Ar····Li^+	analytical			numerical		
def2-SVP	$\alpha_\perp$	$\alpha_\parallel$	α_{iso}	$\alpha_\perp$	$\alpha_\parallel$	α_{iso}
monomer A (Ar)	4.3702	4.3702	4.3702	4.3702	4.3702	4.3702
monomer B (Li^+)	0.1593	0.1593	0.1593	0.1593	0.1593	0.1593
A + B	4.5295	4.5295	4.5295	4.5295	4.5295	4.5295
frz + pol {u}	4.5072	4.5759	4.5301	--	--	--
frz + pol {p}	4.5042	4.5581	4.5222	4.5036	4.5696	4.5256
frz + pol + CT(A → all) {u}	-0.7249	4.3565	0.9689	--	--	--
frz + pol + CT(A → all) {p}	4.7040	5.5191	4.9757	--	--	--
frz + pol + CT(B → all) {u}	0.1594	0.1995	0.1728	--	--	--
frz + pol + CT(B → all) {p}	0.1594	0.1586	0.1591	--	--	--
frz + pol + CT(all → all) [blocked] {u}	-0.5567	4.5025	1.1297	--	--	--
frz + pol + CT(all → all) [blocked] {p}	4.8409	5.7540	5.1452	--	--	--
frz + pol + CT(all → all) [super]	5.2142	7.8649	6.0978	5.2142	7.8649	6.0978

Ar····Li^+	analytical			numerical		
def2-SVPD	$\alpha_\perp$	$\alpha_\parallel$	α_{iso}	$\alpha_\perp$	$\alpha_\parallel$	α_{iso}
monomer A (Ar)	10.3735	10.3735	10.3735	10.3735	10.3735	10.3735
monomer B (Li^+)	0.1603	0.1603	0.1603	0.1603	0.1603	0.1603
A + B	10.5338	10.5338	10.5338	10.5338	10.5338	10.5338
frz + pol {u}	10.1052	12.1433	10.7846	--	--	--
frz + pol {p}	10.0787	10.6399	10.2658	10.0875	10.6599	10.2783
frz + pol + CT(A → all) {u}	9.9728	8.0653	9.3370	--	--	--
frz + pol + CT(A → all) {p}	10.0157	10.4900	10.1738	--	--	--
frz + pol + CT(B → all) {u}	0.1607	3.7873	1.3696	--	--	--
frz + pol + CT(B → all) {p}	0.1606	0.1614	0.1609	--	--	--
frz + pol + CT(all → all) [blocked] {u}	10.0971	10.0052	10.0664	--	--	--
frz + pol + CT(all → all) [blocked] {p}	10.1395	10.8004	10.3598	--	--	--
frz + pol + CT(all → all) [super]	10.0724	11.0645	10.4031	10.0724	11.0645	10.4031