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## Understanding protein complex formation: the role of charge distribution in the encounter complex

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# Understanding protein complex formation:

## The role of charge distribution in the encounter complex

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**To my family**

*“A li pccnunn mj”*

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# Abbreviations

$\Delta\chi$	magnetic susceptibility anisotropy tensor
$\tau_c$	rotational correlation time
A $\beta$	amyloid $\beta$
AdR	adrenodoxin reductase
Adx	adrenodoxin
ATP	adenosine triphosphate
BPTI	bovine pancreatic trypsin inhibitor
ca.	circa
CcP	cytochrome <i>c</i> peroxidase
CL	crosslinked complex
CLaNP	caged lanthanide NMR probe
Cc	cytochrome <i>c</i>
Cc6	cytochrome <i>c</i> <sub>6</sub>
CpdI	Compound I
CpdII	Compound II
Cytf	cytochrome <i>f</i>
DOTAM	1,4,7,10-tetraazacyclododecane-1,4,7,10-tetraacetamide
DOTP	1,4,7,10-tetraazacyclododecane-1,4,7,10-tetrakis (methylenephosphonate)
EDTA	ethylenediaminetetraacetic acid
EIN	Enzyme I
EM	electron microscopy
Fd	ferredoxin
EPR	electron paramagnetic resonance
FRET	fluorescence resonance energy transfer
FTR	ferredoxin:thioredoxin reductase
HPr	histidine-containing phosphocarrier protein
HSQC	heteronuclear single quantum coherence
IFN- $\gamma$	interferon gamma

$k_a$	association rate constant
$K_B$	binding constant
$K_D$	dissociation constant
$k_{ex}$	exchange rate
$k_{off}$	dissociation rate constant
$k_{on}$	association rate constant
Lac	lactose
LBP	lanthanide-binding peptide
MTS	1-acetoxy-2,2,5,5-tetramethyl-d3-pyrroline-3-methyl-methanethiosulfonate
MTSL	1-oxyl-2,2,5,5-tetramethyl-2,5-dihydropyrrol-3-ylmethyl-methanethiosulfonate
NADPH	nicotinamide adenine dinucleotide phosphate (reduced state)
NOE	nuclear Overhauser enhancement
NOESY	nuclear Overhauser spectroscopy
NS2Bc	C-terminal segment of NS2B
NS2B-NS3pro	NS2B-NS3 protease
P450cam	cytochrome P450cam
Pc	plastocyanin
PCS	pseudocontact shift
PDB	protein data bank
Pdx	putidaredoxin
piRDC	paramagnetically induced residual dipolar coupling
PRE	paramagnetic relaxations enhancement
PPI	protein-protein interaction
RD	relaxation dispersion
RDC	residual dipolar coupling
RMSD	root mean square deviation
SAXS	small-angle X-ray scattering
SNAP	synaptosomal-associated protein
SNARE	soluble NSF attachment protein
sPRE	solvent paramagnetic relaxations enhancement



Syt1	synaptotagmin-1
Trx	thioredoxin
WT	wild type
XRD	X-ray diffraction