Table 1S: Structural parameters of cis-3-chlorostyrene (distances in Å and angles in degrees)

	HF	**MP2**	**B3PW91**			**B3LYP**		
	6-31G*	**6-31G***	**6-31G***	**6-311G****	**6-311++G****	**6-31G***	**6-311G****	**6-311++G****
C_1-C_2	1.3942	1.4034	1.4043	1.4016	1.4019	1.4066	1.4043	1.4044
C_1-C_3	1.4809	1.4722	1.4696	1.4683	1.4685	1.4726	1.4720	1.4718
C_3-C_4	1.3215	1.3426	1.3376	1.3340	1.3350	1.3385	1.3348	1.3358
C_2-C_5	1.3789	1.3920	1.3873	1.3840	1.3842	1.3889	1.3853	1.3859
C_5-C_6	1.3845	1.3955	1.3944	1.3915	1.3917	1.3963	1.3930	1.3934
C_6-C_7	1.3828	1.3954	1.3920	1.3889	1.3895	1.3941	1.3911	1.3916
C_7-C_8	1.3849	1.3942	1.3918	1.3893	1.3898	1.3938	1.3914	1.3918
C_8-C_1	1.3909	1.4036	1.4025	1.3997	1.4000	1.4047	1.4021	1.4023
C_2-H_9	1.0724	1.0865	1.0846	1.0827	1.0828	1.0844	1.0816	1.0818
C_3-H_{10}	1.0775	1.0899	1.0901	1.0883	1.0884	1.0898	1.0875	1.0875
C_4-H_{11}	1.0746	1.0848	1.0859	1.0839	1.0841	1.0855	1.0831	1.0831
C_4-H_{12}	1.0752	1.0859	1.0870	1.0852	1.0852	1.0866	1.0842	1.0842
C_5-Cl_{13}	1.7459	1.7431	1.7494	1.7482	1.7489	1.7619	1.7625	1.7612
C_6-H_{14}	1.0732	1.0861	1.0849	1.0829	1.0831	1.0845	1.0820	1.0821
C_7-H_{15}	1.0750	1.0873	1.0868	1.0848	1.0849	1.0864	1.0839	1.0839
C_8-H_{16}	1.0755	1.0882	1.0874	1.0853	1.0855	1.0870	1.0844	1.0844
C_2-C_1-C_3	122.3069	121.5519	122.6682	122.5887	122.5980	122.6627	122.6216	122.6379
C_8-C_1-C_3	119.1698	119.5769	119.0052	119.0699	119.0275	119.0333	119.0921	119.0407
C_1-C_3-C_4	126.8884	125.2545	127.5090	127.4123	127.4205	127.5506	127.5129	127.5174
C_1-C_2-C_5	119.9080	119.7529	119.9178	119.9483	119.8900	119.9270	119.9165	119.9181
C_2-C_5-C_6	121.6689	121.5673	121.7916	121.7482	121.8208	121.8080	121.8585	121.8300
C_5-C_6-C_7	118.4933	118.6023	118.3727	118.4233	118.3787	118.3684	118.3656	118.3789
C_6-C_7-C_8	120.4901	120.5393	120.5377	120.5308	120.5353	120.5351	120.5291	120.5337
C_7-C_8 -C_1	120.9164	120.6669	121.0535	121.0081	121.0007	121.0574	121.0441	121.0179
C_8-C_1-C_2	118.5234	118.8712	118.3267	118.3414	118.3745	118.3041	118.2863	118.3214
C_5-C_2-H_9	119.3221	119.6586	119.2729	119.2094	119.2510	119.3249	119.2662	119.2735
C_1-C_2-H_9	120.7699	120.5884	120.8093	120.8423	120.8589	120.7481	120.8173	120.8084
C_4-C_3-H_{10}	118.3909	118.8627	118.0953	118.1471	118.1157	118.1256	118.1042	118.0693
C_1-C_3-H_{10}	114.7087	115.8536	114.3957	114.4405	114.4638	114.3238	114.3829	114.4132
C_3-C_4-H_{11}	120.7919	121.0813	120.7838	120.7339	120.7120	120.8071	120.7781	120.7478
C_3-C_4-H_{12}	122.9726	122.2325	123.0461	122.8761	122.9037	123.0306	122.9202	122.9533
C_2-C_5-Cl_{13}	119.1472	119.1320	119.1115	119.1437	119.1108	119.1071	119.0870	119.1029
C_7-C_6-H_{14}	121.2084	121.2399	121.3640	121.3662	121.3541	121.3448	121.3487	121.3209
C_5-C_6-H_{14}	120.2984	120.1577	120.2633	120.2105	120.2673	120.2867	120.2858	120.3002
C_8-C_7-H_{15}	119.9170	119.9949	119.9569	120.0010	119.9910	119.9593	120.0002	119.9865
C_6-C_7-H_{15}	119.5928	119.4658	119.5053	119.4682	119.4737	119.5056	119.4707	119.4798
C_1-C_8-H_{16}	119.5097	119.4071	119.1920	119.1804	119.2125	119.1807	119.1907	119.2271
C_7-C_8-H_{16}	119.5739	119.9260	119.7544	119.8115	119.7868	119.7620	119.7652	119.7550
C_2-C_1-C_3-C_4	18.3891	27.4839	0.0	0.0	0.0	0.0	0.0	0.0
E/Hartrees	-766.485459	-766.483180	-769.072059	-769.168710	-769.173175	-769.244318	-769.349041	-769.353664

Table 2S: Structural parameters of trans-3-chlorostyrene (distances in Å and angles in degrees)

	HF	**MP2**	**B3PW91**			**B3LYP**		
	6-31G*	**6-31G***	**6-31G***	**6-311G****	**6-311++G****	**6-31G***	**6-311G****	**6-311++G****
C_1-C_2	1.3911	1.4030	1.4026	1.3998	1.4002	1.4048	1.4023	1.4026
C_1-C_3	1.4809	1.4723	1.4697	1.4684	1.4687	1.4728	1.4722	1.4720
C_3-C_4	1.3215	1.3426	1.3377	1.3341	1.3350	1.3386	1.3348	1.3359
C_2-C_5	1.3826	1.3928	1.3906	1.3877	1.3880	1.3922	1.3891	1.3897
C_5-C_6	1.3803	1.3944	1.3906	1.3873	1.3875	1.3924	1.3886	1.3892
C_6-C_7	1.3869	1.3964	1.3956	1.3929	1.3875	1.3978	1.3953	1.3957
C_7-C_8	1.3813	1.3936	1.3887	1.3859	1.3863	1.3908	1.3879	1.3883
C_8-C_1	1.3942	1.4042	1.4044	1.4018	1.4019	1.4068	1.4043	1.4043
C_2-H_9	1.0740	1.0876	1.0861	1.0841	1.0843	1.0858	1.0831	1.0832
C_3-H_{10}	1.0775	1.0899	1.0901	1.0883	1.0884	1.0897	1.0874	1.0875
C_4-H_{11}	1.0746	1.0848	1.0859	1.0840	1.0841	1.0855	1.0831	1.0832
C_4-H_{12}	1.0751	1.0858	1.0869	1.0850	1.0851	1.0865	1.0841	1.0841
C_5-Cl_{13}	1.7451	1.7427	1.7485	1.7473	1.7480	1.7610	1.7619	1.7602
C_6-H_{14}	1.0732	1.0861	1.0850	1.0830	1.0832	1.0845	1.0820	1.0821
C_7-H_{15}	1.0751	1.0873	1.0869	1.0849	1.0851	1.0865	1.0840	1.0840
C_8-H_{16}	1.0738	1.0870	1.0858	1.0839	1.0840	1.0854	1.0829	1.0829
C_2-C_1-C_3	118.5613	118.8767	118.3562	118.382	118.3706	118.4190	118.4279	118.4080
C_8-C_1-C_3	122.9310	122.2686	123.3340	123.2865	123.2684	123.2943	123.2877	123.2833
C_1-C_3-C_4	126.8011	125.1697	127.3279	127.2305	127.2437	127.3504	127.3200	127.3305
C_1-C_2-C_5	120.2381	120.0229	120.2849	120.3008	120.2418	120.2872	120.2498	120.2668
C_2-C_5-C_6	121.3511	121.3115	121.4196	121.3756	121.4474	121.4449	121.5096	121.4612
C_5-C_6-C_7	118.4913	118.5977	118.3621	118.4181	118.3720	118.3630	118.3543	118.3753
C_6-C_7-C_8	120.8100	120.8035	120.9256	120.9177	120.9222	120.9081	120.9043	120.9121
C_7-C_8 -C_1	120.6019	120.4097	120.6979	120.6562	120.6555	120.7100	120.6976	120.6758
C_8-C_1-C_2	118.5077	118.8547	118.3098	118.3315	118.3611	118.2868	118.2843	118.3087
C_5-C_2-H_9	119.5161	119.7305	119.6230	119.6164	119.6555	119.6618	119.6699	119.6596
C_1-C_2-H_9	120.2458	120.2466	120.0921	120.0828	120.1028	120.0510	120.0802	120.0736
C_4-C_3-H_{10}	118.3580	118.8365	118.0793	118.1129	118.0781	118.1211	118.0918	118.0402
C_1-C_3-H_{10}	114.8301	115.9656	114.5929	114.6566	114.6782	114.5285	114.5882	114.6294
C_3-C_4-H_{11}	120.7857	121.0701	120.7764	120.7231	120.7000	120.8121	120.7721	120.7445
C_3-C_4-H_{12}	122.9626	122.2277	123.0049	122.8252	122.8571	122.9684	122.8601	122.9062
C_2-C_5-Cl_{13}	119.1731	119.2365	119.1491	119.1801	119.1455	119.1490	119.1181	119.1457
C_7-C_6-H_{14}	121.0945	121.2139	121.2640	121.2590	121.2506	121.2402	121.2386	121.2183
C_5-C_6-H_{14}	120.4142	120.1885	120.3738	120.3229	120.3774	120.3969	120.4071	120.4064
C_8-C_7-H_{15}	119.8010	119.8471	119.7873	119.8433	119.8287	119.7960	119.8571	119.8239
C_6-C_7-H_{15}	119.3890	119.3494	119.2871	119.2389	119.2491	119.2959	119.2456	119.2640
C_1-C_8-H_{16}	120.0648	119.7564	119.9576	120.0039	120.0288	119.9279	120.0035	120.0227
C_7-C_8-H_{16}	119.3333	119.8339	119.3445	119.3399	119.3157	119.3621	119.2988	119.3014
C_2-C_1-C_3-C_4	197.6024	207.1749	180.0	180.0	180.0	180.0	180.0	180.0
E/Hartrees	-766.485434	-766.483157	-769.072037	-769.168658	-769.173094	-769.244298	-769.348991	-769.353591

Table 3S: Potential parameters $\{V_{Ni}\}$ i=1-6, kcal.mol^{-1}, for 3-chlorostyrene

	V_1	V_2	V_3	V_4	V_5	V_6
Relaxed	0.06	3.80	0	-0.61	0	-0.02
Restricted	0.67	3.98	0.20	-0.72	0.05	-0.08

Table 4S: Calculated and experimental frequencies for 3-chlorostyrene, in cm^{-1}

	B3LYP/6-311++G**		Fateley IR and Raman	Singh Raman	Tripathi IR	Ribeiro-Claro IR and Raman	This work					
							Raman liquid		INS solid		IR liquid	
	cis	*trans*					*cis*	*trans*	*cis*	*trans*	*cis*	*trans*
A´												
ν_1	3224.4	3225.1		3122	3098	3098	3091	3091			3090	3090
ν_2	3205.8	3205.4	3080		3070	3080	3085	3085			3086	3086
ν_3	3204.3	3192.8				3065					3070	3070
ν_4	3184.5	3190.4	3057	3066		3040	3065	3065			3062	3062
ν_5	3168.2	3173.8	3013	3033	3017	3015	3031	3031			3036	3036
ν_6	3144.4	3145.2	2982	3006	2996	3000	3011	3011			3011	3011
ν_7	3135.0	3136.0	2924			2982					2983	2983
ν_8	1686.6	1686.8	1631	1630	1634	1628	1632	1632			1632	1632
ν_9	1632.8	1633.7	1593	1592	1596	1596	1595	1595			1594	1594
ν_{10}	1603.0	1602.7	1565	1565	1566	1568	1568	1565			1565	1565
ν_{11}	1505.1	1511.7	1477	1478	1469	1480	1476	1478	1495	1495	1475	1478
ν_{12}	1464.1	1466.1	1430	1433	1432	1433	1432	1432	1436	1436	1430	1431
ν_{13}	1447.1	1430.0	1414	1409	1416	1415	1414	1398	1421	1400	1414	1396
ν_{14}	1343.5	1346.5	1305	1306	1307	1308	1306	1306	1313	1313	1302	1306
ν_{15}	1340.4	1339.8	1288		1276	1280			1281	1281	12781	1274
ν_{16}	1297.0	1306.4	1267		1264	1262	1261	1261	1261	1261	1263	1263
ν_{17}	1223.1	1223.5	1202	1201	1204	1205	1202	1202	1200	1200	1201	1201
ν_{18}	1191.9	1194.8	1165	1169	1167	1170	1168	1163	1171	1171	1165	1165
ν_{19}	1114.8	1125.7		1138	1108	1110	1105	1105	1098	1103	1096	1105
ν_{20}	1100.7	1100.2	1081		1064	1083	1081	1081	1086	1086	1081	1081
ν_{21}	1058.8	1046.1	1027	1036	1044/1029	1045	1043	1028	1054	1033	1041	1027
ν_{22}	1012.0	1011.0	998	996	990	1000	999	999	998	998	999	999
ν_{23}	852.8	847.8	846	845		840	842	842	834	834	839	839
ν_{24}	691.0	694.0	681	784	789	682	680	685	686	693	680	685
ν_{25}	560.7	575.9	556	558	687	560	558		551	568	555	570
ν_{26}	455.7	466.2		500?	556	450	448	450	452	452		
ν_{27}	409.2	400.3	425		498	412	412	406	413	409	412	405
ν_{28}	330.7	303.0		303	406	309	330	306	331	306		
ν_{29}	169.2	185.4				190	175	186	188	195		
A´´												
ν_{30}	1024.2	1027.0		1306		990	986	986	988	988	987	987
ν_{31}	987.2	986.3	988			980	945	942	949	949		
ν_{32}	938.0	937.6		938	916	915	914	910	903	903	915	915
ν_{33}	915.0	911.5	913	909		882			890	890	881	881
ν_{34}	893.7	898.1	880	845	842/848	850	847	845	846	846	846	846
ν_{35}	803.8	800.8	789			790	788	785	801	793	788	788
ν_{36}	727.3	729.2	710	718	712	688	711	709	714	711	710	710
ν_{37}	660.9	663.8	649	681		650	650	650	650	650	648	648
ν_{38}	510.1	501.8	568	452	420	500			499	491		
ν_{39}	427.9	438.8	425	404		407			421	427	421	426
ν_{40}	216.8	208.2	215	219		219	219	219	231	231		
ν_{41}	169.9	178.8	187?	177		172	175	181	188	192		
ν_{42}	29.5	26.6	<33									

Table 5S: Force constants after the refinement of 3-chlorostyrene[a]

	Initial		**Final**	
	cis	***trans***	***cis***	***trans***
A´				
$F_{1,1}$	5.997	5.864	4.744	4.767
$F_{2,2}$	6.271	6.384	6.271	6.384
$F_{3,3}$	6.292	6.162	6.021	7.085
$F_{4,4}$	5.816	5.957	6.512	5.742
$F_{5,5}$	6.024	5.908	5.988	5.249
$F_{6,6}$	5.589	5.717	4.009	4.928
$F_{7,7}$	5.156	5.152	6.093	5.991
$F_{8,8}$	9.325	9.323	7.870	7.671
$F_{9,9}$	5.528	5.585	5.065	5.176
$F_{10,10}$	5.552	5.547	5.151	5.058
$F_{11,11}$	5.625	5.623	5.207	5.209
$F_{12,12}$	3.450	3.453	3.685	3.673
$F_{13,13}$	5.636	5.584	5.180	5.155
$F_{14,14}$	5.412	5.415	4.895	4.895
$F_{15,15}$	5.590	5.588	5.151	5.153
$F_{16,16}$	5.546	5.555	5.084	5.086
$F_{17,17}$	1.374	1.373	1.227	1.051
$F_{18,18}$	1.291	1.293	1.212	1.246
$F_{19,19}$	1.302	1.301	1.427	1.586
$F_{20,20}$	0.759	1.252	0.605	1.264
$F_{21,21}$	0.779	0.727	0.668	0.785
$F_{22,22}$	0.822	0.708	0.857	0.799
$F_{23,23}$	1.193	1.023	1.774	1.223
$F_{24,24}$	0.689	0.745	0.650	0.658
$F_{25,25}$	0.542	0.544	0.544	0.513
$F_{26,26}$	0.568	0.596	0.500	0.460
$F_{27,27}$	0.551	0.531	0.597	0.486
$F_{28,28}$	0.569	0.557	0.560	0.490
$F_{29,29}$	0.689	0.491	0.634	0.467
A´´				
$F_{30,30}$	0.412	0.416	0.377	0.483
$F_{31,31}$	0.283	0.281	0.275	0.254
$F_{32,32}$	0.300	0.298	0.265	0.281
$F_{33,33}$	0.280	0.280	0.229	0.269
$F_{34,34}$	0.351	0.356	0.604	0.341
$F_{35,35}$	0.273	0.275	0.300	0.233
$F_{36,36}$	0.155	0.156	0.074	0.107
$F_{37,37}$	0.439	0.218	0.341	0.221
$F_{38,38}$	0.113	0.116	0.107	0.111
$F_{39,39}$	0.114	0.388	0.126	0.330
$F_{40,40}$	0.280	0.282	0.280	0.282
$F_{41,41}$	0.333	0.337	0.391	0.427
$F_{42,42}$	0.346	0.287	0.401	0.276

[a] Units are consistent with energy measured in aJ, lenghts in Å, and angles in radians

Table 6S: Vibrational frequencies for cis-3-chlorostyrene after scaling

	Experimental	Scaled	Assignment
A´			
ν_1	3091	3083	C_bH st.
ν_2	3085	3082	C_bH st.
ν_3	3070	3074	C_eH_2 st., C_bH st.
ν_4	3063	3062	C_bH st.
ν_5	3034	3046	C_bH st.
ν_6	3011	3000	C_eH_2 st., C_eH st.
ν_7	2983	2990	C_eH st.
ν_8	1632	1637	$(C\text{-}C)_e$ st.
ν_9	1594	1595	$(C\text{-}C)_b$ st., benz. asym. def.
ν_{10}	1568	1566	$(C\text{-}C)_b$ st., C_bH rock., benz. asym. def.
ν_{11}	1475	1473	C_bH rock., $(C\text{-}C)_b$ st.
ν_{12}	1429	1429	C_eH rock., $(C\text{-}C)_b$ st., C_bH rock.
ν_{13}	1414	1412	C_eH rock., vinyl st.
ν_{14}	1302	1311	C_bH rock., $(C\text{-}C)_b$ st.
ν_{15}	1278	1283	C_eH rock., $(C\text{-}C)_b$ st.
ν_{16}	1262	1262	C_eH rock., C_bH rock.
ν_{17}	1202	1190	vinyl st., benz. trig. def., C_eH rock., $(C\text{-}C)_b$ st., C_bH rock.
ν_{18}	1168	1167	C_bH rock., $(C\text{-}C)_b$ st.
ν_{19}	1096	1092	$(C\text{-}C)_b$ st., C_bH rock.
ν_{20}	1081	1078	$(C\text{-}C)_b$ st., C_bCl st.
ν_{21}	1042	1041	C_eH rock.
ν_{22}	999	997	benz. trig. def.
ν_{23}	840	845	C_bCl st., vinyl st., benz. asym. def., C_eH rock.
ν_{24}	680	687	benz. asym. def., C_bCl st.
ν_{25}	555	554	benz. asym. def., vinyl sym. def., vinyl rock.
ν_{26}	448	451	vinyl rock., benz. asym. def., vinyl st., vinyl sym. def.
ν_{27}	412	409	C_bCl st., benz. asym. def.
ν_{28}	330	331	C_bCl rock., vinyl sym. def.
ν_{29}	175	170	vinyl rock., C_bCl rock., vinyl sym. def.
A´´			
ν_{30}	986	987	vinyl wag., $(C\text{-}C)_e$ tors.
ν_{31}	945	940	C_bH wag., benz. puck.
ν_{32}	914	914	$(C\text{-}C)_e$ wag.
ν_{33}	881	883	C_bH wag., benz. wag., benz. puck.
ν_{34}	847	856	C_bH wag., benz. puck.
ν_{35}	788	782	C_bH wag., benz. puck., benz. wag.
ν_{36}	711	709	C_bH wag., benz. puck., benz. wag.
ν_{37}	649	649	benz. puck., C_bCl wag.
ν_{38}	499(INS)	500	benz. asym. tors., C_bCl wag., benz. wag.
ν_{39}	421	426	benz. asym. tors.
ν_{40}	218	217	benz. asym. tors.
ν_{41}	175	167	C_bCl wag., C_bH wag., benz. wag., benz. asym. tors.
ν_{42}	-	30	vinyl tors.

Table 7S: Vibrational frequencies for trans-3-chlorostyrene after scaling

	Experimental	Scaled	Assignment
A´			
ν_1	3091	3082	C_eH_2 st.
ν_2	3085	3077	C_bH st.
ν_3	3070	3065	C_bH st.
ν_4	3063	3063	C_bH st.
ν_5	3034	3047	C_bH st.
ν_6	3011	3006	C_eH_2 st., C_eH st.
ν_7	2983	2997	C_eH st.
ν_8	1632	1636	$(C\text{-}C)_e$ st., C_eH rock.
ν_9	1594	1595	$(C\text{-}C)_b$ st., benz. asym. def., C_bH rock.
ν_{10}	1565	1563	$(C\text{-}C)_b$ st., benz. asym. def., C_bH rock.
ν_{11}	1478	1475	C_bH rock., $(C\text{-}C)_b$ st.
ν_{12}	1431	1429	C_eH rock.
ν_{13}	1397	1398	C_bH rock., $(C\text{-}C)_b$ st., C_eH rock.
ν_{14}	1306	1307	C_bH rock., $(C\text{-}C)_b$ st., C_eH rock.
ν_{15}	1274	1281	C_bH rock., $(C\text{-}C)_b$ st.
ν_{16}	1262	1265	$(C\text{-}C)_b$ st., C_eH rock., C_bH rock.
ν_{17}	1202	1189	C_eH rock., vinyl st.
ν_{18}	1163	1166	vinyl st., benz. trig. def., C_eH rock., $(C\text{-}C)_b$ st., C_bH rock.
ν_{19}	1105	1102	C_bH rock., $(C\text{-}C)_b$ st., C_bCl st., C_bH rock.
ν_{20}	1081	1079	$(C\text{-}C)_b$ st.
ν_{21}	1027	1026	C_eH rock., benz. trig. def.
ν_{22}	999	995	benz. trig. def., (C-C)b st.
ν_{23}	840	843	C_bCl st., vinyl st., benz. asym. def.
ν_{24}	685	690	benz. asym. def., C_bCl st.
ν_{25}	570	567	vinyl sym. def., benz. asym. def., vinyl rock., C_eH rock.
ν_{26}	450	460	benz. asym. def., vinyl rock.
ν_{27}	405	404	C_bCl st., benz. asym. def.
ν_{28}	306	306	C_bCl rock., vinyl sym. def.
ν_{29}	186	182	vinyl rock., C_bCl rock., vinyl sym. def.
A´´			
ν_{30}	986	987	vinyl wag., (C-C)e tors.
ν_{31}	942	935	C_bH wag., benz. puck.
ν_{32}	910	911	(C-C)e wag.
ν_{33}	881	883	C_bH wag., benz. wag., benz. puck.
ν_{34}	845	855	C_bH wag., benz. puck.
ν_{35}	785	781	C_bH wag., benz. puck., benz. wag.
ν_{36}	709	707	C_bH wag., benz. wag.
ν_{37}	649	647	benz. puck., C_bCl wag.
ν_{38}	491(INS)	492	benz. asym. tors., C_bCl wag., benz. wag., $(C\text{-}C)_e$ tors., vinyl tors.
ν_{39}	426	465	benz. asym. tors., $(C\text{-}C)_e$ tors., C_bCl wag., benz. wag.
ν_{40}	218	211	benz. asym. tors., benz. wag., C_bH wag.
ν_{41}	180	174	C_bCl wag., benz. asym. tors., C_bH wag.
ν_{42}	-	27	vinyl tors.

Table 8S: Canonical diagonal force constants in terms of simple valence internal coordinates of 3-chlorostyrene (3ClS) and those of benzene (see text)[a]

Force constant	3ClS		Goodman	Pulay	Description
	cis	*trans*			
$F^*_{1,1}$	4.207	4.228	4.892	4.760	$(C\text{-}C)_b$ st.
$F^*_{2,2}$	5.513	5.615			
$F^*_{3,3}$	5.290	6.223			
$F^*_{4,4}$	5.978	5.325			
$F^*_{5,5}$	5.573	4.933			
$F^*_{6,6}$	3.834	4.636			
$F^*_{7,7}$	6.093	5.991	-	-	vinyl st.
$F^*_{8,8}$	7.870	7.671	-	-	$(C\text{-}C)_e$ st.
$F^*_{9,9}$	5.065	5.176	5.547	5.176	C_bH st.
$F^*_{10,10}$	5.151	5.058			
$F^*_{11,11}$	5.207	5.209			
$F^*_{12,12}$	3.685	3.673	-	-	C_bCl st.
$F^*_{13,13}$	5.180	5.155	5.547	5.176	C_bH st.
$F^*_{14,14}$	4.894	4.895	-	-	C_eH st.
$F^*_{15,15}$	5.151	5.153	-	-	
$F^*_{16,16}$	5.084	5.086	-	-	
$F^*_{17,17}$	1.141	1.086	1.369	0.927	$(C\text{-}C)_b$ bend.
$F^*_{18,18}$	1.180	1.096			
$F^*_{19,19}$	1.123	1.194			
$F^*_{20,20}$	1.166	1.249			
$F^*_{21,21}$	1.288	1.304			
$F^*_{22,22}$	1.120	1.150			
$F^*_{23,23}$	1.713	1.413	-	-	$(C\text{-}C)_e$ bend.
$F^*_{24,24}$	0.904	1.066	-	-	vinyl rock.
$F^*_{25,25}$	0.534	0.573	0.993	0.875	C_bH rock.
$F^*_{26,26}$	0.477	0.457			
$F^*_{27,27}$	0.572	0.474			
$F^*_{28,28}$	0.983	0.942	-	-	C_bCl rock.
$F^*_{29,29}$	0.459	0.498	0.993	0.875	C_bH rock.
$F^*_{30,30}$	0.522	0.530	-	-	C_eH rock.
$F^*_{31,31}$	0.492	0.466	-	-	
$F^*_{32,32}$	0.732	0.724	-	-	C_eH bend.
$F^*_{33,33}$	0.343	0.440	-	-	vinyl wag.
$F^*_{34,34}$	0.252	0.233	0.233	-	C_bH wag.
$F^*_{35,35}$	0.242	0.258			
$F^*_{36,36}$	0.211	0.248			
$F^*_{37,37}$	0.551	0.312	-	-	C_bCl wag.
$F^*_{38,38}$	0.274	0.214	0.233	-	C_bH wag.
$F^*_{39,39}$	0.032	0.046		-	$(C\text{-}C)_e$ wag.
$F^*_{40,40}$	0.042	0.061	-	-	C_eH wag.
$F^*_{41,41}$	0.054	0.055	-	-	
$F^*_{42,42}$	0.052	0.053	-	-	
$F^*_{43,43}$	0.192	0.176	0.249	-	$(C\text{-}C)_b$ tors.
$F^*_{44,44}$	0.219	0.208			
$F^*_{45,45}$	0.235	0.186			
$F^*_{46,46}$	0.209	0.179			
$F^*_{47,47}$	0.211	0.196			
$F^*_{48,48}$	0.198	0.187			
$F^*_{49,49}$	0.015	0.032	-	-	vinyl tors.
$F^*_{50,50}$	0.435	0.531	-	-	$(C\text{-}C)_e$ tors.

[a]units consistent with energy in aJ, lenghts in Å, angles in radians