

Table S1. Raman Frequencies and Assignments for n-Alkanethiols ($C_nH_{2n+1}SH$) at MP Ag

C_3SH	C_4SH	C_5SH	C_8SH	C_9SH	$C_{12}SH$	$C_{18}SH$	Mode
625vw	626w	626m	659vw	630vw		623vw	$\nu(C-S)_G$
704s	703s	698vs	702s	706s	706vs	705s	$\nu(C-S)_T$ *
	741sh	742sh					$r(CH_2)$
	775sh	774sh					$r(CH_2)$
806w	806m	807m	807w	808m	801w	805vw	*
		821sh					$r(CH_2)$
		845w	849vw				$r(CH_3)_G$
	867w	878sh					$r(CH_3)_G$
887sh/w	890m	894m	889sh	891sh/w	893sh/w	892sh/w	$r(CH_3)_T$
913m	915m	915m	909m	916m	908m	914m	*
932sh		929sh	922sh	931sh	930sh/w		*
	968vw	963w					$r(CH_2)$
		994vw					$r(CH_2)$
	1008vw		1008sh				$\nu(C-C)_T$
		1023vw	1030m	1026w			$\nu(C-C)_T$
1025m	1050w	1055m				1065w	$\nu_s(C-C)_T$
	1068w						*
		1077w	1078w	1083w			*
					1080m	1101w	$\nu(C-C)_T$
1086m	1094m	1106m	1118sh				$\nu(C-C)_T$
1132vs	1132s	1133vs	1129s	1132s			*
					1127vs	1130s	$\nu_s(C-C)_T$ *
		1176sh					$t(CH_2)$

* Contaminant band

Table S1. Raman Frequencies and Assignments for n-Alkanethiols ($C_nH_{2n+1}SH$) at MP Ag (cont'd)

C_3SH	C_4SH	C_5SH	C_8SH	C_9SH	$C_{12}SH$	$C_{18}SH$	Mode
1199s	1199s	1199s	1199m	1199s	1196m	1201s	*
	1215sh				1211sh	1216 sh	$t(CH_2)_T$
				1231sh			$t(CH_2)_T$
1255vs	1252s	1250vs	1253s	1252s	1252s		*
1284sh				1288sh		1284vs	*
1294vs	1293vs	1294vs	1296vs	1296vs	1294vs		*
	1332sh	1335sh					*
1351m	1349s	1350vs	1352m	1352m	1347s	1350m	*
1387vs	1383vs	1383vs	1391vs	1391s	1388s	1389s	*
						1578sh/s	*
1600vs	1596vs	1596vs	1600vs	1600vs	1598vs	1598vs	*
2728	2732	2731	2731	2729		2727	
2855	2854	2858	2851	2854	2850	2851	$\nu_s(CH_2)$
					2860	2859	$\nu_s(CH_2)$
2872	2876	2877					$\nu_s(CH_3)$
	2882	2882	2875	2876	2876	2882	$\nu_a(CH_2)$
2897	2898	2898			2904	2902	$\nu_a(CH_2)$
2916	2915	2916	2912	2917		2913	$\nu_s(CH_2,FR)$
2932	2935	2934			2928	2929	$\nu_s(CH_2,FR)$
2964	2964	2964	2960	2963	2960	2961	$\nu_a(CH_3)$

* Contaminant band

Table S2. Raman Frequencies and Assignments for Solid $C_8D_{17}SH$ and $C_8D_{17}SH$ at MP Ag

Solid $C_8D_{17}SH$	$C_8D_{17}SH$ at MP Ag	Mode
606vw		$\nu(C-S)_G$
631vw		$r(CD_2)_T$
674s		$r(CD_2)_T$
691m	661vs	$\nu(C-S)_T$
712sh/vw	709sh/w	$r(CD_2)_T^*$
728sh/vw		$r(CD_3)_T$
751vw		$r(CD_3)$
	774w	$r(CD_3)_T$
	808w	*
830w		$t(CD_2)_T$
856vw		$t(CD_2)$
889sh/vw		$t(CD_2)_T$
	914sh	*
919s	921m	$t(CD_2)_T$
937sh/vw		$w(CD_2)$
961sh		$s(CD_2)$
	973vw	$s(CD_2)$
987s		$s(CD_2)$
1030vw		$\nu(C-C)_T$
1057m	1054vw	$\delta_a(CD_3)$
1110sh	1114m	$\nu(C-C)_T$
1139s	1134vs	$\nu(C-C)_T^*$
1161sh/vw		
1193sh/vw		

* Contaminant band

 ν = stretch; δ = bend; r = rock; t = twist; s = scissor; FR = Fermi resonance

Table S2. Raman Frequencies and Assignments for Solid $C_8D_{17}SH$ and $C_8D_{17}SH$ at MP Ag (cont'd)

Solid $C_8D_{17}SH$	$C_8D_{17}SH$ at MP Ag	Mode
	1200w	
1247w		$\nu(C-C)_T$
	1256m	
	1288sh	
	1296s	
	1353w	
	1391s	
	1599s	
2055	2052sh	
2074	2068	$\nu_s(CD_3, FR)$
2105vs	2107vs	$\nu_s(CD_2)$
2130	2124sh	$\nu_s(CD_3, FR)$
2143	2147sh	$\alpha-\nu_s(CD_2)$
2155		$\alpha-\nu_a(CD_2)$
2201		$\nu_a(CD_2)$
2220	2214	$\nu_a(CD_3)$

* Contaminant band

 ν = stretch; δ = bend; r = rock; t = twist; s = scissor; FR = Fermi resonance