

References where the mathematical symbols are defined:

(basic) D. G. Fedorov, K. Kitaura, J. Phys. Chem. A 111 (2007) 6904-6914,

(PCM specific) D. G. Fedorov, K. Kitaura, J. Phys. Chem. A 116 (2012) 704-719.

Note that starting 2012, PCM properties are printed in terms of internal solute energies

$E_X'' = E_X' - \Delta E_X^{es}$, where ΔE_X^{es} is the solute-solvent electrostatic interaction for $X = I$ or IJ .

also, FIXPVA cav+disp+rep energies very slightly readjusted in 2011 (new tessellation).

One-body FMO properties.

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	E"corr	E_I''	E"uncorr	DX	DY	DZ
1(frg00001,L1)	-76.190713244		-76.006738877	-1.78955	0.75817	1.64693
2(frg00002,L1)	-76.190700157		-76.006773118	1.36181	1.05519	-1.87377
3(frg00003,L1)	-76.190636992		-76.006721605	0.30259	-2.20909	-1.22534

Total energy of the molecule: Ecorr (1)= -228.572050393 $\sum_I E_I''$

Total energy of the molecule: Euncorr(1)= -228.020233599

Total energy of the molecule: Edelta (1)= -0.551816794

Dipole moment D(xyz),DA(1)= -0.1251576 -0.3957289 -1.4521729 1.5103218

Monomer surface areas (in A**2), charges (a.u.) and solute-solvent energies (kcal/mol).

I	surf_cav	disp/rep	surf_es	cover,%	q_cav	eps_eff	Ges	Gcav	Gdisp	Grep	Gsol
	σ_I^{cav}	$\sigma_I^{disp} = \sigma_I^{rep}$	σ_I^{es}	S_I	q_I	ϵ_I	$\Delta E_{I(I)}^{es}$	ΔE_I^{cav}	$\Delta E_{I(I)}^{disp}$	$\Delta E_{I(I)}^{rep}$	ΔE_I^{solv}
1 (frg00001)	27.5	64.1	32.7	33.3	0.0000	0.000	-6.116	3.526	-3.266	1.079	-4.777
2 (frg00002)	27.5	64.0	32.8	33.4	0.0061	0.000	-6.045	3.532	-3.266	1.076	-4.704
3 (frg00003)	27.5	63.4	32.7	33.3	-0.0061	0.000	-6.129	3.527	-3.256	1.078	-4.780

Total Gsol(1)= -14.261 kcal/mol.

Shift to convert internal to QM energy, Des(1)= -15.369 kcal/mol.

Total energy of the molecule: Ecor_es(1)= -228.596542184 $\sum_I E_I''$ (= $\sum_I E_I'' + Des(1)$), as printed prior to 2012

Total energy of the molecule: Ecor+so(1)= -228.594776089 $\sum_I (E_I'' + \Delta E_I^{solv})$

Pair ES surface (A**2) and solute-solvent pair interactions (kcal/mol):

I	J	surf_es	cover,%	dGes2	dGes3	dGdisp	dGrep	dGsol
		σ_{IJ}^{es}	S_{IJ}	ΔE_{IJ}^{es2}	ΔE_{IJ}^{es3}	ΔE_{IJ}^{disp}	ΔE_{IJ}^{rep}	ΔE_{IJ}^{solv}
2	1	65.6	66.7	1.159	0.015	-0.698	0.032	0.508
3	1	65.4	66.6	1.193	0.005	-0.690	0.031	0.540
3	2	65.6	66.7	0.569	0.011	-0.700	0.038	-0.083

Total Gsol(2)= -13.296 kcal/mol.

Shift to convert internal to QM energy, Des(2)= -15.338 kcal/mol.

Two-body FMO properties.

I	J	DL	Z	R	Q(I->J)	E"corr	E"uncorr	E"IJ-E"I-E"J,corr/uncorr	dDIJ*VIJ,unc	Gsol	tot,corr	
				R_{IJ}	ΔQ_{IJ}	$\Delta E_{IJ}''$	$\Delta E_{IJ}''^{RHF}$		$Tr(\Delta \mathbf{D}^{IJ} \mathbf{V}^{IJ})$	ΔE_{IJ}^{solv}	ΔE_{IJ}^{int}	
2	1	C1	0	0.76	0.0285	-152.395159486	-152.024694305	-0.01374608	-0.01118231	-0.00074728	0.508	-8.587
3	1	C1	0	0.76	-0.0276	-152.395087295	-152.024666590	-0.01373706	-0.01120611	-0.00072459	0.540	-8.535
3	2	C1	0	0.77	0.0255	-152.393671340	-152.023394087	-0.01233419	-0.00989937	-0.00068220	-0.083	-8.251

Total energy of the molecule: Ecorr (2)=-228.614021800 $\sum_I E_I'' + \sum_{I>J} (E_{IJ}'' - E_I'' - E_J'' + Tr(\Delta \mathbf{D}^{IJ} \mathbf{V}^{IJ}))$

Total energy of the molecule: Ecor_es(2)=-228.638464541 $\sum_I E_I' + \sum_{I>J} (E_{IJ}' - E_I' - E_J' + Tr(\Delta \mathbf{D}^{IJ} \mathbf{V}^{IJ}))$ as earlier

Total energy of the molecule: Ecor+so(2)= -228.635209840 $\sum_I (E_I'' + \Delta E_{IJ}^{solv}) + \sum_{I>J} (E_{IJ}'' - E_I'' - E_J'' + Tr(\Delta \mathbf{D}^{IJ} \mathbf{V}^{IJ})) + \Delta E_{IJ}^{solv}$

Total energy of the molecule: Euncorr(2)= -228.054675455

Total energy of the molecule: Edelta (2)= -0.559346345

Dipole moment D(xyz),DA(2)= -0.1472843 -0.3832508 -1.4534028 1.5102826

Charge transfer for each fragment:

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

1	0	0.0009 =	2->	0.0285	3->	-0.0276
2	0	-0.0030 =	1->	-0.0285	3->	0.0255
3	0	0.0021 =	1->	0.0276	2->	-0.0255

Total absolute monomer transf. charge = 0.006060 $\Delta \bar{Q}$

Total amount of absolute transf. charge = 0.081689 ΔQ

ELECTROSTATIC INTERACTION	=	-15.338	KCAL/MOL	ΔG_{es}
PIEROTTI CAVITATION ENERGY	=	10.584	KCAL/MOL	ΔG_{cav}
DISPERSION FREE ENERGY	=	-11.875	KCAL/MOL	ΔG_{disp}
REPULSION FREE ENERGY	=	3.333	KCAL/MOL	ΔG_{rep}
TOTAL INTERACTION	=	-13.296	KCAL/MOL	$\Delta G_{es} + \Delta G_{cav} + \Delta G_{disp} + \Delta G_{rep}$

The first energy printed below is the best in FMO/PCM.

Free corr energy in solvent=	-228.635209840	$G_{FMO2-MP2/PCM}$	This is the final energy of FMO-MP2/PCM.
Internal corr energy in solvent=	-228.614021800	$G'_{FMO2-MP2/PCM}$	$= G_{FMO2-MP2/PCM} - \sum_I \Delta E_I^{solv} - \sum_{I>J} \Delta E_{IJ}^{solv}$
Free uncorr energy in solvent=	-228.075863495	$G_{FMO2-RHF/PCM}$	
Internal uncorr energy in solvent=	-228.054675455	$G'_{FMO2-RHF/PCM}$	

Solvent q and n-body Mulliken solute atomic charges Q(n)

IAT	IFG	Z	surface	cover,%	q(ASC)	Q(1)	Q(2)
			σ_{α}^{es}	s_{α}^{es}	q_{α}	Q_{α}^{FMO1}	Q_{α}^{FMO2}
1	1	8.0	32.73	71.5	0.000015	-0.999729	-1.002453
2	1	1.0	0.00	0.0	0.000000	0.500836	0.509644
3	1	1.0	0.00	0.0	0.000000	0.498893	0.493733
4	2	8.0	32.84	71.8	0.006094	-0.998937	-1.004276
5	2	1.0	0.00	0.0	0.000000	0.499763	0.507704
6	2	1.0	0.00	0.0	0.000000	0.499174	0.493542
7	3	8.0	32.71	71.5	-0.006109	-0.999854	-1.000967
8	3	1.0	0.00	0.0	0.000000	0.500201	0.508502
9	3	1.0	0.00	0.0	0.000000	0.499653	0.494571