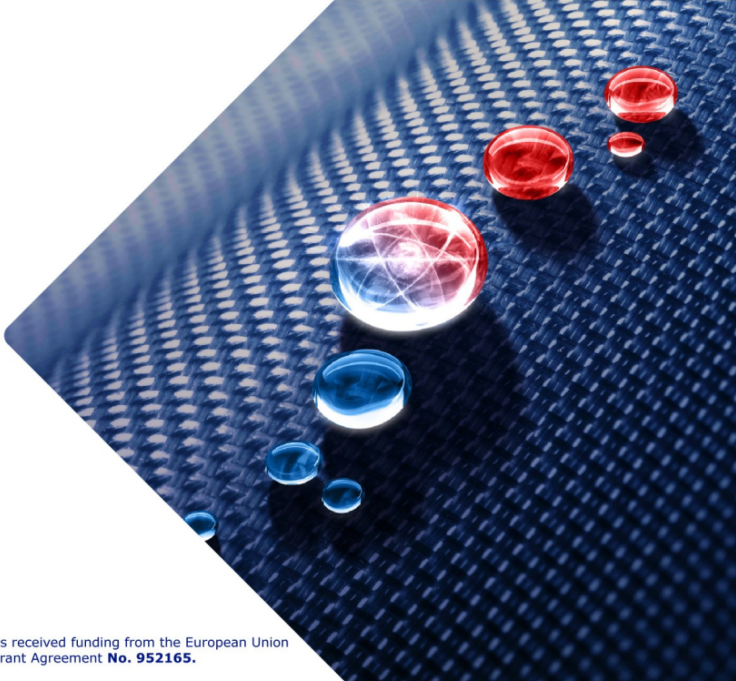


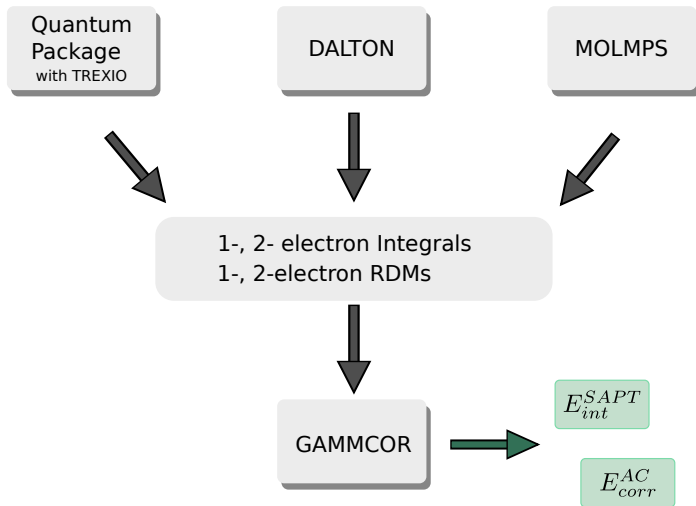
GammCor Code Tutorial

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- 1 Install GammCor code
- 2 Run tests
- 3 Do exercises and discuss the results
 - SAPT (Quantum Package, Dalton)
 - AC (MOLMPS)

EXERCISES



```
git clone https://github.com/michalhapka/trex_workshop2023.git  
or at Dragon  
cp /home/michalhapka/trex_workshop2023
```

GET THE CODE



```
git clone https://github.com/pernalk/GAMMCOR.git  
cd GAMMCOR  
git checkout workshop2023
```

INSTALLATION
GUIDE



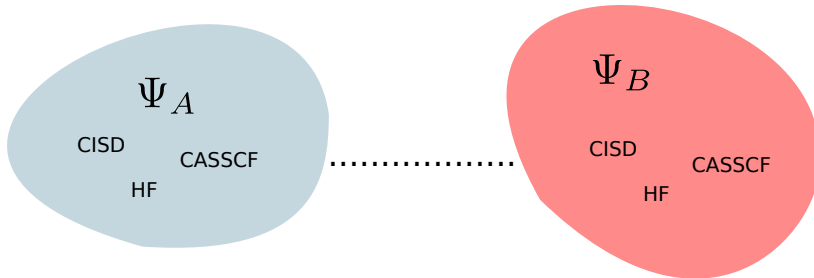
<https://qchem.gitlab.io/gammcor-manual/>

INSTALLATION
AT DRAGON

```
env FC=gfortran CXX=g++ CC=gcc cmake -S. -Bbuild -Cconfig_gnu  
cd build  
make -j 4  
ctest -V
```

<https://qchem.gitlab.io/gammmcor-manual>

$$E_{int}^{SAPT} = E_{elst}^{(1)} + E_{exch}^{(1)} + E_{ind}^{(2)} + E_{exch-ind}^{(2)} + E_{disp}^{(2)} + E_{exch-disp}^{(1)}$$



1 step

Quantum Package



$\Psi_A \Psi_B$

two HDF5 files (one for each monomer)

2 step

$\Psi_A \Psi_B$

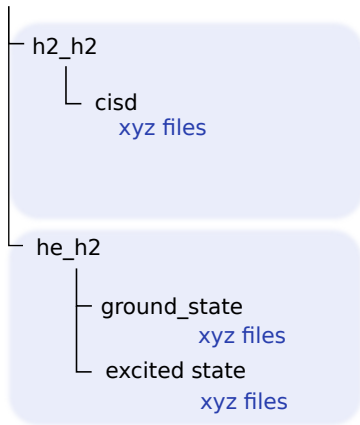


GammCor



E_{int}^{SAPT}

/trex_workshop2023/SAPT



EXERCISE 1

EXERCISE 2

Table 1: Results of SAPT calculations for H₂-H₂ dimer. Energy units are microhartree.

	$E_{\text{elst}}^{(1)}$	$E_{\text{exch}}^{(1)}$	$E_{\text{ind}}^{(2)}$	$E_{\text{exch-ind}}^{(2)}$	$E_{\text{disp}}^{(2)}$	$E_{\text{exch-disp}}^{(2)}$	$E_{\text{int}}^{\text{SAPT}}$
<i>R</i> = 1.44 a.u.							
HF	−62.29	89.96	−5.169	1.706	−154.2	6.911	−123.0
CISD	−52.70	88.98	−4.591	2.014	−151.5	6.111	−111.6
CAS(2,2)	−47.82	81.28	−4.030	1.637	−143.6	5.693	−106.8
CAS(2,8)	−52.61	88.43	−4.565	1.980	−151.7	6.094	−112.4
<i>R</i> = 7.20 a.u.							
HF	−185.4	445.0	−39.72	26.29	−320.6	33.55	−40.89
CISD	−47.28	210.0	−8.408	6.044	−165.6	10.45	5.193
CAS(2,2)	−44.87	201.1	−7.994	5.465	−161.1	10.15	2.748
CAS(2,8)	−47.17	209.4	−8.388	5.992	−165.9	10.43	4.335

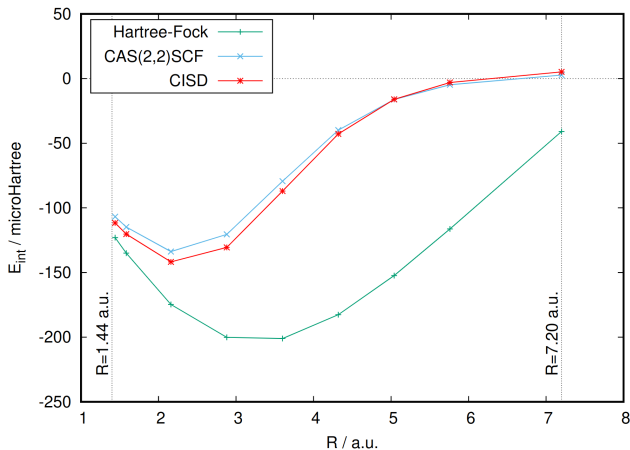


Figure 1: SAPT interaction energy curves for H_2-H_2 . R denotes the covalent bond length in one the monomers.

Table 2: Results of SAPT(CISD)/aug-cc-pVDZ calculations for He-H₂ and He-H₂* dimers. Energy unit is millihartree.

	$E_{\text{elst}}^{(1)}$	$E_{\text{exch}}^{(1)}$	$E_{\text{ind}}^{(2)}$	$E_{\text{exch-ind}}^{(2)}$	$E_{\text{disp}}^{(2)}$	$E_{\text{exch-disp}}^{(2)}$	$E_{\text{int}}^{\text{SAPT}}$
ground state							
$R = 4.0$ a.u.	-1.103	5.740	-0.375	0.395	-0.956	0.114	3.816
$R = 6.6$ a.u.	-0.004	0.029	-0.001	0.001	-0.050	0.001	-0.024
excited state							
$R = 4.0$ a.u.	-0.558	0.776	-1.080	0.099	-1.076	-0.003	-1.843
$R = 6.6$ a.u.	-0.026	-0.060	-0.036	-0.003	-0.204	-0.005	-0.334

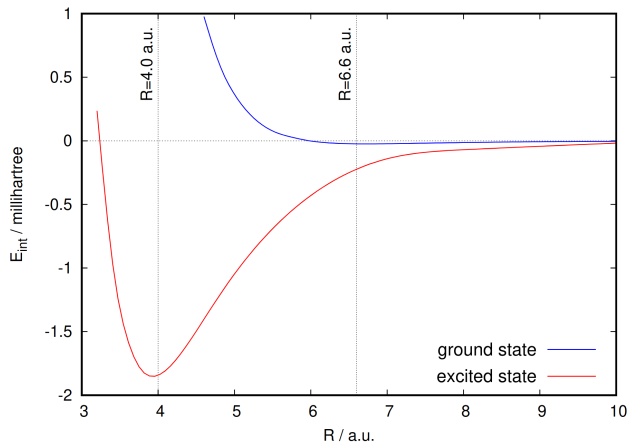


Figure 2: He-H₂ in T-shaped geometry. R denotes the distance between the He atom and COM of the H₂ molecule.

