System: Benzene

Point Group: D2h

N. Electrons: 42

Multiplicity: 1

Level: MCSCF

		IRREP							
		ag	b3u	b2u	b1g	b1u	b2g	b3g	au
SCF	DOCC	6	5	4	3	1	1	1	0
	OPSH	0	0	0	0	0	0	0	0
MCSCF	DOCC	6	5	4	3	0	0	0	0
	RAS	0	0	0	0	0	0	0	0
	CAS	0	0	0	0	3	1	1	1
	AUX	0	0	0	0	0	0	0	0
MRCI	FC	2	2	1	1	0	0	0	0
	FV	0	0	0	0	0	0	0	0
	DOCC	4	3	3	2	0	0	0	0
	ACT	0	0	0	0	3	1	1	1
	AUX	0	0	0	0	0	0	0	0
	INT	4	3	3	2	3	1	1	1

State	Multiplicity	N. electrons	Symmetry
1	1	42	Ag
2	1	42	B2u
3	3	42	B3u

Number of distinct rows (DRTs):	3

	1	2	3	4	5	6	7	8
D_{2h}	a_g	b_{3u}	b_{2u}	b_{1g}	b_{1u}	b_{2g}	b_{3g}	a_u
D_2	a	b_2	b_1	b_3				
C_{2h}	a_g	b_u	a_u	b_g				
C_{2v}	a_1	b_1	b_2	a_2				
C_i	a_g	a_u						
C_s	a´	a´´						
C_2	a	b						
C_1	a							