

```

> ESTexp:=7918.1*icm2eV;
      ESTexp := 0.981719

> E1:=ReadValue("CASsto.out","EIGENVALUE",'format'="%f")*hartree2eV;
E2:=ReadValue("CASsto_triplet.out","EIGENVALUE",'format'="%f")*hartree2eV;
E2-E1;
printpsi("CASsto.out");
      E1 := -4019.300387
      E2 := -4020.339045
      -1.038659

0.780  11111ab0   2   2
0.390  11111010   1   3
-0.390 11111100   1   1
-0.193 111ab110   2  17

> E1:=ReadValue("CASc3.out","EIGENVALUE",'format'="%f")*hartree2eV;
E2:=ReadValue("CASc3_triplet.out","EIGENVALUE",'format'="%f")*hartree2eV;
E2-E1;
      E1 := -4074.149556
      E2 := -4075.104676
      -0.955120

> E1:=ReadValue("XMCQDPT2c3.out"," E(MP2)=", 'format'="%f")*hartree2eV;
E2:=ReadValue("XMCQDPT2c3_triplet.out"," E(MP2)=", 'format'="%f")*hartree2eV;
E2-E1;
      E1 := -4085.066670
      E2 := -4086.093871
      -1.027200

```

### *Excited singlet*

```

> E1:=ReadValue("CASsto_excl.out","1)          EIGENVALUE",'format'="%f")*hartree2eV;
printpsi("CASsto_excl.out",1);
E2:=ReadValue("CASsto_excl.out","2)          EIGENVALUE",'format'="%f")*hartree2eV;
printpsi("CASsto_excl.out",2);
E2-E1;
      E1 := -4019.300387

0.956  11111ab0   2   2
-0.237 111ab110   2  17
      E2 := -4018.744186

0.668  11111100   1   1
0.668  11111010   1   3
-0.191 11110110   1  10
-0.191 11101110   1  26
      0.556201

```