

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. Comp. Chem. 28 (2007) 222-237.

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,CI), 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)	ElJ-El-EJ	dDIJ*VIJ	total	Ees	Eex	Ect+mix	Edisp
				R_{IJ}	ΔQ_{IJ}	$\Delta E'_{IJ}$	$Tr(\Delta \mathbf{D}^{IJ} \mathbf{V}^{IJ})$	ΔE_{IJ}^{int}	ΔE_{IJ}^{ES}	ΔE_{IJ}^{EX}	ΔE_{IJ}^{CT+mix}	ΔE_{IJ}^{DI}
2	1	C1	0	0.76	0.0282	-8.296	-0.455	-8.751	-9.826	5.191	-2.516	-1.599
3	1	C1	0	0.76	-0.0270	-8.250	-0.439	-8.690	-9.860	5.204	-2.460	-1.573
3	2	C1	0	0.77	0.0251	-7.566	-0.414	-7.980	-8.903	4.734	-2.293	-1.517

Total energy of the molecule: Ecorr (2)= -228.616323629 $E^{FMO2-MP2}$

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

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

Interaction energy relative to PL state:
 Eint = EES + EEX + E(CT+mix) + EDI
 Eint = E(FMO2) - E(FMO1) - E(BDA)
 Eint - interaction relative to PL state using PL state densities.

Electrostatic (PL state, incl. EPLs)	EES	-28.590	$\sum_{I>J} \Delta E_{IJ}^{ES}$
Exchange (PL state)	EEX	15.128	$\sum_{I>J} \Delta E_{IJ}^{EX}$
Charge transfer (PL state)	E(CT+mix)	-7.270	$\sum_{I>J} \Delta E_{IJ}^{CT+mix}$
Dispersion (PL state)	EDI	-4.689	$\sum_{I>J} \Delta E_{IJ}^{DI}$
Total interaction (PL state)	Eint	-25.420	$\sum_{I>J} \Delta E_{IJ}^{int}$

Dipole moment D(xyz),DA(2)= -0.1306606 -0.3288742 -1.2622253 1.3108941 **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 **$\Delta \overline{Q}$**
 Total amount of absolute transf. charge = 0.080338 **ΔQ**

n-body Mulliken atomic charges Q(n)

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