TABLE 1: Zero-point vibrational energies within the harmonic approximation for the most stable structures of $C_6H_5X/C_6H_5X^-$ (X=N, S, NH, PH, CH_2, SiH_2) in eV [a]

Compounds	B3LYP	BLYP	BHLYP	B3P86	BP86	B3PW91	BPW91
C_6H_5S	2.457	2.385	2.545	2.469	2.388	2.466	2.398
$C_6H_5S^-$	2.428	2.350	2.521	2.440	2.354	2.436	2.365
Δ (C_6H_5S-$C_6H_5S^-$)	0.030	0.034	0.024	0.030	0.033	0.030	0.033
C_6H_5N	2.476	2.402	2.559	2.487	2.406	2.484	2.417
$C_6H_5N^-$	2.433	2.352	2.529	2.447	2.357	2.443	2.369
Δ (C_6H_5N-$C_6H_5N^-$)	0.043	0.050	0.030	0.041	0.049	0.041	0.048
C_6H_5NH	2.816	2.733	2.912	2.829	2.737	2.825	2.749
$C_6H_5NH^-$	2.774	2.682	2.883	2.790	2.689	2.786	2.702
Δ (C_6H_5NH-$C_6H_5NH^-$)	0.042	0.050	0.028	0.039	0.048	0.039	0.047
C_6H_5PH	2.677	2.597	2.773	2.690	2.600	2.685	2.612
$C_6H_5PH^-$	2.632	2.548	2.733	2.646	2.553	2.642	2.565
Δ (C_6H_5PH-$C_6H_5PH^-$)	0.045	0.048	0.040	0.044	0.047	0.044	0.047
$C_6H_5CH_2$	3.121	3.036	3.220	3.132	3.036	3.127	3.049
$C_6H_5CH_2^-$	3.054	2.962	3.165	3.066	2.963	3.061	2.976
Δ ($C_6H_5CH_2$-$C_6H_5CH_2^-$)	0.067	0.075	0.055	0.066	0.073	0.065	0.073
$C_6H_5SiH_2$	2.874	2.789	2.978	2.885	2.789	2.880	2.802
$C_6H_5SiH_2^-$	2.807	2.718	2.914	2.820	2.722	2.816	2.735
Δ ($C_6H_5SiH_2$-$C_6H_5SiH_2^-$)	0.067	0.071	0.064	0.065	0.068	0.065	0.067

[a]All results obtained with the DZP++ basis set.

TABLE 2: the total energy of the C_6H_5X / $C_6H_5X^-$ and ZPVE value in hartress

Total energy	B3LYP	BLYP	BHLYP	B3P86	BP86	B3PW91	BPW91
C_6H_5N	-286.34649	-286.22691	-286.18377	-287.20507	-286.33788	-286.23562	-286.30911
	0.090986	0.088279	0.094051	0.091407	0.088421	0.091277	0.088824
	-286.25550	-286.13863	-286.08972	-287.11366	-286.24946	-286.14434	-286.22029
$C_6H_5N^-$	-286.39685	-286.27604	-286.21962	-287.27557	-286.39482	-286.28479	-286.36078
	0.089422	0.086425	0.092944	0.089917	0.086633	0.089777	0.087057
	-286.30743	-286.18962	-286.12668	-287.18565	-286.30819	-286.19501	-286.27372
C_6H_5S	-629.83771	-629.71268	-629.67956	-630.87654	-629.85583	-629.69700	-629.80284
	0.09031	0.087642	0.093526	0.090747	0.087741	0.090617	0.088134
	-629.74740	-629.62504	-629.58603	-630.78580	-629.76809	-629.60638	-629.71470
$C_6H_5S^-$	-629.92086	-629.79131	-629.75401	-630.98049	-629.94324	-629.78051	-629.88566
	0.089223	0.086377	0.092644	0.089651	0.086519	0.089519	0.08692
	-629.83163	-629.70493	-629.66137	-630.89083	-629.85672	-629.69099	-629.79874
C_6H_5NH	-286.99718	-286.87195	-286.82607	-287.87744	-286.99100	-286.88691	-286.959632
	0.103489	0.100426	0.107001	0.103964	0.100582	0.10381	0.101032
	-286.89369	-286.77153	-286.71907	-287.77348	-286.89042	-286.783101	-286.85860
$C_6H_5NH^-$	-287.052293	-286.92485	-286.86798	-287.95303	-287.05202	-286.94158	-287.01574
	0.10195	0.098575	0.105963	0.102517	0.098811	0.102367	0.0993
	-286.95034	-286.82627	-286.76202	-287.85051	-286.95321	-286.83921	-286.91644
C_6H_5PH	-573.60031	-573.46739	-573.43901	-574.63605	-573.60998	-573.46140	-573.55899
	0.098395	0.095422	0.101918	0.098841	0.095554	0.098688	0.095978
	-573.50358	-573.37375	-573.33858	-574.53882	-573.51615	-573.36432	-573.46473
$C_6H_5PH^-$	-573.65342	-573.51780	-573.48160	-574.70925	-573.66873	-573.51430	-573.61290
	0.096733	0.093644	0.10043	0.097223	0.093828	0.09708	0.094269
	-573.55669	-573.42416	-573.38117	-574.61203	-573.57490	-573.41722	-573.51863
$C_6H_5CH_2$	-270.95091	-270.81330	-270.78541	-271.83371	-270.93918	-270.84778	-270.90916
	0.114689	0.111575	0.118323	0.11509	0.111578	0.11491	0.112061

	-270.83622	-270.70172	-270.66709	-271.71862	-270.82760	-270.73287	-270.79710
$C_6H_5CH_2^-$	-270.98045	-270.84156	-270.80139	-271.88286	-270.97495	-270.87618	-270.93977
	0.112236	0.108836	0.116308	0.112682	0.108877	0.112504	0.109376
	-270.86821	-270.73272	-270.68508	-271.88286	-270.86607	-270.76367	-270.83039
$C_6H_5SiH_2$	-522.33079	-522.18958	-522.16733	-523.36163	-522.32901	-522.19173	-522.28039
	0.105624	0.102481	0.109426	0.106013	0.102511	0.105844	0.102961
	-522.22517	-522.08710	-522.05790	-523.25562	-522.22650	-522.08588	-522.17743
$C_6H_5SiH_2^-$	-522.38403	-522.24006	-522.21151	-523.43341	-522.386475	-522.24324	-522.33249
	0.103146	0.099877	0.107076	0.103626	0.100017	0.103468	0.100496
	-522.28088	-522.14018	-522.1044368	-523.32978	-522.28646	-522.13978	-522.23199

TABLE 3: Optimized geometry for the C_6H_5N and the corresponding anion $C_6H_5N^-$. All bond distances are in Å, all bond angles are in degree and all results were obtained with the DZP ++ basis set.

C_6H_5N	B3LYP	BLYP	BHLYP	B3P86	BP86	B3PW91	BPW91
c_1-c_2 (c_4-c_5)	1.390	1.399	1.381	1.386	1.396	1.387	1.395
c_1-c_6 (c_5-c_6)	1.439	1.455	1.425	1.434	1.450	1.434	1.448
c_1-c_7(c_5-c_{11})	1.088	1.095	1.080	1.087	1.097	1.088	1.095
c_2-c_3(c_3-c_4)	1.410	1.421	1.400	1.405	1.417	1.406	1.416
c_2-c_8(c_4-c_{10})	1.089	1.097	1.081	1.089	1.098	1.089	1.096
c_3-c_9	1.089	1.096	1.080	1.088	1.097	1.089	1.095
c_6-n_{12}	1.335	1.340	1.331	1.332	1.337	1.335	1.338
A (1,6,5)	118.7	118.4	119.0	118.8	118.5	118.8	118.4
A (2,3,4)	120.1	120.0	120.2	120.1	120.0	120.1	120.0
A (6,5,11)	118.6	118.4	118.8	118.5	118.4	118.6	118.4
A (3,4,5)	120.6	120.8	120.5	120.6	120.7	120.6	120.7
$C_6H_5N^-$	B3LYP	BLYP	BHLYP	B3P86	BP86	B3PW91	BPW91
c_6-n_{12}	1.318	1.328	1.307	1.314	1.325	1.315	1.324

TABLE 4: Optimized geometry for the C_6H_5S and the corresponding anion $C_6H_5S^-$. All bond distances are in Å, all bond angles are in degree and all results were obtained with the DZP ++ basis set.

C_6H_5S	B3LYP	BLYP	BHLYP	B3P86	BP86	B3PW91	BPW91
c_1-c_2 (c_4-c_5)	1.394	1.404	1.384	1.390	1.401	1.391	1.399
c_1-c_6 (c_5-c_6)	1.426	1.440	1.414	1.422	1.436	1.423	1.434
c_1-c_7(c_5-c_{11})	1.088	1.096	1.080	1.088	1.097	1.089	1.095
c_2-c_3(c_3-c_4)	1.407	1.419	1.396	1.403	1.415	1.404	1.414
c_2-c_8(c_4-c_{10})	1.089	1.097	1.080	1.088	1.098	1.089	1.096
c_3-c_9	1.089	1.097	1.081	1.089	1.098	1.089	1.096
c_6-s_{12}	1.723	1.735	1.712	1.713	1.726	1.715	1.724
A (2,3,4)	120.2	120.1	120.2	120.2	120.2	120.2	120.2
A (3,4,5)	120.1	120.2	120.1	120.1	120.1	120.1	120.1
A (1,6,5)	118.2	118.1	118.4	118.3	118.2	118.3	118.2
A (6,5,11)	118.5	118.4	118.6	118.4	118.3	118.4	118.3
$C_6H_5S^-$	B3LYP	BLYP	BHLYP	B3P86	BP86	B3PW91	BPW91
c_6-s_{12}	1.745	1.757	1.737	1.733	1.746	1.735	1.744
A (2,3,4)	117.9	117.9	117.9	117.8	117.8	117.8	117.8
A (3,4,5)	121.1	121.1	121.1	121.1	121.1	121.1	121.1
A (1,6,5)	115.2	115.2	115.4	115.2	115.1	115.2	115.1
A (6,5,11)	117.7	117.7	117.8	117.6	117.5	117.6	117.6

TABLE 5: Optimized geometry for the $C_6H_5CH_2$ and the corresponding anion $C_6H_5CH_2^-$. All bond distances are in Å, all bond angles are in degree and all results were obtained with the DZP ++ basis set.

$C_6H_5CH_2$	B3LYP	BLYP	BHLYP	B3P86	BP86	B3PW91	BPW91
c_1-c_2 (c_4-c_5)	1.392	1.402	1.382	1.388	1.399	1.389	1.397
c_1-c_6 (c_5-c_6)	1.431	1.444	1.420	1.426	1.439	1.427	1.438
c_1-c_7(c_5-c_{11})	1.090	1.098	1.081	1.089	1.099	1.090	1.097
c_2-c_3(c_3-c_4)	1.409	1.420	1.399	1.404	1.416	1.405	1.414
c_2-c_8(c_4-c_{10})	1.090	1.097	1.081	1.089	1.098	1.090	1.096
c_3-c_9	1.089	1.097	1.080	1.088	1.098	1.089	1.096
c_6-c_{12}	1.413	1.419	1.406	1.409	1.417	1.412	1.417
c_{12}-h_{13}(c_{12}-h_{14})	1.088	1.095	1.079	1.087	1.096	1.088	1.094
A (2,3,4)	119.5	119.5	119.5	119.5	119.5	119.5	119.5
A (3,4,5)	120.5	120.5	120.5	120.5	120.5	120.5	120.5
A (1,6,5)	117.4	117.3	117.5	117.5	117.3	117.4	117.3
A (6,5,11)	118.8	118.8	118.9	118.8	118.8	118.9	118.8
A (13,12,14)	117.8	117.7	118.0	117.9	117.8	117.9	117.7
$C_6H_5CH_2^-$	B3LYP	BLYP	BHLYP	B3P86	BP86	B3PW91	BPW91
c_1-c_2 (c_4-c_5)	1.390	1.402	1.378	1.386	1.399	1.387	1.397
c_1-c_6 (c_5-c_6)	1.454	1.464	1.443	1.448	1.460	1.450	1.459
c_1-c_7(c_5-c_{11})	1.094	1.102	1.084	1.093	1.103	1.093	1.100
c_2-c_3(c_3-c_4)	1.417	1.428	1.405	1.412	1.424	1.413	1.423
c_2-c_8(c_4-c_{10})	1.095	1.103	1.086	1.094	1.104	1.095	1.102
c_3-c_9	1.090	1.098	1.081	1.089	1.099	1.090	1.097
c_6-c_{12}	1.399	1.411	1.387	1.394	1.407	1.396	1.406
c_{12}-h_{13}(c_{12}-h_{14})	1.090	1.097	1.082	1.089	1.099	1.090	1.097
A (2,3,4)	116.7	116.8	116.5	116.6	116.7	116.6	116.6
A (3,4,5)	122.1	122.0	122.3	122.2	122.1	122.2	122.1

A (1,6,5)	113.7	113.7	113.7	113.6	113.7	113.6	113.6
A (6,5,11)	118.0	118.0	118.1	118.0	117.9	118.0	118.0
A (13,12,14)	117.5	117.4	117.7	117.7	117.5	117.6	117.5

Table 6: Predicted harmonic vibrational frequencies (cm^{-1}) for the C_6H_5N radical and its anion.

Sym.	B3LYP		BLYP		BHLYP		B3P86		BP86		B3PW91		BPW91		Expt.
	neutral	anion	neutral	anion	neutral	anion	neutral	anion	neutral	anion	neutral	anion	neutral	anion	Neutral[a]
b_1	204.8	172.5	191.8	164.6	218.8	181.2	204.4	172.7	190.6	163.8	204.5	172.5	191.8	165.2	
b_2	372.9	387.0	360.7	373.5	389.9	403.4	369.0	383.6	354.9	368.7	369.2	383.8	356.5	370.3	
a_2	396.3	416.9	383.3	396.1	410.7	438.2	394.2	417.5	379.5	396.6	393.5	416.8	380.3	398.8	
b_1	480.8	482.7	464.5	464.1	497.8	504.8	478.6	481.0	460.3	459.8	478.4	479.8	462.3	461.2	
a_1	517.2	511.8	501.3	494.9	535.3	532.5	516.2	510.7	498.6	492.0	515.4	509.9	500.1	493.5	
b_2	607.0	611.3	588.3	592.7	629.1	634.8	605.1	609.9	584.4	589.3	604.5	609.0	586.1	590.9	
b_1	673.3	669.9	651.4	642.3	695.7	698.5	673.2	668.5	648.7	634.7	672.8	665.2	651.8	637.0	654.0
b_1	761.2	685.8	736.8	659.2	786.6	719.2	758.7	688.0	730.6	658.5	757.7	686.6	733.7	661.5	746.0
a_2	824.6	767.9	797.9	746.0	853.9	794.9	820.2	765.5	789.1	738.5	820.4	764.2	793.5	741.8	
b_1	910.5	781.1	881.4	749.5	940.6	817.2	906.6	780.7	872.5	744.5	905.8	778.9	876.9	748.4	885
a_1	827.6	809.2	796.2	776.5	858.9	845.7	834.8	817.9	802.6	784.4	833.1	815.8	805.8	787.2	
a_1	968.4	954.3	938.1	924.2	1002.1	990.8	972.9	956.8	940.1	924.2	971.2	955.2	942.9	926.9	
b_1	993.7	924.4	959.5	882.0	1029.8	978.8	990.0	923.3	950.2	875.4	988.8	922.0	955	880.5	964.0
a_2	981.3	932.9	949.4	892.3	1016.6	985.8	976.9	929.8	939.4	883.4	976.0	928.7	944.2	888.4	
b_2	1089.5	1061.7	1054.4	1024.3	1127.7	1105.0	1094.7	1067.7	1058.0	1028.7	1093.8	1066.6	1063	1033.6	1079.0
a_1	1024.5	1016.0	990.9	981.0	1059.0	1055.9	1033.2	1025.7	998.2	989.1	1031.8	1024.0	1002.8	993.5	1008.0
b_2	1166.5	1141.7	1137.9	1107.5	1197.8	1183.5	1166.9	1140.1	1134.4	1102.8	1167.0	1140.5	1140.1	1108.9	
b_2	1280.2	1239.1	1232.1	1191.6	1328.6	1290.8	1289.7	1249.1	1240.1	1199.3	1288.7	1247.3	1246.6	1205.1	1250.0
a_1	1163.7	1172.3	1138.0	1140.4	1197.0	1213.8	1165.9	1171.5	1136.3	1135.8	1165.0	1172.0	1141.3	1142.1	1148.0
a_1	1303.3	1390.2	1281.1	1342.4	1332.7	1447.7	1320.2	1398.4	1297.3	1348.4	1310.2	1396.4	1294.6	1354.1	1286.0
b_2	1343.5	1341.3	1308.7	1298.2	1379.7	1391.6	1359.1	1345.6	1318.5	1296.5	1355.5	1343.9	1323.8	1302.5	1309.0
b_2	1437.5	1471.0	1391.3	1422.4	1493.7	1524.5	1446.6	1489.9	1400.2	1439.7	1444.2	1486.4	1405.5	1445.7	
a_1	1453.2	1477.5	1401.8	1410.1	1517.0	1554.5	1457.6	1498.4	1401.9	1427.6	1456.5	1495.0	1408.5	1434.4	1408.0
b_2	1557.4	1516.3	1494.7	1454.9	1624.9	1590.5	1573.0	1531.9	1506.6	1467.2	1570.5	1528.6	1513.5	1473.3	1524.0
a_1	1587.0	1612.2	1531.0	1547.4	1644.5	1685.6	1604.3	1633.3	1545.9	1565.7	1600.7	1629.8	1551.7	1572.7	1552.0

a_1	3184.3	3105.7	3097.3	3014.2	3286.3	3212.1	3205.2	3128.0	3107.9	3026.4	3200.8	3123.3	3124.7	3043.1
b_2	3190.8	3108.5	3103.3	3016.5	3293.3	3215.6	3211.5	3130.7	3113.6	3028.5	3207.3	3126.0	3130.4	3045.2
a_1	3205.8	3158.4	3121.4	3070.7	3305.8	3261.8	3225.6	3178.9	3130.8	3080.6	3221.4	3174.5	3147.3	3097.3
b_2	3214.0	3158.8	3131.1	3071.1	3312.9	3262.2	3232.9	3178.9	3139.1	3080.5	3228.9	3174.6	3155.9	3097.2
a_1	3217.4	3173.4	3134.2	3085.7	3316.7	3277.0	3236.1	3194.8	3142.0	3096.9	3232.0	3190.2	3158.6	3113.1

[a]Assigned from IR spectrum:[54]

Table 7: Predicted harmonic vibrational frequencies (cm^{-1}) for the C_6H_5S radical and its anion.

Sym.	B3LYP		BLYP		BHLYP		B3P86		BP86		B3PW91		BPW91	
	neutral	anion	neutral	anion	neutral	anion	neutral	anion	neutral	anion	neutral	anion	neutral	anion
b_1	163.8	167.8	155.0	159.6	174.0	177.8	162.6	167.7	152.7	158.5	162.4	167.4	153.3	159.1
b_2	297.5	293.9	288.7	285.2	309.1	303.9	297.1	294.0	287.5	284.6	296.5	293.4	287.9	285.1
a_2	386.0	421.9	370.0	409.7	404.6	437.7	382.5	420.6	364.2	406.7	381.8	419.4	365.0	407.3
a_1	426.4	421.6	412.7	407.6	441.5	436.5	429.6	426.1	415.6	411.7	428.3	425.0	416.4	412.9
b_1	467.4	485.8	453.7	469.5	483.9	506.1	463.9	483.6	447.8	465.1	463.3	482.7	449.1	466.2
b_2	611.4	619.9	592.3	601.5	634.7	643.5	609.3	617.9	588.1	597.4	608.4	616.9	589.5	598.7
b_1	681.0	691.7	658.2	667.2	707.1	721.8	680.8	693.0	655.0	665.7	680.0	691.6	657.7	668.2
a_1	726.7	707.8	701.8	683.6	755.3	735.1	732.5	714.0	706.6	688.5	730.5	712.2	708.5	690.8
b_1	774.9	734.3	755.1	709.9	799.2	764.9	770.6	730.7	746.3	701.1	769.5	728.8	748.9	703.5
a_2	856.7	840.1	831.9	816.0	888.1	873.7	851.2	834.3	820.9	804.8	851.0	833.6	824.9	807.9
b_1	951.4	870.2	923.3	838.0	984.9	911.2	946.2	865.1	912.6	827.4	945.2	863.9	916.7	831.2
a_1	995.8	986.3	963.5	954.2	1029.7	1025.5	1000.3	990.4	966.5	956.8	998.2	988.5	969.1	959.2
a_2	997.3	962.6	965.6	927.5	1035.9	1008.6	992.8	958.8	955.3	918.0	991.9	957.9	960.1	922.9
b_1	1008.0	953.2	973.2	915.2	1049.0	1003.7	1004.9	951.6	964.5	908.0	1003.7	950.5	969.3	912.9
a_1	1033.4	1032.1	999.7	996.4	1070.8	1074.5	1040.8	1040.0	1004.9	1002.3	1038.8	1038.3	1008.9	1006.3
a_1	1082.1	1094.8	1041.8	1050.9	1124.6	1145.1	1095.2	1109.6	1054.7	1064.8	1091.2	1106.6	1057.2	1069.1
b_2	1091.9	1070.1	1057.5	1034.8	1131.9	1112.9	1096.3	1074.5	1059.5	1036.8	1095.3	1073.5	1064.4	1041.6
b_2	1170.6	1150.3	1140.6	1118.0	1204.6	1190.1	1170.6	1148.3	1136.8	1112.0	1170.7	1148.8	1142.6	1118.2
a_1	1191.2	1177.6	1158.6	1144.0	1232.1	1221.4	1191.3	1176.5	1154.9	1139.1	1191.0	1176.6	1160.3	1144.8
b_2	1302.7	1281.2	1261.7	1242.0	1343.7	1319.2	1305.0	1284.6	1259.0	1239.8	1303.9	1283.3	1264.7	1245.2
b_2	1347.9	1338.2	1314.7	1301.6	1381.8	1377.0	1370.0	1355.1	1335.0	1316.2	1365.1	1351.3	1339.3	1321.0
b_2	1449.2	1447.8	1402.5	1401.1	1506.8	1505.5	1456.4	1457.8	1407.5	1409.1	1454.1	1455.2	1412.9	1414.8
a_1	1470.3	1469.4	1420.5	1418.0	1532.7	1535.3	1473.6	1473.9	1419.1	1417.8	1472.0	1472.3	1425.2	1424.2
b_2	1576.1	1567.5	1510.3	1500.2	1649.6	1648.6	1593.2	1585.4	1524.0	1515.7	1590.0	1582.0	1530.4	1521.6
a_1	1597.5	1606.5	1538.2	1542.8	1662.4	1681.9	1614.9	1626.5	1553.1	1560.4	1611.0	1622.9	1558.8	1566.7

a_1	3183.8	3124.4	3097.5	3032.8	3285.6	3231.3	3204.5	3146.4	3107.9	3044.6	3200.3	3142.0	3124.6	3061.5
b_2	3192.2	3130.3	3105.6	3038.1	3294.5	3238.2	3212.4	3152.0	3115.5	3049.6	3208.4	3147.6	3132.3	3066.4
a_1	3203.3	3165.4	3118.1	3076.5	3305.0	3270.2	3222.1	3185.9	3126.5	3086.5	3218.3	3181.7	3143.2	3103.3
b_2	3211.1	3172.0	3126.2	3082.2	3312.8	3279.2	3228.7	3190.0	3133.1	3089.6	3225.2	3186.5	3150.0	3106.8
a_1	3216.3	3179.6	3131.9	3091.0	3317.4	3285.2	3234.0	3197.9	3138.7	3098.9	3230.2	3194.0	3155.4	3115.7

Table 8: Predicted harmonic vibrational frequencies (cm^{-1}) for the C_6H_5NH radical and its anion.

Sym.	B3LYP		BLYP		BHLYP		B3P86		BP86		B3PW91		BPW91	
	neutral	anion	neutral	anion	neutral	anion	neutral	anion	neutral	anion	neutral	anion	neutral	anion
a"	197.6	175.8	187.2	169.2	209.7	183.7	196.5	176.1	185.3	168.6	196.3	175.6	185.8	169.5
a"	386.7	425.7	373.7	412.0	401.5	443.0	384.1	425.1	369.5	409.9	383.2	424.0	370.0	410.5
a'	413.4	413.1	401.0	399.3	428.9	429.8	411.0	410.9	397.2	395.9	410.9	410.9	398.5	397.3
a"	486.1	490.2	470.0	471.7	503.1	512.9	483.8	488.4	465.8	467.5	483.3	487.3	467.4	468.9
a'	527.3	523.8	512.3	507.8	544.6	543.5	526.6	522.9	510.0	505.4	525.6	522.0	511.2	506.6
a'	609.9	615.2	591.4	596.9	632.0	638.4	608.4	614.2	588.0	593.8	607.5	613.1	589.4	595.3
a"	672.0	648.6	649.4	625.1	696.4	675.8	672.9	654.2	648.4	629.0	670.3	654.5	648.0	634.0
a"	673.8	680.0	652.9	655.6	699.9	708.6	673.7	680.0	649.3	650.2	672.2	677.6	651.7	652.8
a"	779.0	693.8	756.4	664.4	802.5	728.2	777.3	694.9	751.0	662.6	775.9	692.9	753.9	665.5
a'	825.9	793.3	796.3	766.5	857.1	825.3	830.9	791.9	802.2	760.4	830.5	790.1	804.8	763.8
a"	835.4	812.9	811.8	782.4	862.4	848.2	833.1	814.2	803.2	781.9	831.1	812.7	806.7	785.4
a"	918.0	815.7	890.3	788.5	947.4	849.6	914.0	821.0	881.2	789.0	912.9	818.6	885.2	791.5
a'	979.7	968.8	951.5	940.3	1011.9	1003.8	980.2	970.8	952.1	939.5	979.2	968.8	954.3	941.9
a"	984.3	924.0	953.2	883.8	1019.0	977.1	983.1	922.8	943.6	877.2	980.8	921.6	948.4	882.1
a"	995.9	941.0	963.6	902.7	1031.0	991.5	992.2	938.5	954.6	894.7	990.9	937.3	959.1	899.5
a'	1023.8	1018.5	990.1	983.1	1059.1	1059.1	1031.7	1027.2	996.5	990.2	1030.2	1025.6	1000.9	994.6
a'	1084.4	1058.4	1050.3	1023.3	1123.0	1100.7	1089.1	1063.8	1053.0	1026.4	1088.3	1062.6	1057.8	1031.0
a'	1161.8	1136.4	1130.2	1102.1	1193.9	1179.2	1162.6	1135.9	1129.2	1098.8	1162.3	1136.2	1134.3	1104.6
a'	1162.8	1167.7	1134.9	1133.5	1198.4	1211.6	1164.6	1167.3	1132.2	1129.5	1164.0	1167.4	1137.3	1134.9
a'	1175.5	1169.2	1146.8	1136.6	1213.9	1212.0	1175.6	1168.1	1142.8	1131.0	1175.3	1168.3	1148.0	1137.6
a'	1314.2	1331.8	1285.4	1290.7	1339.3	1387.4	1331.0	1326.5	1294.7	1280.1	1324.0	1326.4	1298.9	1286.5
a'	1344.3	1360.0	1307.6	1317.6	1379.1	1396.9	1342.5	1375.1	1305.3	1325.4	1341.8	1372.2	1308.7	1331.4
a'	1361.5	1372.9	1331.3	1322.5	1402.8	1433.7	1383.6	1387.1	1352.9	1339.5	1378.5	1384.0	1356.5	1344.2
a'	1464.1	1482.7	1418.5	1432.0	1520.7	1542.9	1471.1	1495.7	1423.2	1442.6	1468.3	1492.8	1428.3	1448.7
a'	1480.1	1506.8	1434.7	1447.7	1537.3	1575.7	1486.1	1524.4	1437.5	1460.0	1483.9	1521.3	1442.8	1467.2

a'	1567.9	1541.3	1504.7	1478.2	1636.0	1616.6	1584.4	1559.6	1518.1	1494.1	1581.0	1555.8	1524.1	1499.8
a'	1588.7	1624.2	1535.2	1562.6	1645.7	1693.2	1605.6	1646.5	1549.8	1582.4	1601.7	1642.5	1555.1	1589.0
a'	3174.9	3098.4	3088.6	3006.8	3276.6	3205.4	3193.8	3119.4	3096.7	3017.2	3190.0	3114.9	3113.9	3034.1
a'	3184.9	3108.2	3096.6	3017.1	3286.9	3214.3	3205.4	3129.8	3108.4	3029.1	3201.0	3125.2	3125.2	3045.7
a'	3193.3	3125.5	3106.5	3035.1	3295.6	3231.9	3213.3	3145.4	3116.0	3044.0	3209.1	3140.9	3132.8	3060.7
a'	3205.9	3155.4	3120	3065.2	3307.5	3261.9	3225.3	3175.3	3128.8	3074.1	3221.2	3171.0	3145.5	3091.1
a'	3215.0	3168.6	3129.8	3080.0	3316.2	3273.1	3233.7	3190.0	3137.5	3091.1	3229.8	3185.4	3154.3	3107.0
a'	3433.2	3403.1	3307.4	3268.9	3588.6	3557.2	3467.6	3436.9	3326.0	3291.6	3466.3	3434.6	3349.5	3315.1

Table 9. Predicted harmonic vibrational frequencies (cm^{-1}) for the C_6H_5PH radical and its anion.

Sym.	B3LYP		BLYP		BHLYP		B3P86		BP86		B3PW91		BPW91	
	neutral	anion	neutral	anion	neutral	anion	neutral	anion	neutral	anion	neutral	anion	neutral	anion
a"	164.3	162.4	158.0	156.6	172.1	169.9	163.5	162.7	156.2	156.1	163.2	162.2	156.9	156.7
a'	257.5	257.3	250.2	250.0	267.2	265.5	255.3	255.8	247.2	247.7	254.9	255.3	247.4	248.1
a"	302.2	316.8	300.7	315.7	311.0	312.0	304.6	326.3	302.0	322.6	298.9	323.8	297.5	323.8
a'	399.5	397.6	386.6	384.8	414.7	410.5	402.9	402.4	389.6	??	401.4	401.0	390.1	389.9
a"	411.9	415.7	400.0	403.3	427.6	431.3	410.1	414.5	396.6	388.9	408.7	413.3	396.7	401.1
a"	468.0	474.7	455.0	458.1	483.9	495.5	464.6	471.9	449.2	400.4	464.0	471.3	450.6	454.5
a'	618.9	622.0	600.8	603.8	641.3	645.4	616.9	620.1	596.7	599.9	615.9	619.2	598.1	601.3
a"	695.1	688.8	672.3	664.6	721.1	714.6	695.9	689.8	670.4	668.6	695.4	688.7	673.5	665.4
a'	705.5	876.5	682.4	847.3	733.4	914.3	709.3	875.9	684.7	??	707.2	874.4	686.1	846.6
a"	763.1	689.0	742.2	666.0	789.6	719.4	759.7	693.1	734.2	680.9	758.9	691.1	737.1	670.3
a"	865.7	716.1	841.4	688.4	897.3	749.7	860.7	713.3	830.8	801.9	860.7	712.1	835.1	684.0
a'	891.3	980.2	863.3	948.3	928.5	1018.6	890.2	985.6	859.1	843.2	888.8	983.6	862.2	954.6
a"	938.6	839.0	909.5	813.5	974.8	872.2	933.6	832.0	898.8	808.3	932.9	832.2	903.3	805.5
a"	995.2	850.3	962.2	819.2	1033.2	892.2	991.1	844.6	952.4	902.7	990.5	844.2	957.4	812.1
a"	997.8	947.9	965.8	910.0	1036.5	998.3	1001.8	945.5	961.5	916.3	1000.0	945.4	966.6	907.9
a"	1004.6	961.5	968.7	926.0	1048.1	1008.0	1002.7	957.2	968.4	951.9	1001.8	957.0	970.9	921.3
a'	1037.8	1029.6	1003.9	993.4	1075.2	1072.5	1045.8	1037.7	1009.6	999.5	1043.8	1035.9	1013.4	1003.7
a'	1096.4	1079.6	1055.8	1044.2	1140.2	1122.5	1104.9	1084.5	1066.0	1046.9	1103.9	1083.5	1069.1	1051.7
a'	1100.1	1090.1	1066.2	1050.0	1141.1	1136.0	1108.2	1102.8	1068.6	1060.8	1104.8	1099.7	1073.4	1064.9
a'	1172.4	1151.8	1143.0	1119.4	1206.2	1191.6	1172.1	1149.8	1138.7	1113.6	1172.3	1150.3	1144.5	1119.7
a'	1198.8	1187.6	1166.0	1154.4	1240.1	1230.8	1198.7	1186.7	1162.4	1149.9	1198.7	1187.0	1168.0	1155.7
a'	1315.8	1292.7	1277.9	1252.8	1348.0	1331.7	1320.1	1296.8	1275.6	1251.8	1319.1	1295.7	1281.6	1257.6
a'	1351.6	1347.8	1318.0	1310.3	1391.9	1388.1	1371.5	1362.5	1338.6	1322	1367.0	1359.1	1343.0	1327.0
a'	1452.4	1450.0	1405.3	1404.1	1510.4	1506.0	1458.8	1461.4	1409.1	1413.9	1456.8	1458.6	1414.5	1419.5
a'	1488.0	1473.4	1437.8	1422.9	1550.9	1538.6	1491.6	1477.1	1436.5	1422.1	1490.0	1475.4	1443.0	1428.3

a'	1593.0	1557.3	1527.3	1489.8	1665.5	1639.8	1611.4	1574.2	1542.9	1504.2	1608.3	1571.3	1549.7	1510.2
a'	1609.8	1608.6	1546.8	1546.8	1679.5	1681.4	1628.3	1628.5	1562.5	1564.3	1624.6	1624.9	1568.6	1570.6
a'	2350.4	2272.4	2262.0	2188.0	2453.0	2369.2	2371.2	2297.7	2275.7	2207.4	2364.8	2290.5	2287.3	2218.0
a'	3173.8	3121.2	3087.9	3029.9	3275.3	3228.4	3192.6	3142.7	3096.7	3041.3	3189.1	3138.5	3113.9	3058.5
a'	3178.7	3125.8	3092.3	3034.0	3280.6	3233.4	3197.1	3146.7	3100.7	3045.4	3193.7	3142.8	3117.7	3062.3
a'	3189.0	3148.0	3103.4	3057.8	3290.9	3255.2	3207.9	3167.9	3112.0	3067.3	3204.1	3164.6	3128.7	3085.0
a'	3195.8	3156.4	3109.8	3066.9	3298.4	3263.3	3215.6	3174.1	3118.9	3074	3211.7	3170.8	3135.7	3091.6
a'	3207.7	3173.1	3122.6	3084.7	3309.4	3277.1	3227.5	3194.2	3131.2	3095.6	3223.4	3189.6	3147.9	3112.0

Table 10. Predicted harmonic vibrational frequencies (cm^{-1}) for the $C_6H_5CH_2$ radical and its anion.

Sym.	B3LYP		BLYP		BHLYP		B3P86		BP86		B3PW91		BPW91		Expt.
	neutral	anion	neutral	anion	neutral	anion	neutral	anion	neutral	anion	neutral	anion	neutral	anion	Neutral[a]
b_1	204.2	173.8	197.4	170.1	211.8	178.3	203.1	173.9	195.2	169.0	202.7	173.2	195.7	169.5	
b_2	354.5	351.9	346.2	343.0	366.3	363.3	350.1	347.4	340.2	337.0	350.4	347.5	341.3	338.1	
a_2	393.2	428.6	382.5	415.1	406.0	445.7	390.3	427.8	377.8	412.6	389.2	426.5	378.2	413.2	
b_1	489.9	471.4	477.7	457.2	502.8	489.0	485.1	465.3	470.3	447.3	484.3	463.6	471.4	447.5	430.0
a_2	508.8	532.6	502.2	510.6	523.8	559.5	504.2	536.6	495.3	512.0	501.1	537.9	494.0	518.5	
a_1	526.6	520.8	512.7	506.1	543.2	539.3	525.3	519.2	509.7	502.8	524.4	518.4	510.8	503.9	
b_2	618.5	619.6	601.1	602.0	639.3	642.0	617.0	618.3	597.5	598.7	616.0	617.3	599.0	600.1	
b_1	687.8	554.8	668.0	538.9	708.3	571.1	686.9	542.0	663.8	517.1	685.7	537.3	666.1	516.3	667.0
b_1	750.1	668.0	738.9	644.6	762.4	694.0	741.5	665.0	725.2	635.3	737.8	662.0	725.6	636.8	710.9
b_1	810.5	697.3	798.4	671.7	823.9	727.9	802.5	696.1	783.5	667.0	798.4	694.0	783.5	668.8	762.0
a_1	826.5	807.1	800.0	779.0	854.4	839.7	832.7	814.5	805.0	785.2	830.6	812.4	807.4	787.5	
a_2	853.3	812.8	831.0	790.8	878.8	840.7	847.7	807.3	820.1	780.2	846.9	805.6	823.4	781.9	
b_1	919.3	825.8	892.9	801.1	947.9	853.8	914.3	820.6	882.1	790.2	913.0	817.8	885.8	791.9	882.0
b_2	971.4	951.5	944.7	923.1	1005.5	988.3	970.4	950.4	940.5	918.9	970.0	949.7	944.6	922.9	948.1
a_2	989.2	945.5	957.8	906.9	1018.8	996.5	985.0	941.8	947.6	897.6	983.8	940.7	952.2	901.9	
a_1	986.6	968.9	957.6	941.3	1025.4	1002.5	990.6	971.0	959.2	940.8	988.5	969.0	961.6	943.0	
b_1	997.6	936.1	964.3	896.1	1034.6	988.2	994.1	933.6	955.1	888.5	992.5	932.3	959.6	892.8	
a_1	1032.8	1016.4	999.2	981.2	1067.9	1056.9	1041.1	1025.7	1005.8	988.9	1039.7	1024.1	1010.4	993.3	
b_2	1111.4	1088.2	1079.9	1055.2	1148.8	1129.3	1114.0	1090.8	1079.6	1054.9	1113.3	1090.1	1084.5	1059.8	1015.0
b_2	1166.9	1146.9	1139.0	1115.4	1316.7	1187.1	1166.8	1143.8	1134.7	1108.3	1167.0	1144.5	1140.5	1114.5	
a_1	1179.5	1180.2	1151.5	1148.7	1214.3	1221.5	1179.8	1178.6	1147.9	1143.2	1179.8	1179.2	1153.6	1149.5	
a_1	1286.1	1325.5	1260.7	1285.3	1198.2	1374.7	1293.4	1329.6	1264.4	1285.6	1288.5	1327.7	1266.1	1291.2	1264.0
b_2	1337.2	1310.5	1299.3	1271.2	1371.6	1357.9	1335.1	1309.6	1291.3	1265.5	1334.7	1308.8	1297.3	1271.2	1305.0
b_2	1354.1	1355.5	1324.1	1315.5	1393.5	1398.2	1378.0	1369.3	1347.1	1325.6	1372.8	1366.0	1351.0	1330.5	
b_2	1466.5	1480.9	1420.1	1432.7	1522.1	1536.0	1473.5	1497.4	1424.5	1447.7	1471.1	1493.8	1429.8	1453.5	1446.0

a_1	1487.5	1464.4	1443.5	1422.3	1542.9	1520.9	1485.6	1460.8	1438.4	1413.3	1485.0	1460.1	1445.0	1419.9	1409.0
a_1	1503.1	1521.1	1467.1	1469.7	1553.6	1582.9	1507.4	1533.4	1464.5	1476.0	1504.1	1530.0	1468.7	1482.5	1469
b_2	1578.4	1526.5	1515.3	1465.2	1645.0	1600.4	1596.7	1542.4	1530.7	1477.9	1593.3	1539.0	1537.1	1483.4	
a_1	1598.6	1627.3	1543.4	1568.9	1656.9	1693.0	1616.8	1648.6	1558.9	1587.6	1612.9	1644.6	1564.4	1594.1	
a_1	3157.1	3100.1	3077.1	3010.0	3251.2	3205.5	3174.0	3122.0	3083.1	3021.9	3170.1	3117.6	3099.8	3038.5	3069.0
a_1	3173.4	3118.7	3087.2	3037.1	3275.2	3214.1	3193.6	3136.8	3096.9	3045.1	3189.7	3132.3	3114.1	3060.9	
b_2	3175.6	3103.1	3089.1	3012.8	3277.7	3209.0	3195.5	3124.7	3098.5	3024.3	3191.9	3120.4	3116.0	3041.0	3111.0
a_1	3188.3	3135.1	3102.6	3046.8	3289.9	3240.6	3208.0	3155.1	3111.8	3055.8	3204.2	3151.3	3128.8	3072.9	
b_2	3193.2	3131.1	3106.9	3040.9	3295.4	3237.6	3213.3	3151.7	3116.6	3051.4	3209.3	3148.0	3133.5	3068.6	
a_1	3207.3	3170.0	3122.2	3081.7	3308.5	3273.9	3226.9	3191.2	3131.2	3092.7	3222.7	3186.4	3147.7	3108.7	
b_2	3257.7	3197.7	3174.0	3115.0	3355.1	3294.1	3278.5	3219.4	3183.4	3125.7	3274.2	3214.4	3200.7	3141.7	

[a]Assigned from IR spectrum:[57]

Table 11. Predicted harmonic vibrational frequencies (cm^{-1}) for the $C_6H_5SiH_2$ radical and its anion.

Sym.	B3LYP		BLYP		BHLYP		B3P86		BP86		B3PW91		BPW91	
	neutral	anion	neutral	anion	neutral	anion	neutral	anion	neutral	anion	neutral	anion	neutral	anion
a'	156.1	156.5	155.9	151.2	162.1	163.1	155.0	156.9	149.6	150.8	154.8	156.4	149.9	151.2
a"	151.3	72.8	151.5	79.4	150.3	58.9	149.4	77.2	152.9	84.1	147.4	78.7	150.8	89.0
a"	200.9	202.7	198.1	198.6	206.8	207.9	195.6	198.7	191.5	194.0	195.6	198.7	191.2	194.2
a'	390.2	352.1	378.3	340.5	404.0	364.8	392.4	358.3	379.9	346.5	390.9	356.3	380.4	347.0
a"	399.6	400.3	386.9	386.8	416.2	418.0	397.0	398.4	382.6	383.4	396.1	397.4	383.2	384.1
a'	449.1	452.9	436.8	438.5	465.0	471.1	444.7	449.5	430.0	433.1	443.9	449.0	430.9	434.3
a'	621.3	655.1	595.5	627.7	672.4	688.3	617.6	653.1	579.4	621.5	618.3	652.1	584.6	623.8
a"	1000.8	624.1	603.5	606.1	644.0	647.3	619.2	622.2	599.2	602.0	618.4	621.2	600.7	603.4
a"	660.1	724.1	641.6	699.7	684.7	755.0	655.7	722.7	633.9	695.1	655.0	721.2	636.3	697.8
a'	699.4	704.2	677.6	679.7	725.9	735.9	701.5	702.8	677.7	675.4	699.4	701.9	679.1	678.1
a'	704.7	679.1	681.6	655.4	732.7	710.6	705.3	678.2	679.9	652.9	704.3	676.8	682.3	654.8
a'	760.3	759.8	738.0	729.5	789.8	799.1	756.5	755.7	729.7	921.3	755.5	754.7	732.3	724.4
a"	876.8	857.9	852.7	832.3	909.3	893.6	871.2	853.5	841.6	822.3	870.3	853.7	844.7	826.8
a'	923.5	891.6	898.8	855.7	957.5	936.5	917.2	887.2	887.7	845.9	916.7	887.1	892.1	850.7
a'	942.9	938.6	913.5	909.6	981.6	978.1	937.7	932.9	902.6	898.9	936.5	931.2	906.3	903.2
a"	999.0	975.3	965.4	939.4	1042.4	1022.6	994.7	971.9	955.3	930.3	993.4	971.9	959.6	935.9
a'	628.4	963.5	969.2	924.4	1038.2	1015.4	1004.1	962.9	963.6	918.4	1002.2	962.8	968.1	924.2
a'	1007.4	994.4	970.9	961.7	1053.2	1033.7	1005.3	998.0	970.9	963.9	1004.0	996.2	973.5	966.5
a'	1041.7	1031.9	1008.0	996.8	1080.9	1074.0	1049.7	1040.0	1013.6	1002.1	1047.8	1037.8	1017.5	1005.7
a"	1095.5	1076.5	1061.4	1041.1	1136.0	1119.0	1101.3	1082.2	1065.1	1044.7	1100.1	1081.1	1069.7	1049.5
a'	1115.2	1082.7	1074.1	1042.0	1161.7	1131.7	1125.3	1092.2	1082.3	1049.8	1122.1	1089.6	1085.8	1053.6
a"	1174.1	1155.2	1144.5	1123.5	1208.3	1193.3	1173.8	1153.8	1140.3	1118.2	1174.0	1154.4	1146.1	1124.3
a'	1202.3	1189.7	1169.2	1155.9	1244.7	1233.7	1202.6	1189.2	1166.0	1152.0	1202.7	1189.4	1171.9	1157.9
a"	1311.5	1296.1	1276.2	1258.6	1338.8	1327.0	1320.7	1303.7	1278.5	1260.0	1319.2	1302.4	1284.4	1265.9
a"	1354.3	1345.2	1319.6	1309.1	1397.2	1387.4	1370.9	1361.0	1337.1	1323.6	1366.6	1357.1	1341.5	1328.4

a"	1448.8	1439.3	1401.9	1392.7	1507.7	1498.1	1455.1	1447.1	1404.8	1398.4	1453.1	1444.8	1410.4	1404.1
a'	1500.2	1484.0	1449.9	1433.0	1563.9	1549.8	1504.2	1487.4	1449.1	1431.6	1502.6	1485.9	1455.5	1437.8
a"	1602.4	1583.0	1537.0	1514.7	1677.7	1663.7	1621.3	1600.7	1553.2	1529.6	1618.1	1597.6	1559.9	1535.8
a'	1621.8	1605.7	1555.6	1540.4	1698.1	1684.4	1640.8	1624.9	1572.0	1557.4	1637.4	1621.4	1578.5	1563.6
a'	2189.9	1937.2	2125.2	1878.8	2266.9	2003.9	2202.7	1956.4	2130.1	1890.7	2195.2	1947.9	2138.0	1898.5
a"	2220.0	1936.5	2159.8	1883.9	2291.4	1995.0	2232.8	1957.4	2164.4	1897.5	2224.5	1948.5	2171.2	1904.5
a'	3167.4	3121.7	3082.0	3029.7	3268.6	3228.7	3186.6	3143.1	3091.0	3041.3	3183.3	3139.2	3108.5	3058.6
a"	3168.4	3126.7	3083.3	3034.9	3269.6	3233.9	3187.4	3147.3	3091.9	3045.7	3184.3	3143.8	3109.7	3063.3
a'	3182.5	3144.2	3096.7	3054.4	3284.3	3250.2	3202.7	3163.9	3106.5	3063.8	3198.7	3160.6	3123.4	3081.5
a"	3191.5	3146.5	3105.0	3055.5	3294.0	3253.7	3211.8	3166.7	3115.1	3065.4	3207.8	3163.2	3131.9	3083.0
a'	3204.5	3168.6	3118.9	3079.7	3306.4	3273.2	3224.3	3189.6	3128.2	3090.5	3220.2	3185.2	3144.8	3107.1