

References where the mathematical symbols are defined:

The fragment molecular orbital method: practical applications to large molecular systems,  
 D. G. Fedorov, K. Kitaura, Eds., CRC Press (2009), in press, chapter 1, or  
 D. G. Fedorov, K. Kitaura, J. Phys. Chem. A 111 (2007) 6904-6914.

One-body FMO properties.

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	Ecorr	$E'_I$	Euncorr	DX	DY	DZ
1(frg00001,L1)	-76.191947612		-76.007836505	-1.77830	0.65969	1.48864
2(frg00002,L1)	-76.191961348		-76.007891466	1.28642	1.11442	-1.69243
3(frg00003,L1)	-76.191905112		-76.007851357	0.38270	-2.11713	-1.05827

Total energy of the molecule: Ecorr (1)= -228.575814072

Total energy of the molecule: Euncorr(1)= -228.023579328

Total energy of the molecule: Edelta (1)= -0.552234744

Dipole moment D(xyz),DA(1)= -0.1091791 -0.3430276 -1.2620705 1.3124061

Two-body FMO properties.

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DL: D=C dynamically correlated (MP2,C1), D=N not dynamically correlated (RHF,DFT). D=S separated dimer: semiclassical interaction (ES), D=M MCSCF. L stands for layer, Z is the monomer charge product, R is the interfragment distance relative to van-der-Waals radii (-1.00 is printed if distances are not computed). dDIJ\*VIJ is the density polarisation contribution. Q(I->J) is the charge transfer amount, printed as zero if not available. Positive values correspond to I in IJ having extra negative charge.

I	J	DL	Z	R	Q(I->J)	Ecorr	Euncorr	EIJ-EI-EJ,corr/uncorr	dDIJ*VIJ,unc	tot,corr	
				$R_{IJ}$	$\Delta Q_{IJ}$			$\Delta E'_{IJ}$	$\Delta E'^{RHF}_{IJ}$	$Tr(\Delta \mathbf{D}^{IJ} \mathbf{V}^{IJ})$	$\Delta E^{int}_{IJ}$
2	1	C1	0	0.76	0.0282	-152.397129212	-152.026399729	-0.01322025	-0.01067176	-0.00072479	-8.751
3	1	C1	0	0.76	-0.0270	-152.397000640	-152.026329054	-0.01314792	-0.01064119	-0.00069990	-8.690
3	2	C1	0	0.77	0.0251	-152.395924095	-152.025383234	-0.01205763	-0.00964041	-0.00065907	-7.980

Total energy of the molecule: Ecorr (2)= -228.616323630  $E^{FMO2-MP2}$

Total energy of the molecule: Euncorr(2)= -228.056616444  $E^{FMO2-RHF}$

Total energy of the molecule: Edelta (2)= -0.559707186

Dipole moment D(xyz),DA(2)= -0.1306606 -0.3288742 -1.2622254 1.3108941  $\mathbf{D}^{FMO2-RHF}$

Charge transfer for each fragment:

IFG QFG DeltaQ and its contributions from JFG, Q(JFG->IFG).

1	0	0.0012 =	2->	0.0282	3->	-0.0270
2	0	-0.0031 =	1->	-0.0282	3->	0.0251

3 0 0.0019 = 1-> 0.0270 2-> -0.0251

Total absolute monomer transf. charge = 0.006128  $\Delta\bar{Q}$   
 Total amount of absolute transf. charge = 0.080338  $\Delta Q$

Three-body FMO properties.

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I	J	K	DL	RMIN	RMAX	Ecorr	deltaE <sub>IJK,corr/uncorr</sub>	dE <sub>IJK</sub> <sup>RHF</sup>	dE <sub>IJK</sub> <sup>D</sup>	tot
							$\Delta E'_{IJK}$	$\Delta E'_{IJK}$	$\Delta E^D_{IJK}$	$\Delta E^{int}_{IJK}$
3	2	1	C1	0.76	0.76	-228.615831053	-0.00159118	-0.00173101	0.00208375	0.309

Total energy of the molecule: Ecorr (3)= -228.615831053  $E^{FMO3-MP2}$

Total energy of the molecule: Euncorr(3)= -228.056263700  $E^{FMO3-RHF}$

Total energy of the molecule: Edelta (3)= -0.559567353

Dipole moment D(xyz),DA(3)= -0.1292292 -0.3294254 -1.2622198 1.3108852  $D^{FMO3-RHF}$

n-body Mulliken atomic charges Q(n)

IAT	IFG	Z	Q(1)	Q(2)	Q(3)
1	1	8.0	-0.959373	-0.961737	-0.962384
2	1	1.0	0.499521	0.508812	0.509189
3	1	1.0	0.459853	0.454091	0.454418
4	2	8.0	-0.957268	-0.962262	-0.963056
5	2	1.0	0.499446	0.507613	0.508127
6	2	1.0	0.457823	0.451585	0.451920
7	3	8.0	-0.957996	-0.958814	-0.959831
8	3	1.0	0.499980	0.508432	0.508997
9	3	1.0	0.458016	0.452280	0.452620