

Data from the paper:

Koch et al. (J. Phys. Chem. C 2017, 121, 30, 16066–16078;

<https://pubs.acs.org/doi/10.1021/acs.jpcc.7b02812>).

	DG / eV	I / eV	H_ab
T(BL1)-T(CS1)	-0.3258	0.8442	0.09035
	-0.3258	0.7505	0.09035
T(BL1)-T(CS2)	-0.2943	0.8152	0.11548
	-0.2943	0.7453	0.11548
T(BL2)-T(CS3)	-0.3066	0.8398	0.12389
	-0.3066	0.7518	0.12389
T(BL2)-T(CS5)	-0.2742	0.8125	0.05245
	-0.2742	0.7363	0.05245
T(BL1)-T(CR1)	-0.4644	2.1770	-
	-0.4644	1.7247	-
T(BL1)-T(CR2)	-0.3815	2.2706	-
	-0.3815	1.6669	-