

Atom type	Ho/n	C	N	O	Fe	H-c
Surface_int (%)	4.18	37.68	26.48	0.00	0.78	30.89
Surface_ext (%)	15.17	33.98	23.84	3.26	0.80	22.95
Contacts (%)						
Ho/n	0.6					
C	3.6	16.3				
N	9.2	15.2	2.0			
O	0.0	1.2	0.0	0.0		
Fe	0.0	1.0	0.0	0.0	0.0	
H-c	5.3	18.0	21.8	2.0	0.5	3.1
Enrichment						
Ho/n	0.95					
C	0.50	1.27				
N	1.84	0.85	0.32			
O	0.00	1.00	0.00	/		
H-c	0.95	0.94	1.62	2.02	1.22	0.43