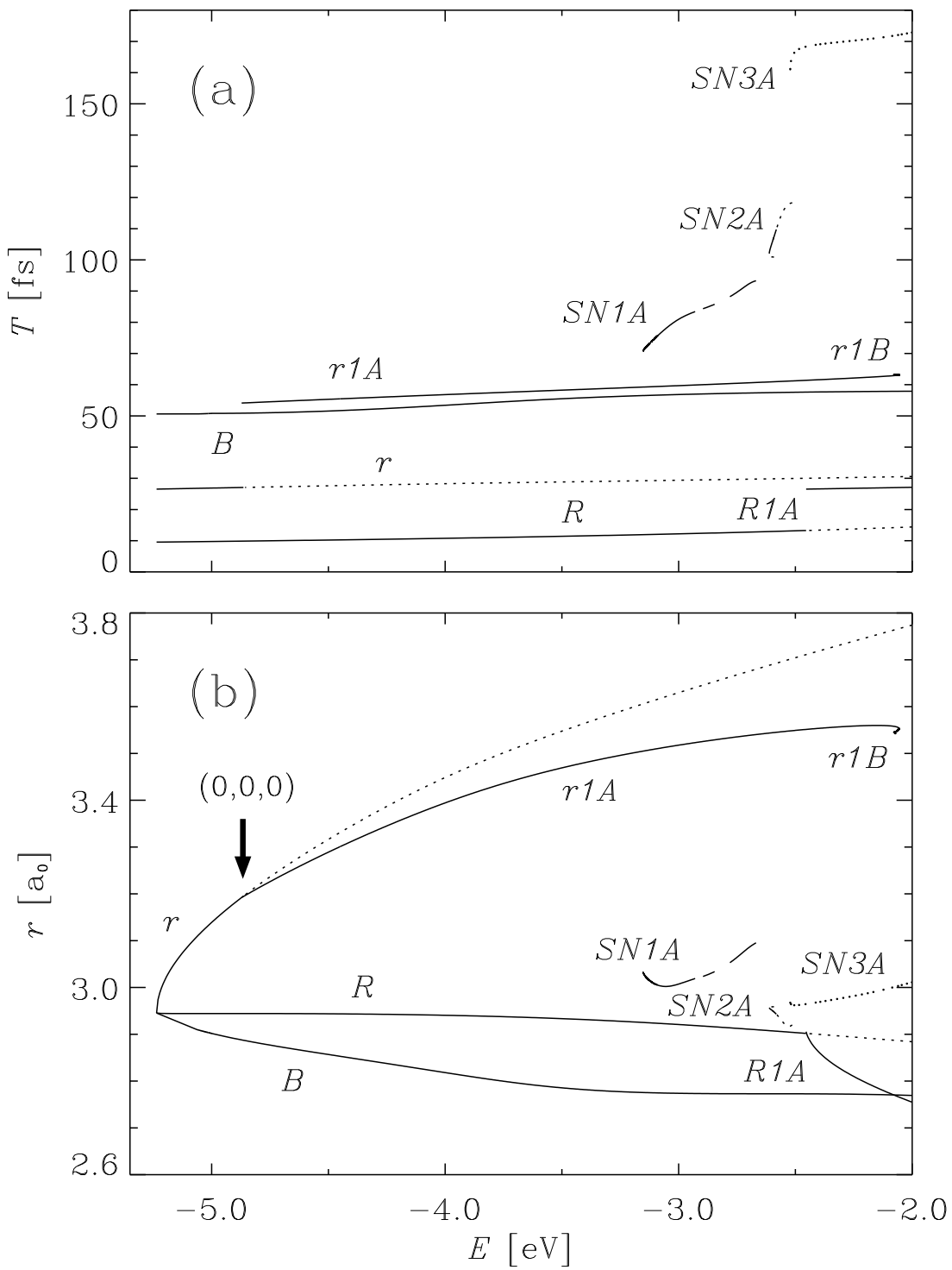
(a)
SN3A
SN2A
SN1A
r1B
r1A
B
r
R
R1A
T [fs]
150
100
50
0
(b)
(0,0,0)
r1B
r1A
r
SN1A
SN3A
R
SN2A
R1A
B
r [a₀]
3.8
3.4
3.0
2.6
−5.0
−4.0
−3.0
−2.0
E [eV]