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 Summary of Multipole Component Variables & Expressions in Tinker  
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#####  
 Math Operations and Symbolic Notation  
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dot            vector dot/inner product (scalar, sum of 3 pair products)  
 crx            vector cross/outer product (vector)  
 ddot           "tensor double dot product" (scalar, sum of 9 pair products)  
 []             significance of variable  
 {}             variable name of older versions of Tinker

#####  
 Sites            Equivalence in Code  
 #####

ii	first multipole	[site number]
i	ipole(i)	[atom number]
xi	x(i)	[x-coordinate]
yi	y(i)	[y-coordinate]
zi	z(i)	[z-coordinate]

kk	second multipole	[site number]
k	ipole(k)	[atom number]
xk	x(k)	[x-coordinate]
yk	y(k)	[y-coordinate]
zk	z(k)	[z-coordinate]

xr	xk - xi	[x-distance]
yr	yk - yi	[y-distance]
zr	zk - zi	[z-distance]

#####  
 Mpoles           Equivalence in Code  
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ci	rpole(1,ii)	[monopole]
dix	rpole(2,ii)	[x-dipole]
diy	rpole(3,ii)	[y-dipole]
diz	rpole(4,ii)	[z-dipole]
qixx	rpole(5,ii)	[xx-quadrupole]
qixy	rpole(6,ii)	[xy-quadrupole]
qixz	rpole(7,ii)	[xz-quadrupole]
qiyy	rpole(8,ii)	[yy-quadrupole]
qiyz	rpole(9,ii)	[yz-quadrupole]
qizz	rpole(10,ii)	[zz-quadrupole]
uix	uind(1,ii)	[x-induced]
uiy	uind(2,ii)	[y-induced]
uiz	uind(3,ii)	[z-induced]

ck	rpole(1,kk)	[monopole]
dkx	rpole(2,kk)	[x-dipole]
dky	rpole(3,kk)	[y-dipole]
dkz	rpole(4,kk)	[z-dipole]

qkxx	rpole(5, kk)	[xx-quadrupole]
qkxy	rpole(6, kk)	[xy-quadrupole]
qkxz	rpole(7, kk)	[xz-quadrupole]
qkyy	rpole(8, kk)	[yy-quadrupole]
qkyz	rpole(9, kk)	[yz-quadrupole]
qkzz	rpole(10, kk)	[zz-quadrupole]
ukx	uind(1, kk)	[x-induced]
uky	uind(2, kk)	[y-induced]
ukz	uind(3, kk)	[z-induced]

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#####
Energy
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#####
Equivalence in Code
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dir	dix*xr + diy*yr + diz*zr	[di-dot-r]	{dri}
qix	qixx*xr + qixy*yr + qixz*zr	[qix-dot-r]	{qrix}
qiy	qixy*xr + qiyy*yr + qiyz*zr	[qiy-dot-r]	{qriy}
qiz	qixz*xr + qiyz*yr + qizz*zr	[qiz-dot-r]	{qriz}
qir	qix*xr + qiy*yr + qiz*zr	[qi-dot-r]	{qrr}

dkr	dkx*xr + dky*yr + dkz*zr	[dk-dot-r]	{drk}
qkx	qkxx*xr + qkxy*yr + qkxz*zr	[qkx-dot-r]	{qrkx}
qky	qkxy*xr + qky*yr + qkyz*zr	[qky-dot-r]	{qrky}
qkz	qkxz*xr + qkyz*yr + qkzz*zr	[qkz-dot-r]	{qrkz}
qkr	qkx*xr + qky*yr + qkz*zr	[qk-dot-r]	{qrrk}

dik	dix*dkx + diy*dky + diz*dkz	[di-dot-dk]	{dik}
qik	qix*qkx + qiy*qky + qiz*qkz	[qi-dot-qk]	{qrrik}
diqk	dix*qkx + diy*qky + diz*qkz	[di-dot-qk]	{diqrk}
dkqi	dkx*qix + dky*qiy + dkz*qiz	[dk-dot-qi]	{dkqri}
qiqk	2.0d0*(qixy*qkxy+qixz*qkxz+qiyz*qkyz) + qixx*qkxx + qiyy*qkyy + qizz*qkzz	[qi-ddot-qk]	{qiqk}

diu	dix*ukx + diy*uky + diz*ukz	[di-dot-uk]	{duik}*
qiu	qix*ukx + qiy*uky + qiz*ukz	[qi-dot-uk]	{quik}*
uir	uix*xr + uiy*yr + uiz*zr	[ui-dot-r]	{uri}
dku	dkx*uix + dky*uiy + dkz*uiz	[dk-dot-ui]	{duik}*
qku	qkx*uix + qky*uiy + qkz*uiz	[qk-dot-ui]	{quik}*
ukr	ukx*xr + uky*yr + ukz*zr	[uk-dot-r]	{urk}

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#####
Gradient
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#####
Equivalence in Code
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dirx	diy*zr - diz*yr	[x of di-crs-r]	{dirx}
diry	diz*xr - dix*zr	[y of di-crs-r]	{diry}
dirz	dix*yr - diy*xr	[z of di-crs-r]	{dirz}

dkrx	dky*zr - dkz*yr	[x of dk-crs-r]	{dkrx}
dkry	dkz*xr - dkx*zr	[y of dk-crs-r]	{dkry}
dkrz	dkx*yr - dky*xr	[z of dk-crs-r]	{dkrz}

dikx	diy*dkz - diz*dky	[x of di-crs-dk]	{dikx}
diky	diz*dkx - dix*dkz	[y of di-crs-dk]	{diky}
dikz	dix*dky - diy*dkx	[z of di-crs-dk]	{dikz}

qirx	qiz*yr - qiy*zr	[x of qi-crs-r]	{qrixr}
qiry	qix*zr - qiz*xr	[y of qi-crs-r]	{qriyr}
qirz	qiy*xr - qix*yr	[z of qi-crs-r]	{qrizr}
qkrx	qkz*yr - qky*zr	[x of qk-crs-r]	{qrkxr}
qkry	qkx*zr - qkz*xr	[y of qk-crs-r]	{qrkyr}
qkrz	qky*xr - qkx*yr	[z of qk-crs-r]	{qrkzr}
qikx	qky*qiz - qkz*qiy	[x of qi-crs-qk]	{qrrx}
qiky	qkz*qix - qkx*qiz	[y of qi-crs-qk]	{qrry}
qikz	qkx*qiy - qky*qix	[z of qi-crs-qk]	{qrrz}
qixk	qixx*qkx + qixy*qky + qixz*qkz	[qix's-dot-qk]	{qikrx}
qiyk	qixy*qkx + qiyy*qky + qiyz*qkz	[qiy's-dot-qk]	{qikry}
qizk	qixz*qkx + qiyz*qky + qizz*qkz	[qiz's-dot-qk]	{qikrz}
qkxi	qkxx*qix + qkxy*qiy + qkxz*qiz	[qkx's-dot-qi]	{qkixr}
qkyi	qkxy*qix + qkyy*qiy + qkyz*qiz	[qiy's-dot-qk]	{qkiry}
qkzi	qkxz*qix + qkyz*qiy + qkzz*qiz	[qiz's-dot-qk]	{qkizr}
qikrx	qizk*yr - qiyk*zr	[x of qik-crs-r]	{qikrxr}
qikry	qixk*zr - qizk*xr	[y of qik-crs-r]	{qikryr}
qikrz	qiyk*xr - qixk*yr	[z of qik-crs-r]	{qikrzr}
qkirx	qkzi*yr - qkyi*zr	[x of qki-crs-r]	{qkirxr}
qkiry	qkxi*zr - qkzi*xr	[y of qki-crs-r]	{qkiryr}
qkirz	qkyi*xr - qkxi*yr	[z of qki-crs-r]	{qkirzr}
diqkx	dix*qkxx + diy*qkxy + diz*qkxz	[di-dot-qkx's]	{diqkx}
diqky	dix*qkxy + diy*qkyy + diz*qkyz	[di-dot-qky's]	{diqky}
diqkz	dix*qkxz + diy*qkyz + diz*qkzz	[di-dot-qkz's]	{diqkz}
dkqix	dkx*qixx + dky*qixy + dkz*qixz	[dk-dot-qix's]	{dkqix}
dkqiy	dkx*qixy + dky*qiiy + dkz*qiyz	[dk-dot-qiy's]	{dkqiy}
dkqiz	dkx*qixz + dky*qiyz + dkz*qizz	[dk-dot-qiz's]	{dkqiz}
diqkrx	diqkz*yr - diqky*zr	[x of diqk-crs-r]	{diqkxr}
diqkry	diqkx*zr - diqkz*xr	[x of diqk-crs-r]	{diqkry}
diqkrz	diqky*xr - diqkx*yr	[x of diqk-crs-r]	{diqkzr}
dkqirx	dkqiz*yr - dkqiy*zr	[x of dkqi-crs-r]	{dkqixr}
dkqiry	dkqix*zr - dkqiz*xr	[y of dkqi-crs-r]	{dkqiyr}
dkqirz	dkqiy*xr - dkqix*yr	[z of dkqi-crs-r]	{dkqizr}
dqikx	diy*qkz - diz*qky + dky*qiz - dkz*qiy - 2.0d0*(qixy*qkxz+qiyy*qkyz+qiyz*qkzz -qixz*qkxy-qiyz*qkyy-qizz*qkyz)	[complex]	{dqiqkx}
dqiky	diz*qkx - dix*qkz + dkz*qix - dkx*qiz - 2.0d0*(qixz*qkxx+qiyz*qkxy+qizz*qkxz -qixx*qkxz-qixy*qkyz-qixz*qkzz)	[complex]	{dqiqky}
dqikz	dix*qky - diy*qkx + dkx*qiy - dky*qix - 2.0d0*(qixx*qkxy+qixy*qkyy+qixz*qkyz -qixy*qkxx-qiyy*qkxy-qiyz*qkxz)	[complex]	{dqiqkz}