Table 2. Comparison of covalent bond rupture energies, distances, and forces for all covalent single bonds present in the experiment as well as for the Au-S bond.

	Theoretical			Experimental		Theoretical (this work)			
Bond	C-O	C-N	C-S	C-C	Au-S[†] Au-Au	C-S (TTF)	C-S (TTF^{2+})	C-C (TTF^{2+})	Deslipping
Bond energy, kcal•mol^{-1}	85-91	69-75	61	83-85	44	55	55	55	46
Rupture distance, Å	1.43	1.38	1.82	1.54	2.4	1.77	1.68	1.47	8.61
Rupture force, nN	4.3	4.1	3.7[‡]	2-13	1.4	>1.0[‡]	>1.0[‡]	>1.0[‡]	0.074[§]

[†]Room temperature experiments measuring the rupture of alkane-thiols on Au surfaces and of gold nanowires have both given rupture forces of 1.4-1.5 ± 0.3 nN. It is unclear whether the Au-S bond is rupturing in experiment involving alkane-thiols on Au surfaces or whether Au-Au rupture is being observed.

[‡]The experimental loading rate for rupture of the C-S bond was not reported. Rupture values for the C-S bonds in TTF as well as C-S and C-C bonds in TTF^{2+} are expected to require >1 nN given the similarities in bond energies and distances to experimental data for the C-S bond and the fact that all published accounts of covalent bond rupture indicate rupture forces much greater than 1 nN.

[§]The value of 0.074 nN is taken from the experimental AFM measurements presented in this work, which has been attributed to deslipping based on experimental and theoretical studies.