

Relative Energies (kcal/mol), $E_{\text{trans}} - E_{\text{cis}}$, of oligomers of size $n = 1-6$. MPWB1K and B3LYP relative energies calculated using geometries obtained using the respective functional and the 6-31G(d) basis set. MPWB1K* and B3LYP* refers to the relative energies after removal of the estimated π - π interactions that occur for $n > 4$.

n	(2FSO) _n			
	MPWB1K	B3LYP	MPWB1K*	B3LYP*
1	2.24	2.17	2.24	2.17
2	6.71	6.69	6.71	6.69
3	11.31	11.21	11.31	11.21
4	16.17	15.65	16.17	15.65
5	23.54	20.59	21.23	20.46
6	34.35	25.16	25.86	24.80

n	(2FOS) _n			
	MPWB1K	B3LYP	MPWB1K*	B3LYP*
1	0.21	0.21	0.21	0.21
2	0.61	0.69	0.61	0.69
3	1.20	1.14	1.20	1.14
4	1.55	1.51	1.55	1.51
5	5.44	2.37	3.37	2.31
6	10.20	3.01	2.40	2.83

n	(FSFO) _n			
	MPWB1K	B3LYP	MPWB1K*	B3LYP*
1	2.32	2.28	2.32	2.28
2	4.40	4.62	4.40	4.62
3	6.81	6.92	6.81	6.92
4	9.36	9.14	9.36	9.14
5	14.78	11.80	12.94	11.99
6	20.70	14.09	14.66	14.24

n	(FOFS) _n			
	MPWB1K	B3LYP	MPWB1K*	B3LYP*
1	0.15	0.20	0.15	0.20
2	2.47	2.52	2.47	2.52
3	4.63	4.84	4.63	4.84
4	6.96	7.04	6.96	7.04
5	12.31	9.71	10.64	9.92
6	18.51	12.01	11.46	11.99