

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*

$E_X'' = E_X' - \Delta E_X^{\text{es}}$ , where  $\Delta E_X^{\text{es}}$  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 $\sigma_I^{\text{cav}}$	disp/rep $\sigma_I^{\text{disp}} = \sigma_I^{\text{rep}}$	surf_es $\sigma_I^{\text{es}}$	cover,% $s_I$	q_cav $q_I$	eps_eff $\epsilon_I$	Ges $\Delta E_{I(I)}^{\text{es}}$	Gcav $\Delta E_I^{\text{cav}}$	Gdisp $\Delta E_{I(I)}^{\text{disp}}$	Grep $\Delta E_{I(I)}^{\text{rep}}$	Gsol $\Delta E_I^{\text{solv}}$
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  $\sum_I E_I''$  (=  $\sum_I E_I'' + \text{Des}(1)$ ), as printed prior to 2012

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

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

I	J	surf_es $\sigma_{IJ}^{\text{es}}$	cover,% $s_{IJ}$	dGes2 $\Delta E_{IJ}^{\text{es}2}$	dGes3 $\Delta E_{IJ}^{\text{es}3}$	dGdisp $\Delta E_{IJ}^{\text{disp}}$	dGrep $\Delta E_{IJ}^{\text{rep}}$	dGsol $\Delta E_{IJ}^{\text{solv}}$
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.

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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
				$R_{IJ}$	$\Delta Q_{IJ}$	$\Delta E''_{IJ}$	$\Delta E''_{IJ}^{\text{RHF}}$			$Tr(\Delta \mathbf{D}^{IJ} \mathbf{V}^{IJ})$	$\Delta E_{IJ}^{\text{solv}}$	$\Delta E_{IJ}^{\text{int}}$
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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  $\sum_I (E''_I + \Delta E_I^{solv}) + \sum_{I>J} (E''_{IJ} - E''_I - E''_J + Tr(\Delta \mathbf{D}^{IJ} \mathbf{V}^{IJ})) + \Delta E_{IJ}^{solv}$

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).		
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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  $\Delta Q$

ELECTROSTATIC INTERACTION	=	-15.338 KCAL/MOL	$\Delta G_{es}$
PIEROTTI CAVITATION ENERGY	=	10.584 KCAL/MOL	$\Delta G_{cav}$
DISPERSION FREE ENERGY	=	-11.875 KCAL/MOL	$\Delta G_{disp}$
REPULSION FREE ENERGY	=	3.333 KCAL/MOL	$\Delta G_{rep}$
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)
			$\sigma_{\alpha}^{es}$	$s_{\alpha}^{es}$	$q_{\alpha}$	$Q_{\alpha}^{FMO1}$	$Q_{\alpha}^{FMO2}$
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