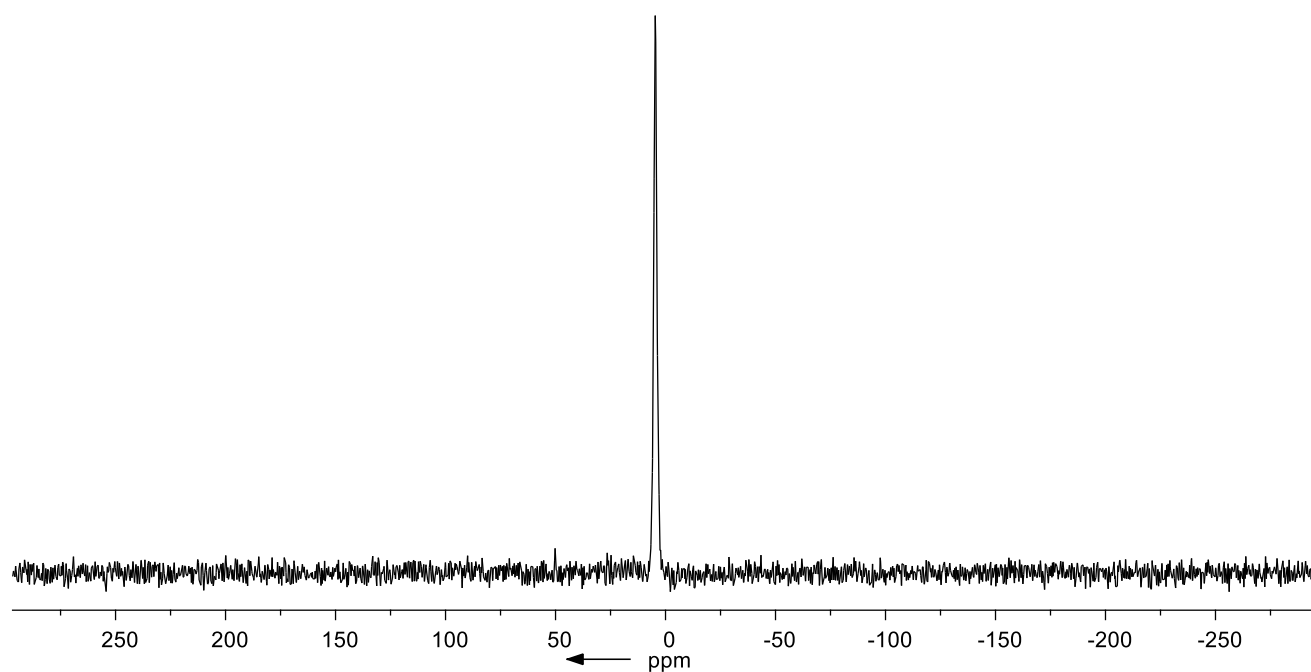


Figure S29. Vibrational spectra of $\text{PPh}_3\text{-BPh}_3$ (top: IR; bottom: Raman)

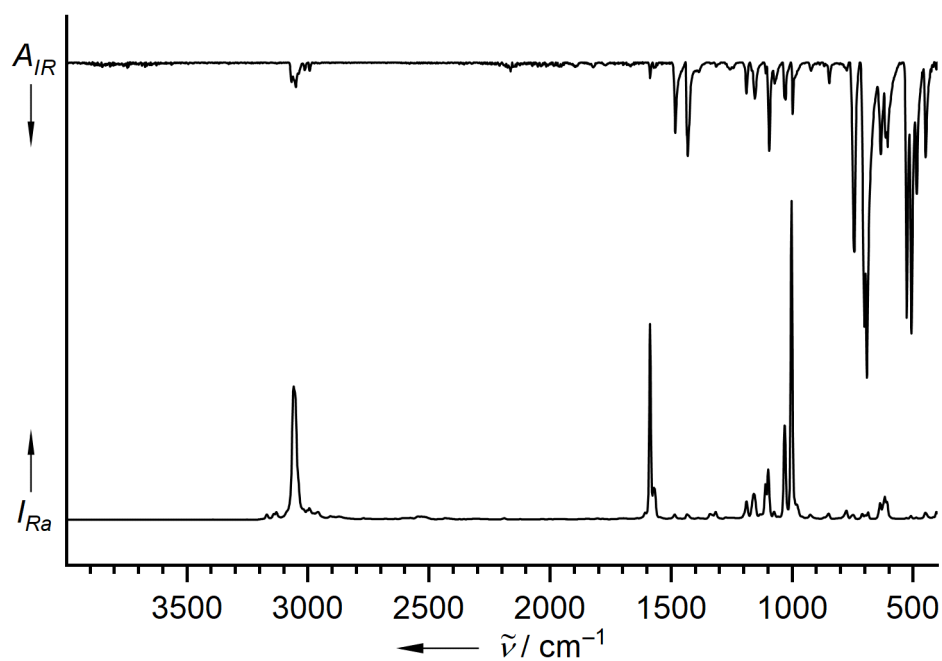
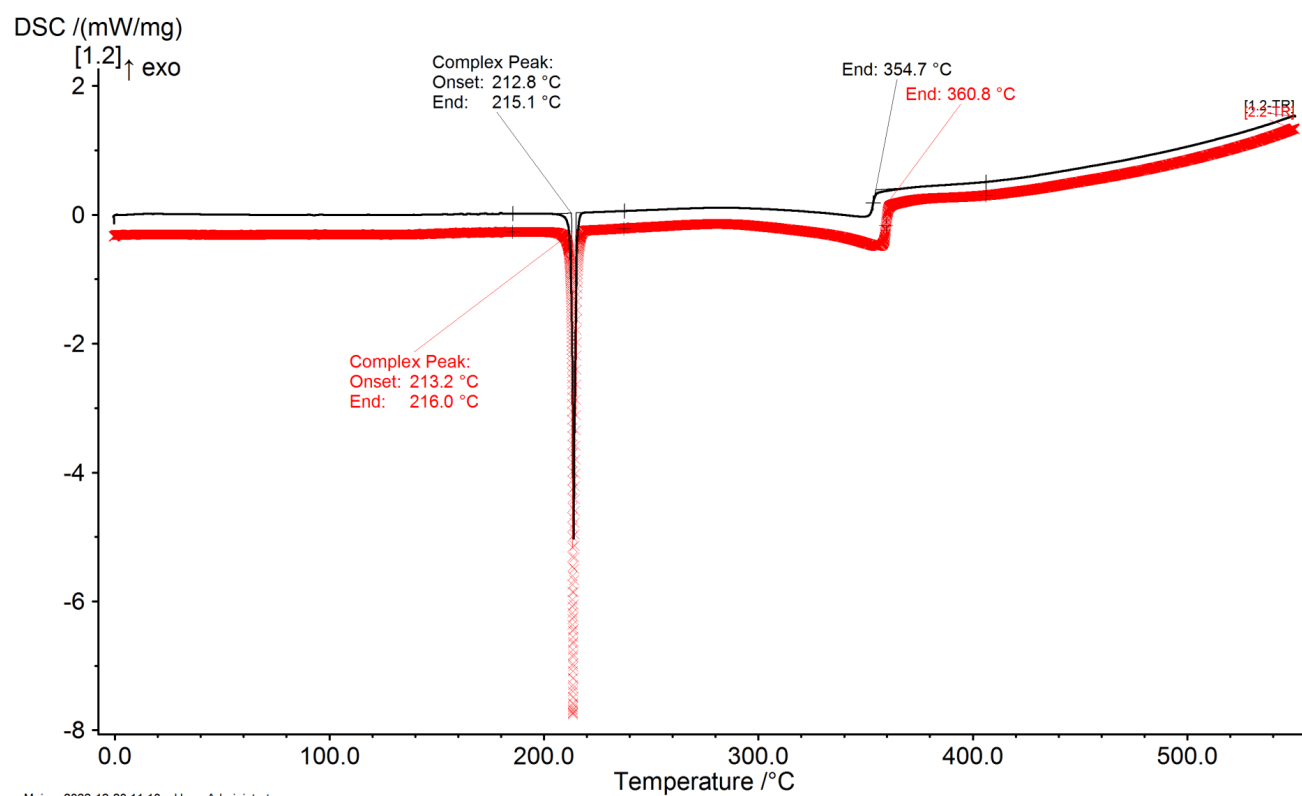


Figure S30. DSC measurement of $\text{PPh}_3\text{-BPh}_3$.



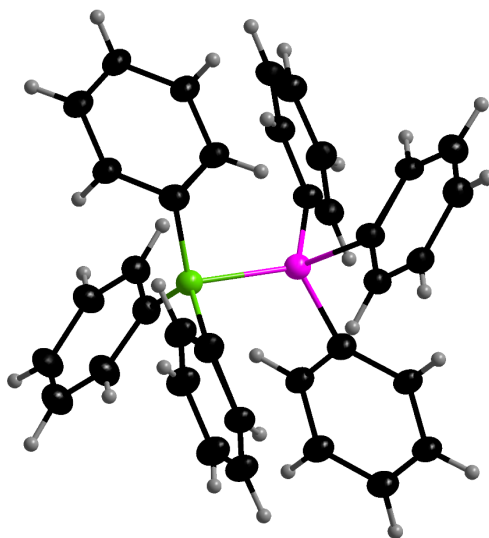
Crystal Structure Determination

Crystal data of PPh₃–BPh₃ were collected on a XtaLAB Synergy-R diffractometer with a hybrid pixel array detector, using Cu_{Kα} radiation (rotating-anode X-ray tube, $\lambda_{\text{Cu}} = 1.54184 \text{ \AA}$). The structure was solved by intrinsic phasing methods (SHELXT) and refinement is based on full-matrix least-squares calculations on F^2 (SHELXL).^[9] All nonhydrogen atoms were refined anisotropically. For CH idealized bond lengths and angles were used. Calculations were carried out using the ShelXle graphical interface.^[10] Molecular structure diagrams were drawn with the program Diamond 4.6.6.^[11] Crystallographic data have been deposited with the Cambridge Crystallographic Data Centre. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S2. Selected crystal data and details of the refinement of the crystal structures of PPh₃–BPh₃.

	PPh ₃ –BPh ₃
Formula	C ₃₆ H ₃₀ PB
M_w	504.38
T (K)	99.97(12)
Crystal system	hexagonal
Space group	$P6_3/c/m$
a (Å)	9.8279(7)
b (Å)	9.8279(7)
c (Å)	8.0179(9)
Volume (Å ³)	607.68(12)
Z	1
ρ (calcd) (Mg m ⁻³)	1.249
μ (mm ⁻¹)	1.070
$F(000)$	266
No. of collected reflections	4248
No. of unique reflections	500
$R(\text{int})$	0.0405
No. of parameters / restraints	116 / 327
$R1$ ($I > 2\sigma(I)$)	0.0536
$wR2$ (all)	0.1562
GOF on F^2	1.107
Largest diff. peak / hole / e Å ⁻³	0.080 / –0.208
CCDC no.	2231981

Figure S31. Crystal structure of $\text{PPh}_3\text{-BPh}_3$ (ellipsoids are drawn at the 25% probability level except for the H atoms that are depicted with arbitrary radii, disorder is omitted for clarity).



7. References

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