MANCHESTER UNIVERSITY COMPUTING MACHINE LABORATORY

Programme Sheet B

ROUTINE Self-Polarisabilities of atoms & bonds. **Date** January 1957

MJAR'½

/	K/½/					E	K/D/				
/	V	A	T	/	set acc for sequence control	/	/	U	S	:	Bring down j = 10 level to S4
E	D	S	/	C	set D for fractions.	E	V	D	T	½	ε_j → Acc.
@	V	I	/	J	call in sequence control and dec input	@	P	U	T	A	store ε_j
A	A	/	Q	O		A	/	½	A	K	c_{vj} → Dec.
:	F	S	/	P		:	/	½	A	F	Acc = c^2_{vj}
S	£	A	W	O	set B3 = 42	S	O	U	/	E	store c^2_{vj}
I	X	A	Y	O	set B5 = 21	I	P	A	/	U	L' = M, M = 0 i.e. L = c^2_{vj}
U	Q	A	T	/	set acc for sequence control	U	M	U	T	I	add in $\sum_i c^2_{vj}$
½	D	S	/	C	set D for fractions	½	M	U	T	A	re-store new $\sum_i c^2_{vj}$
D	V	I	/	J	call in sequence control and dec input	D	J	U	½	:	Bring down k = 10 level to S4
R	R	/	Q	O		R	P	U	T	½	ε_j → Acc
J	F	S	/	P		J	V	D	T	N	A = $\varepsilon_j - \varepsilon_k$
N	/	R	W	½	[/R + B3] → Acc.	N	P	A	T	A	store $\varepsilon_j - \varepsilon_k$
F	V	D	T	A	store in least line pair with vector	F	/	½	A	K	c_{vk} → D
C	/	I	S	:	write up as [/I + B5]	C	/	½	A	F	Acc = c^2_{vk}
K	E	:	Y	Q	1 off B5	K	H	A	/	E	store c^2_{vk}
T	A	:	W	Q	2 off B3	T	½	E	T	:	clear A
Z	L	/	/	T	if B3 is +ve, input again	Z	H	A	/	C	D = c^2_{vk}
L	I	/	/	L	L stop	L	O	U	/	N	A = c^2_{vk} c^2_{vj}
W	"	A	W	O	set B3 = 42	W	H	A	/	E	store c^2_{vk} c^2_{vj} temporarily.
From F@ → H	L	A	/	:	C.R.	H	H	A	/	C	D = c^2_{vk} c^2_{vj}
Y	W	A	/	:	L.F.	Y	P	A	T	/	L = $\varepsilon_j - \varepsilon_k$
P	V	/	/	:	L.S.	P	M	I	/	J	Division
Q	O	A	W	B	Jump B3	Q	Q	E	Q	O	
M O	Q	:	/	C	D = $2^{20} \times 2^{14}$	O	F	S	/	P	
/I B	O	A	/	N	mult by [B3] → $\frac{B3}{2}$ in m.s. position.	B	V	U	T	I	add in total
G	X	/	/	:	print (as letters)	G	V	U	T	A	store $\sum \frac{c^2_{vj} c_{vk}}{\varepsilon_j - \varepsilon_k}$
,,	£	/	/	:	F.S.	,,	E	:	H	Q	1 off B4, chooses next k level
M	Z	A	/	:	space	M	T	E	/	T	if B4 is positive repeat for new k
V/ X	£	/	T	:	clear acc.	X	E	:	Y	Q	1 off B5, chooses next k level
V	M	A	Y	O	set B5 = 10 to count j's	V	X	/	/	T	if B5 is positive, select next j
£	M	A	H	O	set B6 = 10 to count k's	£	T	A	P	O	set B6 for printing

MNA@½ KO½I M:/C KVDE P//T MNAR½

O A I N
/ / / I
/ / / :
£ / / :
Z A / :

MANCHESTER UNIVERSITY COMPUTING MACHINE LABORATORY

Programme Sheet B

ROUTINE *Self-Polarizabilities, Page 2* **Date** ______

K/R/

	@					
	/	A	:	/	C	D = 2
	E	M	U	/	N	$A: 2\sum c_{rj}^{2}$
	@	G	I	/	J	
	A	A	@	Q	O	Print q_r
	:	F	S	/	P	
	S	Z	A	/	:	space
	I	Z	A	/	:	space
	U	S	:	/	C	D = 4
	½	V	U	/	N	$A: 4\sum\sum \frac{c_{rj}^{2} c_{rk}^{2}}{\varepsilon_j - \varepsilon_k}$
	D	G	I	/	J	
	R	R	@	Q	O	print $\pi_{r,r}$
	J	F	S	/	P	
	N	A	:	W	G	2 SH B3
[illegible]	F	L	@	/	T	if +ve, select next r
	C	L	A	/	:	C.R
	K	W	A	/	:	L.F.
	T	W	A	/	:	LF
	Z	W	A	/	:	LF
	L	W	@	/	L	L stop
	W	O	@	/	P	call in band routine
	H	W	/	T	:	Clear A
	Y	M	U	T	A	Empty MU } for new totals
	P	V	U	T	A	Empty VU }
To H/	Q	H	@	/	P	
	O	Q	@	T	:	clear A
	B	V	U	T	A	Empty VU
	G	O	I	/	J	
	,,	/	/	E	A	call in band routine
	M	X	@	/	P	
	X	T	S	/	/	
	V					
	£					

KTJT

A					
/					
E					
@					
A					
:					
S					
I					
U					
½					
D					
R					
J					
N					
F					
C					
K					
T	I	/	/	/	for dec output
Z	/	/	Z	/	space
L	/	/	L	/	C.R.
W	/	/	W	/	L.F.
H	/	/	/	/	dump for c_{rk}^{1}, $c_{rj}^{2} c_{rk}^{1}$
Y	/	/	/	/	
P	/	/	/	/	dump for $\varepsilon_j - \varepsilon_k$
Q	/	/	/	/	
O	/	/	/	/	used in printing index
B	/	/	/	/	
G	/	½	H	A	for sequence control
,,	R	E	/	/	put 22 line pairs in /½ - RD
M	R	/	/	/	constants
X	Y	/	/	/	
V	/	R	H	A	for sequence control
£	R	E	/	/	put 22 line pairs in /R - RJ

MNAR½

Programme Sheet B

ROUTINE bond polarisabilities. **Date** _____

MJA@½

/	K / ½ /				
→ /	"	/	/	:	L.S.
E	£	£	T	:	clear A
@	W	A	/	:	read r
A	V	A	/	E	store r × 2^{34} in VA
:	E	/	/	:	print r
S	D	@	T	:	clear
I	W	A	/	:	read s
U	M	A	/	E	store s × 2^{34} in MA
½	E	/	/	:	print s
D	M	/	/	:	F.S.
R	Z	A	/	:	space
J	A	E	T	:	clear A
N	J	:	/	C	D = 2^6
F	V	A	/	N	M = 2r
C	V	A	/	E	store 2r
K	M	/	T	:	clear A
T	M	A	/	N	M = 2s
Z	M	A	/	E	store 2s
L			T	:	clear A
W	"	A	L	0	B2 = 48
H	M	A	L	Q	take off 2s
Y	E	:	/	0	if true, jump 1 instruction
P	S	/	/	P	if negative, close.
Q	W	A	L	0	B2 = 2r 44
O	A	:	L	Q	B2 = 2r−2 44−2s
B	M	A	W	0	B3 = 2s 44
G	A	:	W	Q	B3 = 2s−2 44−2s
,,	Q	A	Y	0	B5 = 10 − count j's
→ M	Q	A	H	0	B4 = 10 − count k's
→ X	/	U	S	:	bring down j = 10 level
V	V	D	T	½	A = ε_j
£	P	U	T	A	store ε_j

E	K / D /				
/	/	½	L	½	c_{jr} → A
E	O	U	T	A	store c_{jr}
@	/	½	W	½	c_{js} → A
A	Q	U	T	A	store c_{js}
:	J	U	:	:	bring down k = 10 level
S	P	U	T	½	A = ε_j
I	V	D	T	N	A = $\varepsilon_j - \varepsilon_k$
U	O	A	T	A	store $\varepsilon_j - \varepsilon_k$
½	/	½	L	½	c_{kr} → A
D	H	A	T	A	store c_{kr}
R	/	½	W	½	c_{ks} → A
J	P	A	T	A	Store c_{ks}
N	O	U	/	K	D = c_{jr}
F	P	A	/	F	M = $c_{jr} c_{ks}$
C	Q	U	/	K	D = c_{js}
K	H	A	/	F	M = $(c_{jr} c_{ks} + c_{js} c_{kr})$
T	P	A	/	E	store ( )
Z			T	:	clear A
L	P	A	/	K	D = ( )
W	P	A	/	F	M = $( )^2$
H	P	A	/	E	store $( )^2$
Y	P	A	/	C	D = $( )^2$
P	O	A	T	/	L = $\varepsilon_j - \varepsilon_k$
Q	M	I	/	J	}
O	O	E	Q	O	} Division
B	F	S	/	P	}
G	V	U	T	I	add in previous $\Sigma\Sigma \frac{(\ )^2}{\varepsilon_j - \varepsilon_k}$
,,	V	U	T	A	store new total
M	E	:	H	Q	1 off B4, chooses new k level
X	J	/	/	T	
V	E	:	Y	Q	1 off B5, chooses new j level
£	K	/	/	T	

MFA@½ KK½E "/T: MFAR½ .H.

MANCHESTER UNIVERSITY COMPUTING MACHINE LABORATORY

Programme Sheet B

ROUTINE bond polarisabilities Page 2 **Date** _____

@	K/RJ					A	KTJT				
/	A	:	/	C	D=2	/					
E	V	U	/	N	form $2\Sigma\Sigma \left(\frac{\quad}{\varepsilon_j - \varepsilon_k}\right)^2$ in L	E					
@	T	A	P	O	set B6 for printing.	@					
A	Q	I	/	J	Print Π_{xx}, Π_{xz}.	A					
:	:	∂	Q	O		:					
S	F	S	/	P		S					
I	V	U	T	A	clear VU for new summation	I					
U	L	A	/	:	C.R.	U					
½	B	/	/	:	L.F	½					
D	E	/	/	P	back to start	D					
R			/	L	stop.	R					
J	N	E	/	/	44	J					
N						N					
F						F					
C						C					
K						K					
T						T	I	/	/	/	for decoutput
Z						Z	/	/	Z	/	space
L						L	/	/	L	/	C.R.
W						W	/	/	O	/	input
H						H	/	/	/	/	
Y						Y	/	/	/	/	c_{kr}
P						P	/	/	/	/	
Q						Q	/	/	/	/	c_{ks}, ( ), ( )^2
O						O	/	/	/	/	
B						B	/	/	/	/	$\varepsilon_j - \varepsilon_k$
G						G	R	/	/	/	10
,,						,,	T	E	/	/	48
M						M	/	/	/	/	
X						X	/	/	/	/	Dump for $s \times 2^{34}$, 2s
V						V	/	/	/	/	
£						£	/	/	/	/	Dump for $v \times 2^{34}$, 2v

MFAR 1/2

MANCHESTER UNIVERSITY COMPUTING MACHINE LABORATORY

Programme Sheet B

ROUTINE boundorders

Date ________

/ @

/					
E					
@					
A					
:					
S					
I					
U					
½					
D					
R					
J					
N					
F					
C					
K					
T					
Z					
L					
W					
H					
Y					
P					
Q					
O					
B					
G					
,,					
M	/	U	S	:	bring down j = 10 level
X	/	½	@	K	$D = c_{rj} \pm$
V	/	½	A	F	$A = c_{rj} c_{sj} \pm$
£	/	A	/	E	store temporarily

MFA@½

~~KMM~~

KK½E "/T:
KD½E ME/:
KN½E F:/C

KQ½:
NELO
VALQ
NEWO
MAWQ
KJRE
NE//.

MFAR½

KM½:

E A KIDZ

/			T	:	
E	@	A	T	½	$A = \Sigma$
@	/	A	T	C	add in ...
A	@	A	T	A	store new total
:	~~[illegible]~~				one off j clear A
S	E	:	Y	Q	back to M/ ...
I	K	/	/	T	
U	@	A	/	K	$D = \sum_j c_{rj} c_{sj}$
½	A	:	/	F	$A = 2\Sigma c_{rj} c_{sj} = p_{rs}$ in (L).
D	T	A	P	O	set B6 for printing
R	Q	I	/	J	print
J	R	E	Q	O	
N	F	S	/	P	
F	/	A	T	A	clear /A @A
C	@	A	T	A	
K	L	A	/	:	CR
T	B	/	/	:	LF
Z	E	/	/	P	back to start
L					
W					
H					
Y					
P					
Q					
O					
B					
G	~~/ / / V~~				~~V / / /~~
,,	~~/ / / E~~				~~[illegible]~~
M	/	/	/	/	
X	/	/	/	/	Dump for 5×2^{34},
V	/	/	/	/	
£	/	/	/	/	Dump for 5×2^{34},

MKAR½ H

MCA/I

KHS@ ~~//~~ KA@/

TTS (single p.p.)

MANCHESTER UNIVERSITY COMPUTING MACHINE LABORATORY

Programme Sheet 2 (b)

ROUTINE *charges & polarisabilities – Directory etc.*

MJA@½
K/½/   K/DP

Note	I					u			
	R	A	½	½	**/**	R	A	/	½
	R	A	D	½	**E**	D	A	/	½
	D	A	½	½	**@**	½	A	/	½
	D	A	D	½	**A**	U	A	/	½
	½	A	D	½	**:**	I	A	/	½
	½	A	½	½	**S**	S	A	/	½
	U	A	½	½	**I**	:	A	/	½
	U	A	D	½	**U**	A	A	/	½
	I	A	D	½	**½**	@	A	/	½
	I	A	½	½	**D**	E	A	/	½
	S	A	½	½	**R**	/	A	/	½
	S	A	D	½	**J**	R	A	E	½
	:	A	D	½	**N**	D	A	E	½
	:	A	½	½	**F**	½	A	E	½
	A	A	½	½	**C**	U	A	E	½
	A	A	D	½	**K**	I	A	E	½
	@	A	D	½	**T**	S	A	E	½
	@	A	½	½	**Z**	:	A	E	½
	E	A	½	½	**L**	A	A	E	½
	E	A	D	½	**W**	@	A	E	½
	/	A	D	½	**H**	E	A	E	½
	/	A	½	½	**Y**	/	A	E	½
					P	ε_j			
					Q				
bond polarisabilities	£	£	/	/	**O**	c^2_{1j}		c_{j4}	
	F	A	@	/	**B**				
Dec output	U	@	/	/	**G**			c_{j5}	
	W	/	E	@	**"**				
Division	£	E	/	/	**M**	Σc^2_{1j}			
	Y	/	E	@	**X**				
sequence control	£	£	/	/	**V**	$\Sigma\Sigma \frac{c^2_{1j} c^2_{1k}}{\varepsilon_j - \varepsilon_k}$		$\Sigma\Sigma\left(\frac{\ }{\varepsilon_j \varepsilon_k}\right)^2$	
Decinput	L	/	@	/	**£**				

½		D
c_{22j}	**/**	
	E	
	@	
	A	
	:	
	S	
	I	
	U	
	½	c_{2j}
	D	
	R	c_{1j}
	J	
	N	
	F	
	C	
	K	
	T	
	Z	
	L	
	W	
	H	
	Y	
	P	
	Q	
	O	
	B	
	G	
	"	
	M	
	X	
	V	ε_j
	£	

MCA½½

H.

Polarisabilities etc.

Purpose : 1. to read in and store eigenvalues and eigenvectors of 22nd order secular determinant, +ve eigenvalues on left hand and -ve eigenvalues on right hand halves of tracks. Stop on L strip.

2. to calculate automatically and print atom charges and self polarisabilities and print the atom number at the same time. Stop on L strip

3. to read from tape pairs of numbers defining a bond, print them, and calculate the corresponding bond self polarisability. Stop on reading ££.

Starting sequence

MCA/I

KHS@ ££// NA@/

TTS (single prepulse)

E@ @A A: : S SI Iu u½ ½D DR RJ JN NF FC CK KT TZ ZL LW WH HY YP

PE PF WC @J A½ ££

Restart : During atom program

also in middle - set B3 by hand K.C.C.

MCA/I

KHS@ L/// NA@/

TTS

MCA/I
KHS@ W/// NA@/
TTS.

During bond program

MCA/I

KHS@ ₤₤// FA@/

TTS (single prepulse)

Tracks used

1A - RA	for vectors
JA	empty
NA	atom routine
FA	bond routine
CA	directory.
KA	bond order routine

eigenvalues + vectors in decoutput form on tape

eigenvalues /1000

vectors /10

$$q_r = 2\sum_{j=1}^{m} c_{rj}^2$$

$$\pi_{rs} = 4\sum_{j=1}^{m}\sum_{k=m+1}^{n} \frac{c_{rj}^2 c_{sk}^2}{\varepsilon_j - \varepsilon_k}$$

$$\pi_{rs,rs} = 2\sum_{j=1}^{m}\sum_{k=m+1}^{n} \frac{(c_{rj}c_{ck} + c_{sj}c_{rk})^2}{\varepsilon_j - \varepsilon_k}$$

$$p_{rs} = 2\sum_{j=1}^{m} c_{rj}c_{sj}$$