

## SUPPLEMENTARY INFORMATION

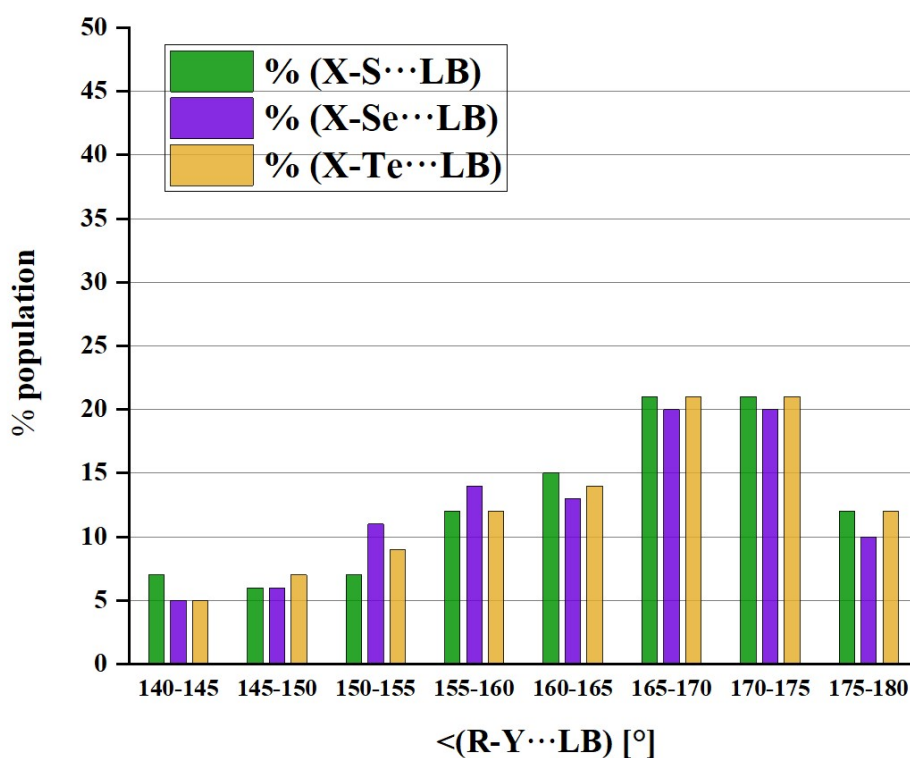
### Directionality in Cation–Anion Interactions Involving Chalconium Cations

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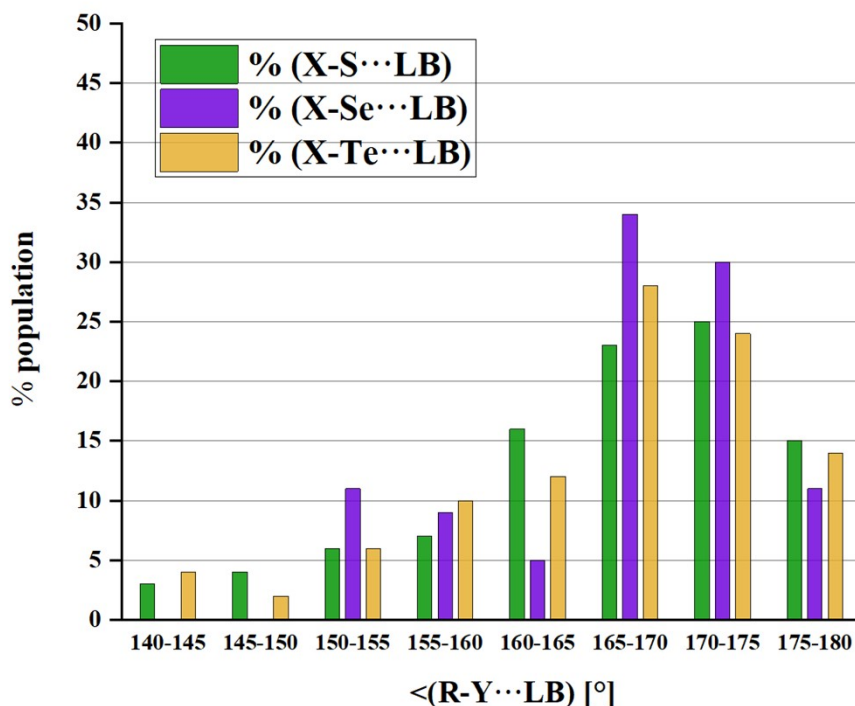


Fig. S1 Bar charts representing the distribution of obtained hits versus the R-Y...LB angle prior to cone correction for all contacts to chalconium cations of (top) all bases and (bottom) anions only.

Table S1. Coordinates of investigated structures from crystal database source.

AMOLUM	Sb	14.94970000	9.54680000	8.68360000
	F	13.17940000	9.54680000	8.01500000
	F	15.36550000	8.23940000	7.46970000
	F	14.45480000	8.26020000	9.91410000
	F	16.70430000	9.54680000	9.31490000
	F	15.36550000	10.85410000	7.46970000
	F	14.45480000	10.83330000	9.91410000
	S	12.16640000	9.54680000	5.59810000
	F	11.77690000	9.54680000	4.14050000
	F	13.18300000	8.43180000	5.50170000
	F	13.18300000	10.66170000	5.50170000
	N	10.60410000	7.64440000	5.60000000
	C	9.74910000	6.92100000	5.54890000
	C	8.64640000	5.98010000	5.48100000
	H	8.99910000	5.07000000	5.39700000
	H	8.08900000	6.18630000	4.70260000
	H	8.10800000	6.04880000	6.29650000
	N	10.60410000	11.44910000	5.60000000
	C	9.74910000	12.17250000	5.54890000
C	8.64640000	13.11340000	5.48100000	
H	8.99910000	14.02350000	5.39700000	
H	8.08900000	12.90720000	4.70260000	
H	8.10800000	13.04470000	6.29650000	
MEKCAI	Se	3.44880000	2.80770000	9.70530000

	C	4.26070000	4.21440000	8.64900000
	H	4.85130000	3.81770000	7.97580000
	H	4.78120000	4.80370000	9.23460000
	H	3.55990000	4.73370000	8.20230000
	C	2.39250000	1.99580000	8.29860000
	C	2.04210000	3.86400000	10.51720000
	H	1.71930000	1.40520000	8.69530000
	H	2.43880000	4.53720000	11.10780000
	H	2.97810000	1.47530000	7.70930000
	H	1.45280000	3.27840000	11.03770000
	H	1.94580000	2.69660000	7.77930000
	H	1.52280000	4.31070000	9.81640000
	Te	6.25650000	6.25650000	12.51300000
	Cl	5.76600000	3.83500000	11.93690000
	Cl	6.83260000	6.74700000	10.09150000
	Cl	8.67800000	5.68040000	13.00350000
	Cl	6.74700000	8.67800000	13.08910000
	Cl	5.68040000	5.76600000	14.93450000
	Cl	3.83500000	6.83260000	12.02250000
	Te	6.25650000	0.00000000	6.25650000
	Cl	5.68040000	0.49050000	8.67800000
	Cl	3.83500000	-0.57610000	5.76600000
	Cl	6.74700000	-2.42150000	6.83260000
	Cl	6.83260000	-0.49050000	3.83500000
	Cl	8.67800000	0.57610000	6.74700000
	Cl	5.76600000	2.42150000	5.68040000
	Te	0.00000000	0.00000000	12.51300000
	Cl	2.42150000	0.57610000	12.02250000
	Cl	-0.49050000	2.42150000	13.08910000
	Cl	0.57610000	-0.49050000	14.93450000
	Cl	-2.42150000	-0.57610000	13.00350000
	Cl	0.49050000	-2.42150000	11.93690000
	Cl	-0.57610000	0.49050000	10.09150000
RILFOL	C	1.79060000	6.77220000	10.53780000
	C	2.26460000	5.52470000	10.93840000
	H	1.93300000	4.72900000	10.53950000
	C	3.23730000	5.47040000	11.94150000
	H	3.57540000	4.62990000	12.22570000
	C	3.70920000	6.63370000	12.52180000
	H	4.36620000	6.59010000	13.20650000
	C	3.22610000	7.86100000	12.10410000
	H	3.55960000	8.65570000	12.50470000
	C	2.26090000	7.94620000	11.11130000
	H	1.92750000	8.79100000	10.83060000
	C	1.31050000	7.90040000	7.60890000
	C	2.68410000	7.93340000	7.60210000
	H	3.17740000	7.46790000	8.26800000
	C	3.34520000	8.65470000	6.61610000
	H	4.29530000	8.67920000	6.59900000
	C	2.61330000	9.34180000	5.65070000
	H	3.06570000	9.84680000	4.98480000
	C	1.23570000	9.29280000	5.65580000
	H	0.74220000	9.76580000	4.99500000
C	0.56450000	8.55450000	6.62470000	
H	-0.38380000	8.49490000	6.61780000	

	C	-0.72340000	8.51400000	9.96270000
	C	-0.59500000	9.80200000	9.47310000
	H	-0.04510000	9.97670000	8.71820000
	C	-1.27900000	10.83540000	10.09620000
	H	-1.21040000	11.71960000	9.75730000
	C	-2.05780000	10.58290000	11.20540000
	H	-2.51280000	11.29770000	11.63680000
	C	-2.17830000	9.30020000	11.69500000
	H	-2.71400000	9.12980000	12.46020000
	C	-1.51030000	8.25410000	11.05990000
	H	-1.59790000	7.36560000	11.38520000
	Te	0.25000000	6.83020000	9.09410000
	C	-0.01430000	4.41260000	6.27200000
	H	-0.91000000	4.52970000	6.65210000
	H	-0.07160000	3.85970000	5.46580000
	H	0.35960000	5.28930000	6.04270000
	C	0.87140000	3.73930000	7.27690000
	C	0.77810000	2.24360000	7.37960000
	H	1.36270000	1.92820000	8.10020000
	H	1.05880000	1.83980000	6.53220000
	H	-0.14740000	1.98680000	7.57300000
	O	1.60120000	4.38810000	8.00560000
	B	-1.36060000	3.77980000	10.89220000
	F	-1.18110000	5.12420000	11.22800000
	F	-2.18660000	3.68920000	9.76700000
	F	-1.94180000	3.10970000	11.94630000
	F	-0.12650000	3.22370000	10.58530000
	B	-3.12790000	6.87340000	6.22580000
	F	-3.30750000	5.52900000	5.89000000
	F	-2.30200000	6.96400000	7.35100000
	F	-2.54680000	7.54350000	5.17170000
	F	-4.36200000	7.42950000	6.53270000