Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary data

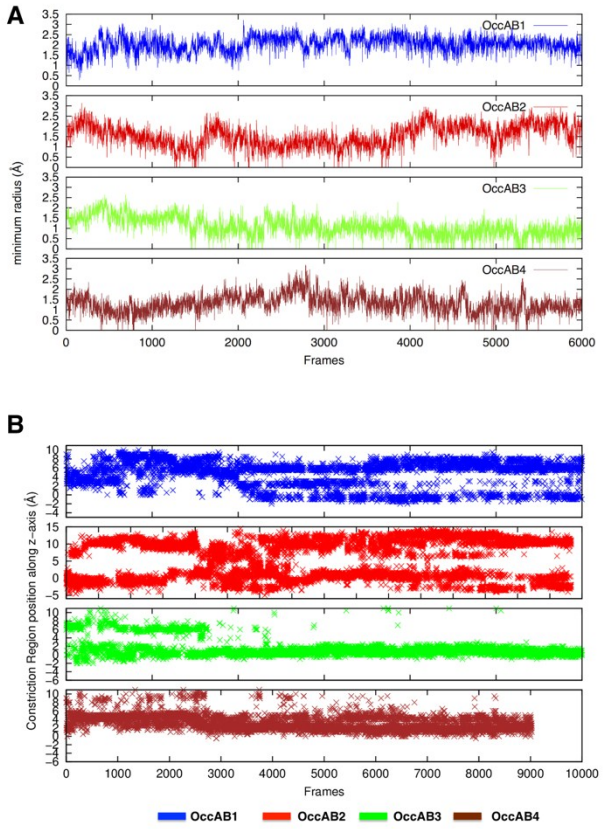

Figure S1: Radius profiles of OccAB. (A) Minimum radius over time simulation. (B) distribution of the minimum radius area (constriction region: CR) along the pore axis (z-axis).

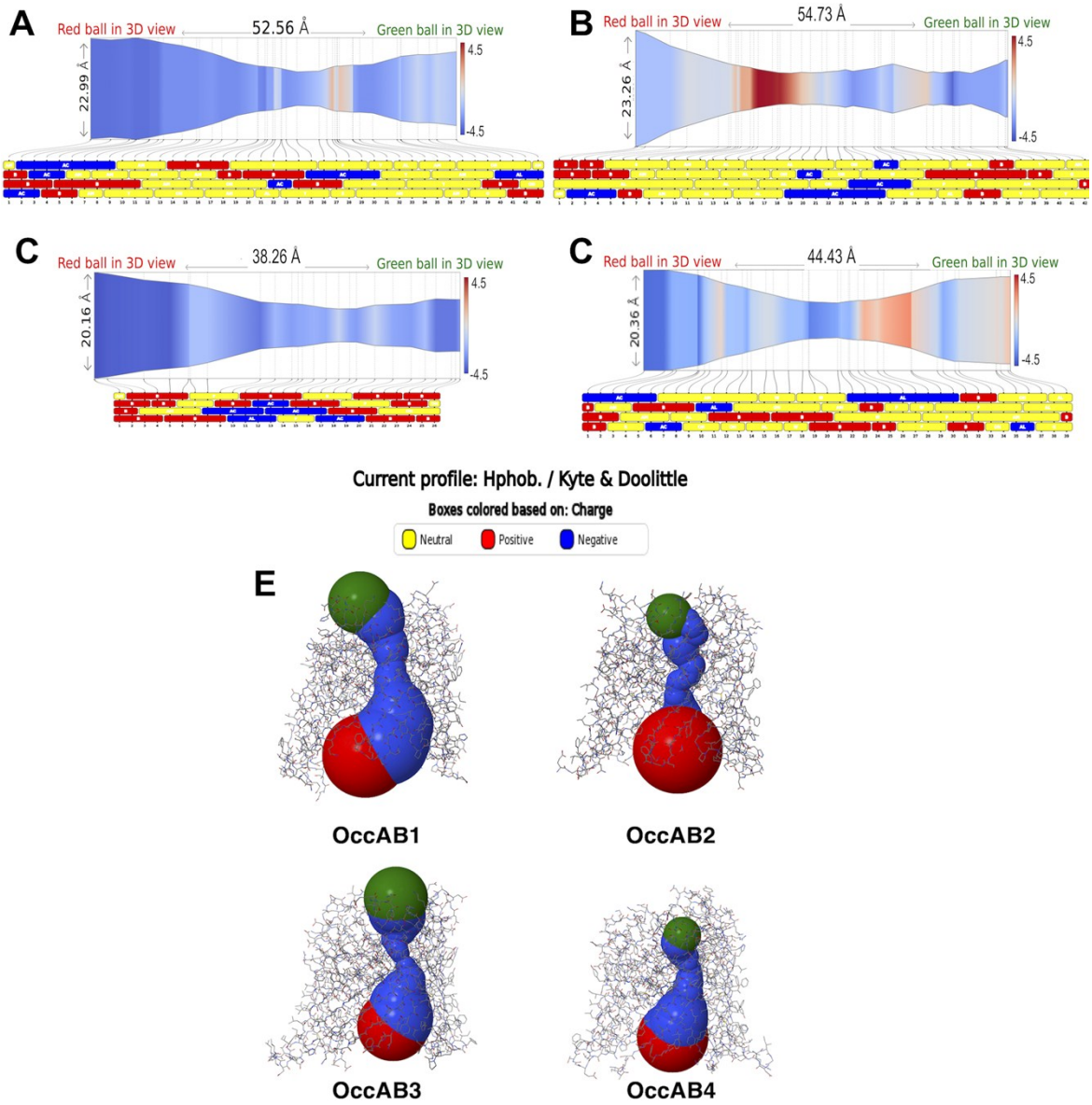

Figure S 2: Structural and biophysical properties of OccAB1-4 channel from *A.baumannii*. TOP (A, B, C and D) The 2D profiles of the radius of OccAB crystals in the figure are colored by hydrophobicity of residues along with the channels. The boxes are colored according to the Amino Acid charge property and labeled by Amino acid. (E) The transmembrane channels identified by ChExVis and extracted in OccAB (5DL5, 5DL6, 5DL7 and 5DL8 crystals) pore shown as sphere (blue), the green ball corresponds to the entrance of the channel (extracellular) and the red ball corresponds to wide pore end (periplasm side).

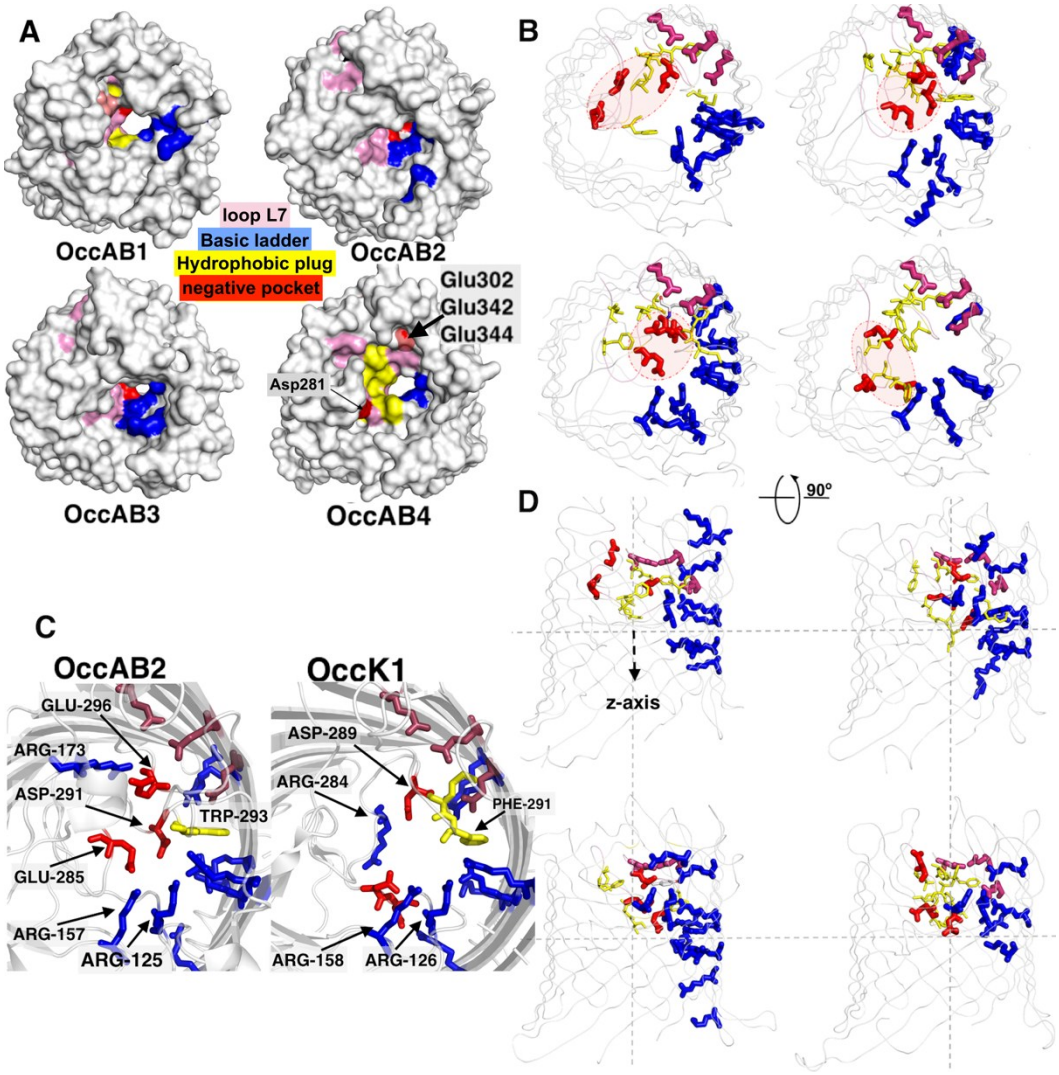

Figure S3: The basic ladder and negative pocket of OccAB porins. (A) surface representation of the Top view of OccAB crystals, (B) (D) the transversal view of the porins shown as ribbon, the residues involved in the "basic ladder' are shown as blue stick, the residues of the negative pocket are shown as red sticks and the barrel negatively, the hydrophobic residues are represented in yellow. The pink colour in the panel A corresponds to the loop L7. (D) Structural comparison between residues lining the pore involved in the conductance state in OccAB2 and OccK1

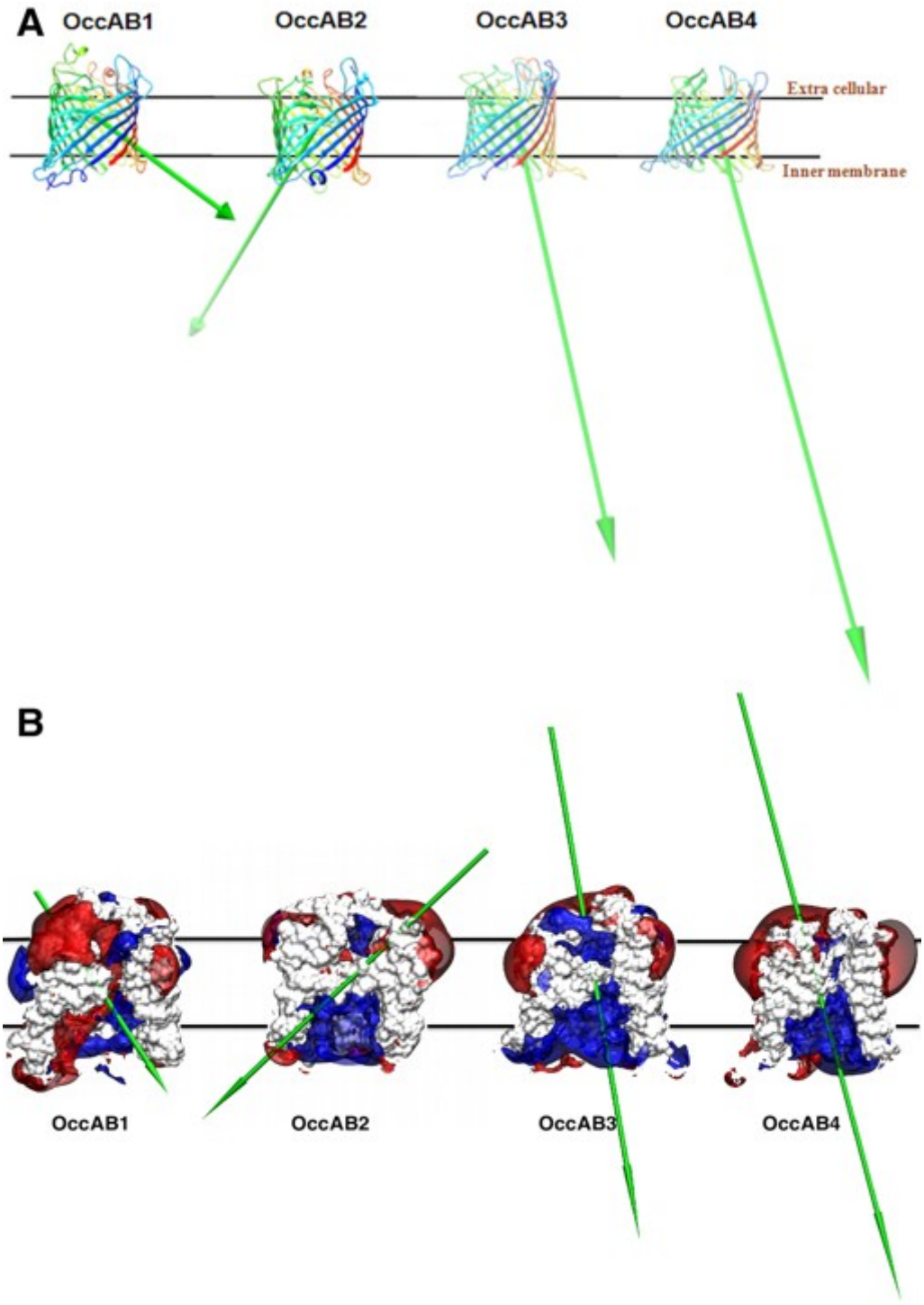

Figure S 4: A Calculated electric dipole moment vector of the OccAB crystals porins which is represented by the green arrow. The center of the arrow corresponds to the Center of Mass of the porin, the tip indicates the positively charged end and the base of the arrow corresponds to the negatively charged end, the length of the arrow corresponds to the magnitude of the macro-dipole moment. B) Half transversal surface representation of OccAB porins with the averaged dipole moment vector over simulation time. As red surface representation is the negative electrostatic potential (in -2 KT/e isocontour), as blue surface is the negative electrostatic potential (in +2 KT/e isocontour) averaged over simulation time.

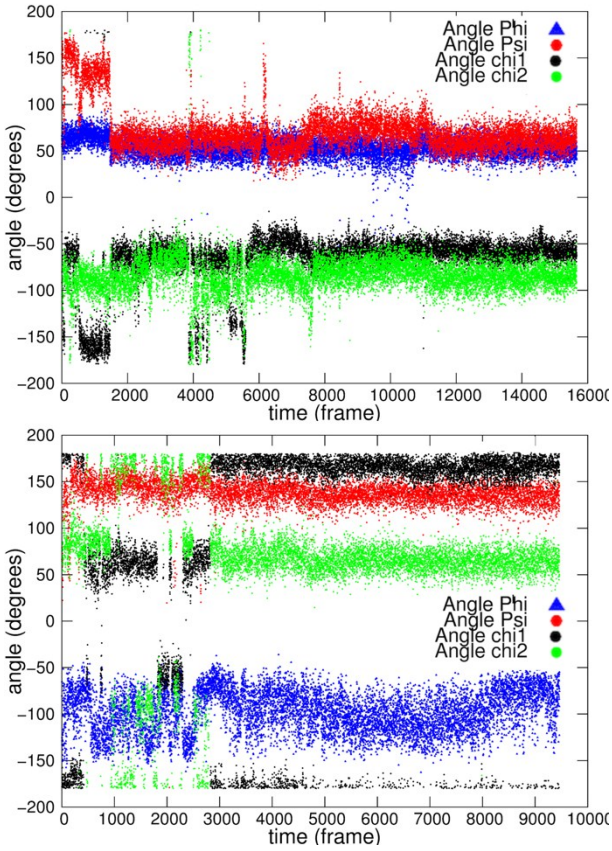

Figure S 5: The flexibility of the pore in OccAB2 and OccAB4. The angles Phi, Psi, Chi1 and Chi2 of Trp293 in OccAB2 (Top) and Trp292 in OccAB4 (bottom) plotted against time showing the flipping of the tryptophan lining the pore during the MD simulations.

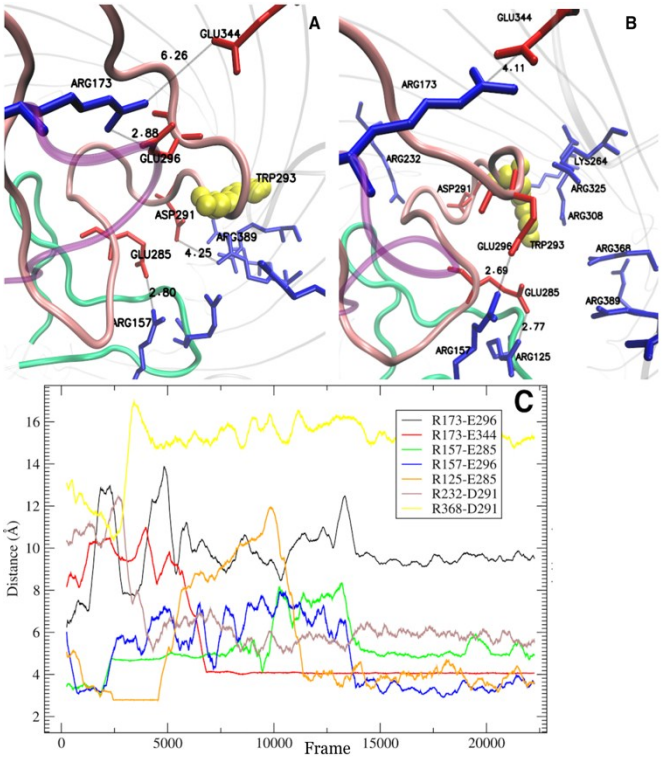

Figure S 6: *The flexibility of the CR of OccAB2. (A) 3D structural arrangement of the main residues in CR1 and CR2 at the starting conformation of the 800ns run of MD simulations equilibrations using the OccAB2 crystal as starting structure, (B) the similar top view at the last frame. (C) the distances between the carbon sidechains of the main residues in the CR1 and CR2 along the*

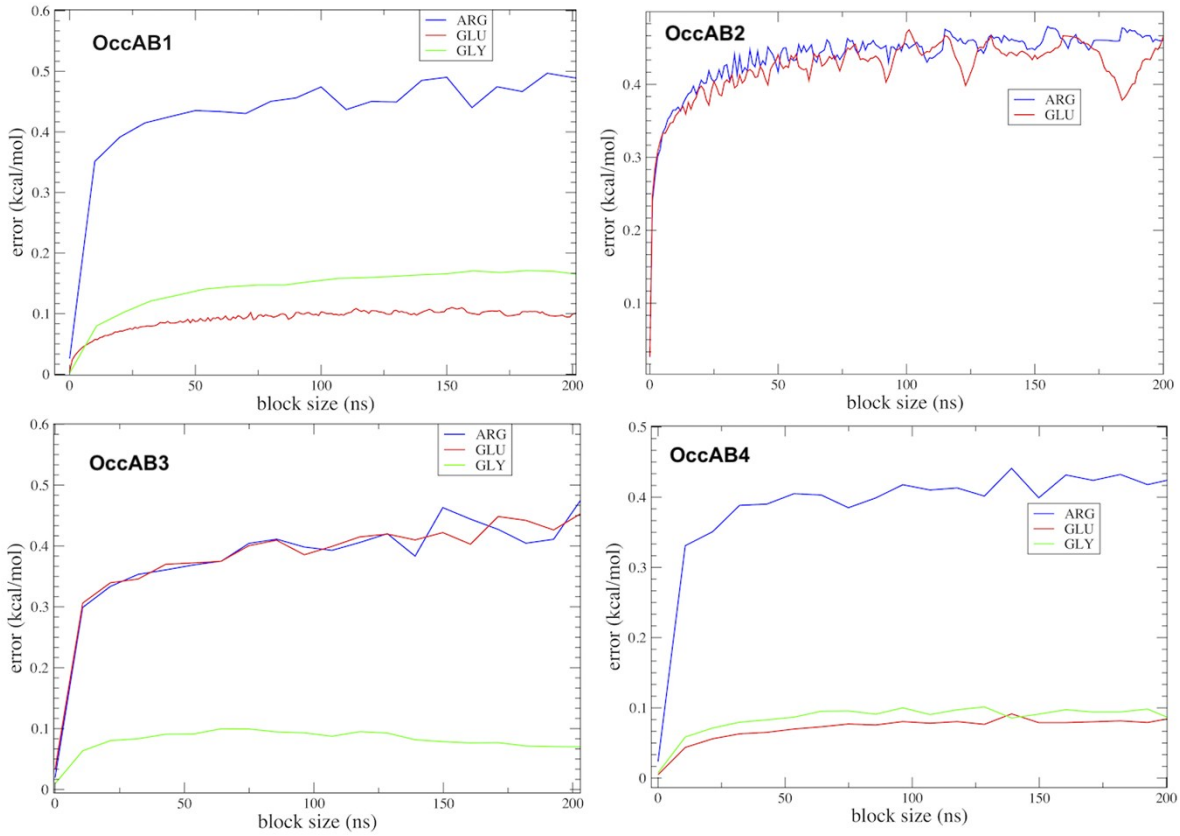

Figure S7: Statistical error for metadynamics simulations calculated with the block average technique. For each trajectory we calculated the average of F(Z) as function of simulation length, see the Methods section. We expect that at long time the average of F(Z) tends to a constant value if at convergence. In all metadynamics simulations the statistical error does not exceed 0.5 kcal/mol, or of the order of k_BT.

Table S1: Statistic values over time trajectories of the distribution of the minimum radius and its position along z-axis (Sd: Standard deviation) from Fig.S1.

Minimum radius Å				
	mean	**Sd**	**min**	**max**
OccAB1	2.03	0.39	0.28	3.21
OccAB2	1.76	0.51	0	3.15
OccAB3	1.08	0.47	0	2.64
OccAB4	1.25	0.43	0	3.19
Constriction region position along z axis Å				
OccAB1	4.73	2.67	-2	10
OccAB2	5.58	5.4	-5	14.5
OccAB3	1.47	2.02	-2	11.5
OccAB4	3.09	1.66	-0.5	11

Table S2: Length and Straightness of the channels calculated by ChExVis[20]

Crystal structure	Length Å	Straightness
OccAB1	52.563	0.883
OccAB2	54.730	0.801
OccAB3	38.257	0.888
OccAB4	44.608	0.891

Table S3: Physico-Chemical properties of OccAB porins for the macro dipole moment calculations, to be compared with OccK8, OmpF and OccK1. OccK8, 2OMPF, OccK1 (604.85D, 271.40 (trimer=540.38), 853.7 D).

	AB1	AB2	AB3	AB4
Number of atom	6288	6251	6388	6239
Total charge	-7.0	-7.0	-2.0	-10.0
Geometrical centre	0.28 -0.88 -0.31	0.15 -0.32 -0.54	-0.29 0.10 -0.27	-0.17 0.08 -0.44
Centre of masses	0.27 -0.86 -0.35	0.127 -0.303 -0.555	-0.28 0.09 -0.28	-0.17 0.06 -0.45
Centre of charges	0.15 -1.03 0.17	0.09 -0.24 -0.13	-0.50 0.14 0.09	-0.22 0.13 0.24
Macro-Dipole moment magnitude	334.94 D	640.05 D	902.75 D	1389.06 D