

# MPWB1K/6-31G(d) optimized geometries

Total energies (Hartrees) for oligomers of size n = 1-6

2FO-S	1	2	3	4	5	6
cis	-980.0968964	-1959.025273	-2937.954072	-3916.882531	-4895.816593	-5874.752013
trans	-980.0965596	-1959.024299	-2937.952157	-3916.88006	-4895.807932	-5874.735763
2FS-O	1	2	3	4	5	6
cis	-980.1052484	-1959.041871	-2937.978519	-3916.91571	-4895.856922	-5874.803502
trans	-980.101681	-1959.031174	-2937.960501	-3916.889934	-4895.819416	-5874.748769
FO-FS	1	2	3	4	5	6
cis	-980.1060055	-1959.044304	-2937.982467	-3916.921161	-4895.864693	-5874.809482
trans	-980.1023731	-1959.036941	-2937.971746	-3916.906713	-4895.841755	-5874.779986
FS-FO	1	2	3	4	5	6
cis	-980.1060661	-1959.043949	-2937.982601	-3916.921625	-4895.865315	-5874.810652
trans	-980.1057723	-1959.040373	-2937.975091	-3916.910072	-4895.845068	-5874.777672

# B3LYP/6-31G(d) optimized geometries

zero-point energies (Hartrees) for oligomers of size n = 1-5

2FO-S	1	2	3	4	5
cis	0.101629	0.183126	0.264549	0.346017	0.427567
trans	0.101608	0.183084	0.264492	0.345863	
2FS-O	1	2	3	4	5
cis	0.10159	0.183087	0.264532	0.345952	0.427525
trans	0.101441	0.182728	0.263983	0.345146	
FO-FS	1	2	3	4	5
cis	0.10152	0.183017	0.264446	0.345801	0.427302
trans	0.101449	0.182827	0.264143	0.345449	0.426725
FS-FO	1	2	3	4	5
cis	0.101576	0.183051	0.264422	0.345839	0.427303
trans	0.101449	0.182827	0.264143	0.345449	

B3LYP/6-31G(d) optimized geometries  
Total energies (Hartrees) for oligomers of size n = 1-6

2FO-S	1	2	3	4	5	6
cis	-980.2827119	-1959.384239	-2938.486007	-3917.587598	-4896.689964	-5875.791998
trans	-980.2823714	-1959.383137	-2938.484188	-3917.585199	-4896.686193	-5875.787199
2FS-O	1	2	3	4	5	6
cis	-980.29054	-1959.399614	-2938.508941	-3917.617996	-4896.727943	-5875.837229
trans	-980.2870859	-1959.388957	-2938.491071	-3917.59306	-4896.69513	-5875.797137
FO-FS	1	2	3	4	5	6
cis	-980.2913154	-1959.401892	-2938.512918	-3917.623761	-4896.73546	-5875.846587
trans	-980.2909961	-1959.39787	-2938.505203	-3917.61255	-4896.71999	-5875.827455
FS-FO	1	2	3	4	5	6
cis	-980.2912453	-1959.401786	-2938.512736	-3917.62364	-4896.735323	-5875.846434
trans	-980.2876086	-1959.394418	-2938.501712	-3917.609082	-4896.716518	-5875.823978