

TABLE 1. Tight-Binding Parameters ε and t for Each Subunit (in eV)^a

subunit	site number	represent	ε	t, t_n	ε (lit.)	t (lit.)
S_1	1	thiol	-4.2	6, 6		
S_2	2-5	methylenes	-14	6	-13.9 ^a	6 ^b , 7.7 ^c
S_3	6-7	amide	-1.3, -1.8	0.5, 1.8		1.8 ^d
S_4	8-9	methylene	-14	6	-13.9 ^a	6 ^b , 7.7 ^c
S_5	10-13	saturated tail group R	-14	6	-13.9 ^a	6 ^b , 7.7 ^c
S_5	10-13	conjugated tail group R	3.5	4, 1	5.9 ^e	4 ^e , 3.6 ^a
S_6	14-N	Ga_2O_3	-4.5 to -11.5			

^a Subunits of the same kind are coupled by t . The coupling of a subunit to a saturated C neighbour is t_n , provided the subunit itself is not a saturated C (including methylene). Literature parameters are presented from (a) Benkő *et al.*³¹ (b) Xu *et al.*³² (c) Wang *et al.*³³ (d) Murrell³⁴ and (e) Salem³⁵ t param-

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