Combining quantum mechanics and machine-learning calculations for anharmonic corrections to vibrational frequencies

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Table S1: Radial Symmetry Function Parameters for e_1 and e_2; $\eta/Bohr^{-2}$, r_s, and $r_c/Bohr$. e_1 and e_2 denote the chemical element of neighbor atoms. X denote a none hydrogen chemical element.

e_1	e_2	η	r_s	r_c
H	H			12.0
		0.001	0	
		0.010	0	
		0.030	0	
		0.060	0	
		0.150	1.9	
		0.300	1.9	
		0.600	1.9	
		1.500	1.9	
		2.500	2.5	
X	H			12.0
		0.001	0.9	
		0.010	0.9	
		0.030	0.9	
		0.060	0.9	
		0.150	0.9	
		0.300	0.9	
		0.600	0.9	
		1.500	0.9	
X	X			12.0
		0.001	0.0	
		0.010	0.0	
		0.030	0.0	
		0.060	0.0	
		0.150	4.0	
		0.300	4.0	
		0.600	4.0	
		1.500	4.0	
		2.500	6.0	

Table S2: Angular Symmetry Function Parameters for $\eta/Bohr^{-2}$, λ, ξ and $r_c/Bohr$. We used the same angular parameters for all kind of atom types

η	λ	ξ	r_c
0.001	-1	4.0	12.0
0.001	+1	4.0	12.0
0.01	-1	4.0	12.0
0.01	+1	4.0	12.0
0.03	-1	1.0	12.0
0.03	+1	1.0	12.0
0.07	-1	1.0	12.0
0.07	+1	1.0	12.0

Table S3: RMSD for Forces/meV/Å and energies/meV of traning and testing sets

Molecule	Force Train	Force Test	Energy Train	Energy Test
H_2O	6.506	14.455	0.146	0.132
KrF_2	17.223	13.620	0.670	0.647
OCSe	5.649	3.990	0.155	0.048
SO_2	13.136	25.867	0.407	0.426
SeO_2	11.613	3.931	0.408	0.121
CSe_2	20.412	21.520	0.391	0.688
TiO_2	12.889	28.717	0.246	0.524
NH_3	7.585	10.537	0.110	0.183
ClF_3	22.766	7.437	0.482	0.334
H_2CO	12.033	8.376	0.250	0.187
H_2O_2	22.608	26.805	0.406	0.441
$GaCl_3$	4.997	9.278	0.132	0.066
AlF_2Cl	8.263	7.015	0.105	0.083
$AlFCl_2$	15.561	15.521	0.263	0.340
$ZnCH_2$	22.115	51.789	0.369	1.026
CH_4	7.057	7.092	0.078	0.012
$CHBr_3$	13.719	24.724	0.236	0.843
$SiBr_4$	5.111	7.680	0.046	0.022
$TiCl_4$	17.804	26.316	0.347	0.292
CBr_4	8.713	10.278	0.095	0.087
CH_2O_2	14.888	26.396	0.222	0.262
CH_2NH	17.038	13.584	0.167	0.050
CH_3OH	12.453	18.849	0.104	0.185
CH_3SeH	17.914	19.430	0.214	0.384
C_2H_3Br	18.851	31.459	0.276	0.738
CH_2CHCl	14.960	31.402	0.198	0.745
SeF_6	17.520	22.812	0.220	0.237
$C_2H_4Br_2$	14.675	16.463	0.107	0.139
GeH_3CH_3	13.847	21.653	0.129	0.318
C_2H_5Br	19.213	49.261	0.147	0.485
C_3H_6	11.271	13.742	0.092	0.116
C_3H_6O	23.223	42.517	0.132	0.542
$C_3H_4O_3$	16.870	46.623	0.091	0.409
C_6H_6	15.631	11.112	0.050	0.041
C_4H_8S	23.233	27.076	0.146	0.136
$C_2H_6O_4S$	17.490	18.351	0.082	0.074
$C_{10}H_8$	23.168	29.026	0.080	0.070
Average	14.811	20.668	0.211	0.309

Table S4: Fundamental frequencies/cm^{-1} calculated using Full B2PLYP, Hybrdid B2PLYP/ANN and Full ANN methods. Experimental values are taken from NIST DataBase

Molecule	Experience	B2PLYP	Hybrid	ANN
H_2O	1595.00	1591.69	1589.34	1579.09
H_2O	3657.00	3660.96	3673.11	3668.21
H_2O	3756.00	3757.75	3757.69	3753.02
KrF_2	235.10	230.91	234.68	226.91
KrF_2	235.10	231.28	234.68	226.91
KrF_2	449.00	453.12	455.05	453.16
KrF_2	592.50	576.03	576.05	578.10
OCSe	463.00	475.31	472.51	470.09
OCSe	463.00	475.31	472.51	470.09
OCSe	643.50	653.62	652.37	653.88
OCSe	2023.50	1985.02	2018.34	2017.65
SO_2	518.00	509.17	502.31	509.14
SO_2	1151.00	1121.48	1117.97	1122.51
SO_2	1362.00	1326.36	1327.41	1323.60
SeO_2	372.50	357.93	355.36	360.33
SeO_2	922.00	905.30	903.10	902.30
SeO_2	965.60	955.84	952.78	952.59
CSe_2	313.10	320.60	317.13	324.25
CSe_2	313.10	320.60	317.13	324.25
CSe_2	369.10	369.03	368.92	372.38
CSe_2	1301.90	1315.66	1315.37	1313.50
TiO_2	323.00	326.79	325.69	313.41
TiO_2	944.00	916.08	916.20	916.34
TiO_2	959.00	915.81	914.89	918.87
NH_3	950.00	967.89	944.08	948.40
NH_3	1627.00	1634.88	1635.27	1630.33
NH_3	1627.00	1633.60	1635.02	1630.73
NH_3	3337.00	3361.41	3369.95	3375.14
NH_3	3444.00	3457.60	3434.44	3434.05
NH_3	3444.00	3460.49	3435.01	3435.39
ClF_3	328.00	308.38	310.55	309.23
ClF_3	328.00	324.40	326.71	314.00
ClF_3	442.00	416.63	415.89	416.49
ClF_3	529.00	514.94	513.28	518.36
ClF_3	702.00	693.23	696.88	692.84
ClF_3	752.00	744.45	747.51	739.72
H_2CO	1167.00	1189.30	1186.74	1170.81
H_2CO	1249.00	1252.84	1250.62	1253.39
H_2CO	1500.00	1511.83	1509.12	1510.50
H_2CO	1746.00	1760.79	1759.53	1761.00
H_2CO	2782.00	2772.68	2790.00	2779.97

Table S4: Fundamental frequencies/cm^{-1} calculated using Full B2PLYP, Hybrdid B2PLYP/ANN and Full ANN methods. Experimental values are taken from NIST DataBase (Continued)

Molecule	Experience	B2PLYP	Hybrid	ANN
H_2CO	2843.00	2843.70	2846.42	2840.81
H_2O_2	878.00	902.66	907.47	899.90
H_2O_2	1274.00	1270.63	1256.18	1273.71
H_2O_2	1394.00	1396.94	1362.74	1392.49
H_2O_2	3615.00	3609.80	3582.05	3612.52
H_2O_2	3614.00	3606.42	3646.11	3558.79
$GaCl_3$	131.00	124.68	125.86	125.58
$GaCl_3$	131.00	124.70	125.87	125.62
$GaCl_3$	143.00	139.50	140.55	140.21
$GaCl_3$	382.00	377.80	377.40	377.47
$GaCl_3$	464.00	466.22	465.53	465.90
$GaCl_3$	464.00	466.24	465.45	465.94
AlF_2Cl	200.00	186.52	187.84	184.50
AlF_2Cl	250.00	235.69	236.97	240.04
AlF_2Cl	260.00	264.83	264.81	264.68
AlF_2Cl	500.00	501.32	503.54	501.13
AlF_2Cl	820.00	818.97	817.44	820.09
AlF_2Cl	900.00	933.81	931.41	934.42
$AlFCl_2$	150.00	151.34	153.18	153.24
$AlFCl_2$	200.00	205.43	204.72	205.24
$AlFCl_2$	220.00	234.82	233.54	233.02
$AlFCl_2$	450.00	431.99	431.69	434.28
$AlFCl_2$	610.00	627.85	625.29	629.36
$AlFCl_2$	850.00	877.34	880.15	875.51
$ZnCH_2$	513.70	501.89	501.98	506.29
$ZnCH_2$	524.80	538.37	568.14	548.79
$ZnCH_2$	543.80	629.66	620.28	612.81
$ZnCH_2$	1341.50	1359.10	1367.89	1346.15
$ZnCH_2$	2958.50	2991.15	2981.05	3000.00
$ZnCH_2$	3047.20	3072.84	3050.98	3061.70
CH_4	1306.00	1307.51	1312.30	1313.03
CH_4	1306.00	1307.45	1312.33	1313.50
CH_4	1306.00	1307.45	1312.34	1313.85
CH_4	1534.00	1528.38	1509.50	1516.47
CH_4	1534.00	1528.27	1509.47	1516.99
CH_4	2917.00	2932.19	2953.98	2954.61
CH_4	3019.00	3016.84	3021.29	3018.91
CH_4	3019.00	3016.22	3020.05	3019.28
CH_4	3019.00	3015.91	3020.87	3019.91
$CHBr_3$	155.00	151.22	151.52	150.26

Table S4: Fundamental frequencies/cm^{-1} calculated using Full B2PLYP, Hybrdid B2PLYP/ANN and Full ANN methods. Experimental values are taken from NIST DataBase (Continued)

Molecule	Experience	B2PLYP	Hybrid	ANN
$CHBr_3$	155.00	151.31	151.60	150.28
$CHBr_3$	222.00	222.32	222.12	227.55
$CHBr_3$	541.00	537.00	536.60	536.54
$CHBr_3$	669.00	647.91	649.98	649.29
$CHBr_3$	669.00	647.63	650.65	649.30
$CHBr_3$	1149.00	1153.84	1155.09	1147.74
$CHBr_3$	1149.00	1153.70	1155.17	1147.74
$CHBr_3$	3042.00	3074.30	3080.68	3082.61
$SiBr_4$	90.00	86.59	86.38	85.12
$SiBr_4$	90.00	86.61	86.41	85.13
$SiBr_4$	137.00	135.45	135.78	135.29
$SiBr_4$	137.00	135.47	135.79	135.30
$SiBr_4$	137.00	135.52	135.86	135.31
$SiBr_4$	249.00	245.94	246.13	246.28
$SiBr_4$	487.00	488.93	488.67	488.37
$SiBr_4$	487.00	488.91	488.93	488.38
$SiBr_4$	487.00	488.86	488.99	488.40
$TiCl_4$	114.00	112.40	112.59	114.08
$TiCl_4$	114.00	112.42	112.52	114.09
$TiCl_4$	136.00	132.76	133.78	127.47
$TiCl_4$	136.00	132.83	133.81	127.50
$TiCl_4$	136.00	132.58	133.78	127.52
$TiCl_4$	389.00	375.98	376.13	374.97
$TiCl_4$	498.00	491.95	493.60	491.50
$TiCl_4$	498.00	492.12	493.43	491.51
$TiCl_4$	498.00	492.18	493.69	491.51
CBr_4	122.00	125.31	126.15	124.12
CBr_4	122.00	125.14	126.16	124.12
CBr_4	182.00	183.25	185.55	185.18
CBr_4	182.00	183.34	185.58	185.18
CBr_4	182.00	183.42	185.67	185.18
CBr_4	267.00	268.21	270.34	269.01
CBr_4	672.00	656.77	652.78	653.14
CBr_4	672.00	656.35	652.91	653.18
CBr_4	672.00	655.93	652.93	653.14
CH_2O_2	625.00	623.11	609.38	614.53
CH_2O_2	638.00	642.52	681.05	662.05
CH_2O_2	1033.00	1038.90	1045.23	1029.98
CH_2O_2	1105.00	1095.18	1097.45	1091.20
CH_2O_2	1229.00	1299.13	1255.29	1248.31

Table S4: Fundamental frequencies/cm^{-1} calculated using Full B2PLYP, Hybrdid B2PLYP/ANN and Full ANN methods. Experimental values are taken from NIST DataBase (Continued)

Molecule	Experience	B2PLYP	Hybrid	ANN
CH_2O_2	1387.00	1383.78	1411.24	1394.77
CH_2O_2	1770.00	1770.81	1771.15	1771.80
CH_2O_2	2943.00	2930.55	2929.01	2923.55
CH_2O_2	3570.00	3553.49	3536.89	3541.98
CH_2NH	1058.00	1063.96	1078.68	1066.59
CH_2NH	1061.00	1085.17	1068.71	1057.10
CH_2NH	1127.00	1142.10	1100.68	1109.04
CH_2NH	1344.00	1343.97	1336.75	1344.66
CH_2NH	1452.00	1467.72	1464.92	1469.26
CH_2NH	1638.00	1659.17	1646.45	1647.39
CH_2NH	2914.00	2886.71	2890.67	2901.73
CH_2NH	3025.00	2962.90	3025.78	2956.77
CH_2NH	3263.00	3301.56	3288.54	3285.55
CH_3OH	-	281.51	258.73	269.82
CH_3OH	1033.00	1027.87	1022.32	1013.19
CH_3OH	1060.00	1073.61	1082.58	1079.21
CH_3OH	-	1154.66	1144.54	1155.20
CH_3OH	1345.00	1332.27	1330.47	1342.43
CH_3OH	1455.00	1460.73	1497.96	1485.38
CH_3OH	1477.00	1471.77	1485.09	1476.66
CH_3OH	1477.00	1482.54	1490.21	1488.32
CH_3OH	2844.00	2841.50	2898.37	2887.10
CH_3OH	2960.00	2921.76	2928.62	2938.11
CH_3OH	3000.00	3002.57	2999.85	3003.39
CH_3OH	3681.00	3679.22	3632.35	3641.25
CH_3SeH	145.00	155.11	175.36	130.37
CH_3SeH	590.00	584.57	585.79	586.97
CH_3SeH	712.00	718.04	708.65	738.47
CH_3SeH	921.00	923.67	936.04	944.72
CH_3SeH	980.00	988.32	982.25	974.44
CH_3SeH	1288.00	1298.85	1292.75	1299.23
CH_3SeH	1433.00	1438.10	1437.43	1420.02
CH_3SeH	1447.00	1452.22	1449.25	1427.40
CH_3SeH	2330.00	2336.59	2379.26	2351.18
CH_3SeH	2955.00	2979.01	2980.42	2974.23
CH_3SeH	3027.00	3039.15	3067.70	3058.30
CH_3SeH	3032.00	3046.16	3076.27	3071.07
C_2H_3Br	344.00	347.83	339.18	328.18
C_2H_3Br	582.00	597.04	586.52	540.69
C_2H_3Br	612.00	605.83	604.61	597.64

Table S4: Fundamental frequencies/cm^{-1} calculated using Full B2PLYP, Hybrdid B2PLYP/ANN and Full ANN methods. Experimental values are taken from NIST DataBase (Continued)

Molecule	Experience	B2PLYP	Hybrid	ANN
C_2H_3Br	901.00	919.03	912.05	896.94
C_2H_3Br	941.00	960.88	936.70	908.79
C_2H_3Br	1005.00	1012.93	1009.30	972.34
C_2H_3Br	1258.00	1268.22	1258.42	1236.51
C_2H_3Br	1373.00	1382.87	1338.97	1388.26
C_2H_3Br	1602.00	1619.06	1599.41	1595.08
C_2H_3Br	3027.00	3053.92	3039.82	3034.56
C_2H_3Br	3087.00	3100.11	3095.28	3093.65
C_2H_3Br	3112.00	3128.97	3116.88	3128.66
CH_2CHCl	395.00	400.30	392.45	383.14
CH_2CHCl	620.00	629.04	619.07	589.65
CH_2CHCl	720.00	710.68	707.50	707.40
CH_2CHCl	896.00	908.45	901.60	891.63
CH_2CHCl	941.00	958.12	941.52	917.07
CH_2CHCl	1030.00	1034.65	1014.37	1003.45
CH_2CHCl	1279.00	1291.54	1277.22	1273.19
CH_2CHCl	1368.00	1377.01	1336.22	1364.61
CH_2CHCl	1608.00	1626.05	1608.51	1607.35
CH_2CHCl	3030.00	3057.31	3045.36	3044.29
CH_2CHCl	3086.00	3091.23	3097.75	3100.48
CH_2CHCl	3121.00	3130.71	3152.74	3153.16
SeF_6	264.00	-	257.19	265.75
SeF_6	264.00	-	257.19	265.75
SeF_6	264.00	-	257.19	265.75
SeF_6	405.00	-	392.90	401.63
SeF_6	405.00	-	392.90	401.63
SeF_6	405.00	-	392.90	401.63
SeF_6	437.00	-	428.64	427.82
SeF_6	437.00	-	428.64	427.82
SeF_6	437.00	-	428.64	427.82
SeF_6	659.00	-	645.75	648.87
SeF_6	659.00	-	645.76	648.87
SeF_6	707.00	-	695.45	696.83
SeF_6	780.00	-	767.24	768.64
SeF_6	780.00	-	767.23	768.64
SeF_6	780.00	-	767.24	768.65
$C_2H_4Br_2$	118.00	103.78	100.39	126.11
$C_2H_4Br_2$	190.00	181.02	180.05	188.78
$C_2H_4Br_2$	193.00	187.04	189.02	189.35
$C_2H_4Br_2$	589.00	592.43	587.11	592.36

Table S4: Fundamental frequencies/cm^{-1} calculated using Full B2PLYP, Hybrdid B2PLYP/ANN and Full ANN methods. Experimental values are taken from NIST DataBase (Continued)

Molecule	Experience	B2PLYP	Hybrid	ANN
$C_2H_4Br_2$	660.00	662.51	659.95	659.33
$C_2H_4Br_2$	753.00	751.73	771.20	792.24
$C_2H_4Br_2$	933.00	946.07	925.73	922.38
$C_2H_4Br_2$	1053.00	1047.80	1073.19	1067.13
$C_2H_4Br_2$	1087.00	1089.53	1082.48	1098.02
$C_2H_4Br_2$	1186.00	1196.58	1188.59	1190.89
$C_2H_4Br_2$	1255.00	1265.55	1260.35	1222.31
$C_2H_4Br_2$	1255.00	1259.99	1282.54	1261.30
$C_2H_4Br_2$	1440.00	1457.86	1391.89	1430.64
$C_2H_4Br_2$	1441.00	1458.00	1410.51	1457.96
$C_2H_4Br_2$	2972.00	3009.87	3012.76	3019.19
$C_2H_4Br_2$	2974.00	3024.36	3025.11	3021.87
$C_2H_4Br_2$	3013.00	3046.51	3076.99	3066.06
$C_2H_4Br_2$	3037.00	3069.28	3095.35	3081.97
GeH_3CH_3	157.00	158.47	135.00	177.37
GeH_3CH_3	506.00	504.65	487.65	537.74
GeH_3CH_3	506.00	500.57	488.11	537.94
GeH_3CH_3	602.00	594.09	601.66	602.05
GeH_3CH_3	843.00	850.83	862.22	874.99
GeH_3CH_3	848.00	845.34	826.63	859.95
GeH_3CH_3	848.00	844.51	827.03	859.77
GeH_3CH_3	900.00	899.64	902.97	856.41
GeH_3CH_3	900.00	899.58	902.69	856.65
GeH_3CH_3	1254.00	1260.29	1210.82	1248.23
GeH_3CH_3	1428.00	1446.89	1384.08	1407.62
GeH_3CH_3	1428.00	1446.90	1386.07	1408.14
GeH_3CH_3	2084.00	2092.67	2100.44	2115.58
GeH_3CH_3	2084.00	2087.48	2100.10	2101.77
GeH_3CH_3	2085.00	2093.36	2128.08	2101.63
GeH_3CH_3	2938.00	2976.39	2932.50	2944.16
GeH_3CH_3	2997.00	3014.05	3037.26	3021.90
GeH_3CH_3	2997.00	3013.37	3034.36	3021.70
C_2H_5Br	247.00	252.51	241.65	276.97
C_2H_5Br	290.00	286.56	284.50	303.25
C_2H_5Br	583.00	566.11	567.62	570.83
C_2H_5Br	770.00	773.51	798.64	819.10
C_2H_5Br	964.00	962.54	989.43	985.08
C_2H_5Br	964.00	1027.29	1015.20	1047.31
C_2H_5Br	1061.00	1063.08	1067.90	1061.87
C_2H_5Br	1248.00	1244.98	1247.88	1221.65

Table S4: Fundamental frequencies/cm^{-1} calculated using Full B2PLYP, Hybrdid B2PLYP/ANN and Full ANN methods. Experimental values are taken from NIST DataBase (Continued)

Molecule	Experience	B2PLYP	Hybrid	ANN
C_2H_5Br	1252.00	1264.37	1270.54	1245.55
C_2H_5Br	1386.00	1391.00	1399.05	1394.83
C_2H_5Br	1451.00	1456.18	1423.41	1420.25
C_2H_5Br	1451.00	1457.03	1449.70	1446.63
C_2H_5Br	1451.00	1467.87	1425.77	1458.94
C_2H_5Br	2880.00	2964.79	2952.78	2939.96
C_2H_5Br	2937.00	2998.15	3011.05	2997.26
C_2H_5Br	2988.00	2999.81	3002.86	2993.48
C_2H_5Br	2988.00	3005.16	3013.40	3011.01
C_2H_5Br	3018.00	3041.32	3052.41	3034.95
C_3H_6	738.00	745.97	766.35	759.85
C_3H_6	738.00	744.55	765.14	759.90
C_3H_6	854.00	862.59	903.60	861.00
C_3H_6	868.00	864.99	880.46	872.25
C_3H_6	868.00	865.64	878.83	872.36
C_3H_6	1028.00	1040.42	1061.01	1064.73
C_3H_6	1028.00	1035.74	1063.92	1064.44
C_3H_6	1067.00	1076.34	1075.15	1077.91
C_3H_6	1127.00	1133.88	1121.98	1059.34
C_3H_6	1189.00	1193.05	1200.98	1206.17
C_3H_6	1191.00	1198.40	1181.47	1189.64
C_3H_6	1191.00	1196.02	1180.79	1189.67
C_3H_6	1440.00	1449.18	1359.31	1372.41
C_3H_6	1440.00	1447.21	1356.15	1372.06
C_3H_6	1499.00	1461.84	1381.09	1447.22
C_3H_6	3019.00	3045.73	3021.18	3014.68
C_3H_6	3019.00	3040.56	3014.03	3015.30
C_3H_6	3027.00	3050.25	3056.71	3055.95
C_3H_6	3082.00	3094.03	3096.73	3087.82
C_3H_6	3082.00	3088.44	3095.39	3088.08
C_3H_6	3102.00	3112.28	3108.83	3102.17
C_3H_6O	-	202.94	210.17	213.52
C_3H_6O	-	367.88	378.08	422.52
C_3H_6O	-	411.63	440.03	405.88
C_3H_6O	-	751.53	754.24	753.49
C_3H_6O	-	828.12	832.11	832.55
C_3H_6O	-	896.75	892.24	915.59
C_3H_6O	-	953.35	954.56	969.43
C_3H_6O	-	1025.84	1010.27	999.90
C_3H_6O	-	1111.31	1087.31	1095.10

Table S4: Fundamental frequencies/cm^{-1} calculated using Full B2PLYP, Hybrdid B2PLYP/ANN and Full ANN methods. Experimental values are taken from NIST DataBase (Continued)

Molecule	Experience	B2PLYP	Hybrid	ANN
C_3H_6O	-	1136.05	1128.44	1116.67
C_3H_6O	-	1146.49	1138.24	1132.78
C_3H_6O	-	1171.04	1159.85	1157.81
C_3H_6O	-	1271.86	1268.19	1265.63
C_3H_6O	-	1380.37	1359.81	1379.67
C_3H_6O	-	1411.83	1393.59	1405.99
C_3H_6O	-	1453.85	1417.31	1418.06
C_3H_6O	-	1469.77	1433.09	1451.79
C_3H_6O	-	1490.97	1453.13	1462.22
C_3H_6O	2942.00	2969.66	2930.10	2940.23
C_3H_6O	2974.00	2944.71	3003.77	2980.58
C_3H_6O	2995.00	2983.71	2994.34	2993.88
C_3H_6O	3001.00	2998.79	3017.30	3010.66
C_3H_6O	3051.00	3009.55	3020.34	3009.80
C_3H_6O	-	3057.76	3061.46	3061.45
$C_3H_4O_3$	-	76.69	45.60	66.29
$C_3H_4O_3$	-	55.03	104.74	162.30
$C_3H_4O_3$	-	245.76	262.69	242.37
$C_3H_4O_3$	-	383.50	388.13	380.05
$C_3H_4O_3$	-	390.33	392.96	402.54
$C_3H_4O_3$	-	526.22	520.35	531.15
$C_3H_4O_3$	604.00	601.97	596.20	606.52
$C_3H_4O_3$	668.00	671.57	679.29	678.74
$C_3H_4O_3$	-	717.36	717.46	716.65
$C_3H_4O_3$	761.00	751.42	751.70	745.23
$C_3H_4O_3$	970.00	963.08	954.76	979.52
$C_3H_4O_3$	1030.00	1019.41	1015.10	1012.66
$C_3H_4O_3$	1133.00	1130.26	1140.69	1142.55
$C_3H_4O_3$	-	1208.53	1209.79	1209.88
$C_3H_4O_3$	1360.00	1358.32	1367.11	1316.15
$C_3H_4O_3$	1391.00	1379.37	1390.89	1396.03
$C_3H_4O_3$	1424.00	1430.07	1393.51	1422.94
$C_3H_4O_3$	-	1420.61	1412.91	1433.04
$C_3H_4O_3$	1737.00	1724.28	1716.93	1718.44
$C_3H_4O_3$	1804.00	1792.67	1796.57	1796.98
$C_3H_4O_3$	2941.00	2950.94	2980.93	2970.18
$C_3H_4O_3$	-	2981.03	2988.76	2981.65
$C_3H_4O_3$	3025.00	3036.43	3039.83	3034.87
$C_3H_4O_3$	3463.00	3432.40	3427.25	3431.77
C_6H_6	398.00	-	404.18	483.52

Table S4: Fundamental frequencies/cm^{-1} calculated using Full B2PLYP, Hybrdid B2PLYP/ANN and Full ANN methods. Experimental values are taken from NIST DataBase (Continued)

Molecule	Experience	B2PLYP	Hybrid	ANN
C_6H_6	398.00	-	404.15	483.55
C_6H_6	608.00	-	629.33	616.66
C_6H_6	608.00	-	629.31	616.80
C_6H_6	674.00	-	688.34	653.59
C_6H_6	707.00	-	692.93	667.79
C_6H_6	847.00	-	861.62	859.22
C_6H_6	847.00	-	861.97	859.52
C_6H_6	976.00	-	975.75	978.19
C_6H_6	976.00	-	975.49	978.44
C_6H_6	990.00	-	987.49	1018.02
C_6H_6	993.00	-	1011.54	1021.18
C_6H_6	1010.00	-	1002.68	1014.36
C_6H_6	1038.00	-	1031.41	1032.66
C_6H_6	1038.00	-	1031.41	1032.68
C_6H_6	1150.00	-	1110.70	1117.67
C_6H_6	1178.00	-	1146.59	1188.57
C_6H_6	1178.00	-	1146.71	1188.70
C_6H_6	1309.00	-	1317.15	1323.85
C_6H_6	1350.00	-	1351.21	1354.03
C_6H_6	1484.00	-	1485.15	1486.67
C_6H_6	1484.00	-	1485.07	1486.68
C_6H_6	1601.00	-	1596.06	1595.89
C_6H_6	1601.00	-	1596.00	1595.87
C_6H_6	3047.00	-	3020.84	3030.12
C_6H_6	3047.00	-	3067.47	3072.20
C_6H_6	3049.00	-	3068.16	3073.25
C_6H_6	3057.00	-	3047.93	3048.87
C_6H_6	3057.00	-	3048.51	3050.34
C_6H_6	3074.00	-	3083.81	3081.30
C_4H_8S	-	111.56	94.36	166.82
C_4H_8S	290.00	287.47	264.17	374.76
C_4H_8S	472.00	472.08	465.72	483.44
C_4H_8S	516.00	518.18	501.93	514.39
C_4H_8S	678.00	674.29	669.35	670.27
C_4H_8S	684.00	680.89	681.95	698.32
C_4H_8S	822.00	827.35	839.38	841.81
C_4H_8S	829.00	880.99	881.32	864.77
C_4H_8S	888.00	886.47	889.99	875.17
C_4H_8S	958.00	884.55	880.47	885.10
C_4H_8S	1023.00	962.12	969.45	972.83

Table S4: Fundamental frequencies/cm^{-1} calculated using Full B2PLYP, Hybrdid B2PLYP/ANN and Full ANN methods. Experimental values are taken from NIST DataBase (Continued)

Molecule	Experience	B2PLYP	Hybrid	ANN
C_4H_8S	1037.00	1031.44	1029.96	1021.74
C_4H_8S	1061.00	1032.21	1047.83	1039.01
C_4H_8S	1125.00	1061.25	1071.87	1117.41
C_4H_8S	1131.00	1132.11	1121.46	1143.62
C_4H_8S	1196.00	1197.32	1191.11	1171.41
C_4H_8S	1213.00	1220.65	1216.19	1202.16
C_4H_8S	1263.00	1265.97	1255.32	1244.42
C_4H_8S	1276.00	1281.39	1265.79	1261.93
C_4H_8S	1305.00	1316.04	1306.14	1298.23
C_4H_8S	1321.00	1332.60	1337.90	1317.87
C_4H_8S	1441.00	1452.95	1415.67	1413.74
C_4H_8S	1451.00	1455.90	1412.44	1426.08
C_4H_8S	1459.00	1463.32	1419.49	1432.21
C_4H_8S	1464.00	1476.50	1429.11	1449.65
C_4H_8S	2862.00	2958.74	2946.38	2948.93
C_4H_8S	2922.00	2966.12	2938.38	2955.33
C_4H_8S	2932.00	2974.74	2958.69	2960.93
C_4H_8S	2940.00	2974.97	2957.15	2964.14
C_4H_8S	2946.00	2965.66	2928.61	2942.54
C_4H_8S	2952.00	2970.07	2938.01	2951.66
C_4H_8S	2962.00	2987.79	2956.35	2969.09
C_4H_8S	2971.00	2989.10	2950.62	2969.80
$C_2H_6O_4S$	-	100.93	2.43	125.09
$C_2H_6O_4S$	-	188.34	144.65	14.24
$C_2H_6O_4S$	-	190.17	175.97	175.95
$C_2H_6O_4S$	-	166.97	176.71	194.81
$C_2H_6O_4S$	-	255.39	256.72	229.58
$C_2H_6O_4S$	-	251.51	255.42	293.82
$C_2H_6O_4S$	-	388.83	387.51	406.65
$C_2H_6O_4S$	-	414.65	416.79	427.04
$C_2H_6O_4S$	-	492.44	495.00	492.22
$C_2H_6O_4S$	-	554.06	557.01	574.92
$C_2H_6O_4S$	-	587.67	593.76	587.35
$C_2H_6O_4S$	758.00	731.64	733.20	764.85
$C_2H_6O_4S$	814.00	797.32	799.45	816.93
$C_2H_6O_4S$	-	996.24	986.56	982.52
$C_2H_6O_4S$	1006.00	1008.89	997.70	1033.11
$C_2H_6O_4S$	-	1162.90	1158.10	1137.03
$C_2H_6O_4S$	-	1170.02	1162.33	1166.45
$C_2H_6O_4S$	-	1177.08	1174.31	1170.81

Table S4: Fundamental frequencies/cm^{-1} calculated using Full B2PLYP, Hybrdid B2PLYP/ANN and Full ANN methods. Experimental values are taken from NIST DataBase (Continued)

Molecule	Experience	B2PLYP	Hybrid	ANN
$C_2H_6O_4S$	-	1178.61	1174.78	1189.39
$C_2H_6O_4S$	1206.00	1196.77	1198.69	1181.60
$C_2H_6O_4S$	1410.00	1412.56	1417.56	1404.99
$C_2H_6O_4S$	-	1447.59	1443.57	1423.99
$C_2H_6O_4S$	-	1454.91	1455.28	1436.83
$C_2H_6O_4S$	-	1464.90	1447.17	1449.54
$C_2H_6O_4S$	-	1464.59	1448.13	1470.35
$C_2H_6O_4S$	-	1478.68	1451.50	1465.12
$C_2H_6O_4S$	-	1481.00	1451.30	1481.09
$C_2H_6O_4S$	-	2995.51	3001.05	3006.67
$C_2H_6O_4S$	-	2991.83	3005.01	3015.93
$C_2H_6O_4S$	-	3027.91	3062.87	3044.70
$C_2H_6O_4S$	-	3028.46	3064.16	3051.16
$C_2H_6O_4S$	-	3051.44	3078.90	3072.50
$C_2H_6O_4S$	-	3051.50	3079.02	3073.28
$C_{10}H_8$	176.00	-	165.72	169.29
$C_{10}H_8$	195.00	-	179.16	181.99
$C_{10}H_8$	359.00	-	339.20	322.73
$C_{10}H_8$	386.00	-	382.42	417.24
$C_{10}H_8$	461.00	-	462.44	503.07
$C_{10}H_8$	476.00	-	473.09	501.89
$C_{10}H_8$	506.00	-	512.28	508.62
$C_{10}H_8$	512.00	-	509.88	536.88
$C_{10}H_8$	581.00	-	603.90	601.00
$C_{10}H_8$	618.00	-	608.73	606.45
$C_{10}H_8$	717.00	-	723.12	723.42
$C_{10}H_8$	753.00	-	734.71	690.52
$C_{10}H_8$	758.00	-	719.49	741.84
$C_{10}H_8$	841.00	-	791.22	762.90
$C_{10}H_8$	782.00	-	788.82	788.48
$C_{10}H_8$	846.00	-	834.48	874.99
$C_{10}H_8$	876.00	-	869.11	891.30
$C_{10}H_8$	970.00	-	921.94	936.48
$C_{10}H_8$	935.00	-	942.26	956.79
$C_{10}H_8$	943.00	-	957.39	944.28
$C_{10}H_8$	958.00	-	954.15	983.53
$C_{10}H_8$	980.00	-	960.21	1000.37
$C_{10}H_8$	1008.00	-	994.72	1001.57
$C_{10}H_8$	1025.00	-	1011.87	1008.52
$C_{10}H_8$	1125.00	-	1127.54	1121.87

Table S4: Fundamental frequencies/cm^{-1} calculated using Full B2PLYP, Hybrdid B2PLYP/ANN and Full ANN methods. Experimental values are taken from NIST DataBase (Continued)

Molecule	Experience	B2PLYP	Hybrid	ANN
$C_{10}H_8$	1145.00	-	1158.44	1152.88
$C_{10}H_8$	1138.00	-	1140.11	1155.63
$C_{10}H_8$	1158.00	-	1137.53	1148.89
$C_{10}H_8$	1209.00	-	1193.29	1198.08
$C_{10}H_8$	1239.00	-	1231.04	1255.79
$C_{10}H_8$	1265.00	-	1235.66	1268.29
$C_{10}H_8$	1361.00	-	1380.21	1371.86
$C_{10}H_8$	1376.00	-	1381.63	1383.89
$C_{10}H_8$	1389.00	-	1393.59	1407.44
$C_{10}H_8$	1460.00	-	1472.28	1461.59
$C_{10}H_8$	1438.00	-	1449.35	1451.64
$C_{10}H_8$	1506.00	-	1517.33	1524.42
$C_{10}H_8$	1577.00	-	1573.35	1565.18
$C_{10}H_8$	1595.00	-	1603.17	1589.55
$C_{10}H_8$	1624.00	-	1635.47	1624.04
$C_{10}H_8$	3031.00	-	3012.22	3027.14
$C_{10}H_8$	3027.00	-	3010.53	3045.82
$C_{10}H_8$	3058.00	-	3036.49	3054.25
$C_{10}H_8$	3060.00	-	3032.72	3045.42
$C_{10}H_8$	3065.00	-	3069.94	3071.29
$C_{10}H_8$	3060.00	-	3052.02	3060.86
$C_{10}H_8$	3092.00	-	3070.91	3054.74
$C_{10}H_8$	3090.00	-	3062.25	3057.29

Table S5: Harmonic frequencies/cm^{-1} calculated using B2PLYP and ANN potentials

Molecule	B2PLYP	ANN
H_2O	1644.97	1635.62
H_2O	3834.21	3829.25
H_2O	3944.41	3940.54
KrF_2	234.76	226.96
KrF_2	234.76	226.96
KrF_2	461.96	460.07
KrF_2	584.54	586.87
OCSe	471.89	469.48
OCSe	471.89	469.48
OCSe	661.90	663.40
OCSe	2043.63	2043.04
SO_2	513.20	519.71
SO_2	1136.97	1141.44
SO_2	1345.44	1341.59
SeO_2	360.54	365.39
SeO_2	916.34	915.35
SeO_2	967.68	967.42
CSe_2	320.90	328.05
CSe_2	320.90	328.05
CSe_2	374.31	377.58
CSe_2	1332.06	1330.26
TiO_2	328.82	316.92
TiO_2	925.43	925.62
TiO_2	926.67	930.87
NH_3	1052.06	1049.97
NH_3	1681.00	1675.13
NH_3	1681.10	1675.72
NH_3	3496.53	3505.60
NH_3	3624.95	3623.51
NH_3	3624.99	3623.72
ClF_3	315.18	313.66
ClF_3	328.40	315.77
ClF_3	423.37	423.97
ClF_3	522.05	526.71
ClF_3	701.94	697.59
ClF_3	757.21	750.15
H_2CO	1208.60	1192.78
H_2CO	1274.96	1277.15
H_2CO	1545.33	1547.08
H_2CO	1790.67	1793.18
H_2CO	2929.62	2922.92
H_2CO	2992.23	2982.80

Table S5: Harmonic frequencies/cm^{-1} calculated using B2PLYP and ANN potentials (Continued)

Molecule	B2PLYP	ANN
H_2O_2	362.07	371.47
H_2O_2	932.80	925.01
H_2O_2	1321.89	1338.33
H_2O_2	1441.45	1464.57
H_2O_2	3800.22	3775.12
H_2O_2	3800.32	3783.65
$GaCl_3$	125.52	125.23
$GaCl_3$	125.54	125.27
$GaCl_3$	140.85	140.56
$GaCl_3$	380.08	380.14
$GaCl_3$	469.90	470.41
$GaCl_3$	469.94	470.43
AlF_2Cl	186.81	183.44
AlF_2Cl	236.33	239.39
AlF_2Cl	265.31	265.18
AlF_2Cl	509.55	506.57
AlF_2Cl	828.06	830.42
AlF_2Cl	945.28	947.92
$AlFCl_2$	151.55	151.58
$AlFCl_2$	204.80	205.35
$AlFCl_2$	234.11	233.59
$AlFCl_2$	437.47	440.07
$AlFCl_2$	635.29	639.01
$AlFCl_2$	883.90	878.50
$ZnCH_2$	511.94	515.82
$ZnCH_2$	541.98	516.74
$ZnCH_2$	631.13	625.35
$ZnCH_2$	1336.66	1303.42
$ZnCH_2$	3112.75	3129.11
$ZnCH_2$	3220.72	3225.95
CH_4	1353.66	1354.31
CH_4	1353.67	1354.86
CH_4	1353.68	1355.00
CH_4	1574.61	1581.20
CH_4	1574.62	1581.72
CH_4	3055.70	3056.27
CH_4	3168.29	3166.50
CH_4	3168.30	3166.59
CH_4	3168.31	3166.73
$CHBr_3$	153.15	151.85
$CHBr_3$	153.18	151.87

Table S5: Harmonic frequencies/cm^{-1} calculated using B2PLYP and ANN potentials (Continued)

Molecule	B2PLYP	ANN
$CHBr_3$	224.73	230.11
$CHBr_3$	541.51	541.34
$CHBr_3$	664.99	663.72
$CHBr_3$	665.40	663.73
$CHBr_3$	1176.99	1169.53
$CHBr_3$	1177.10	1169.53
$CHBr_3$	3208.98	3205.69
$SiBr_4$	86.59	85.33
$SiBr_4$	86.61	85.34
$SiBr_4$	136.03	135.54
$SiBr_4$	136.04	135.56
$SiBr_4$	136.11	135.56
$SiBr_4$	247.57	247.72
$SiBr_4$	492.93	492.59
$SiBr_4$	493.10	492.60
$SiBr_4$	493.13	492.62
$TiCl_4$	113.19	114.80
$TiCl_4$	113.21	114.81
$TiCl_4$	133.60	127.29
$TiCl_4$	133.61	127.32
$TiCl_4$	133.66	127.34
$TiCl_4$	377.55	376.49
$TiCl_4$	497.89	496.92
$TiCl_4$	497.92	496.95
$TiCl_4$	497.93	496.95
CBr_4	125.63	123.58
CBr_4	125.63	123.58
CBr_4	184.87	184.46
CBr_4	184.87	184.46
CBr_4	184.87	184.46
CBr_4	271.16	269.88
CBr_4	668.17	668.70
CBr_4	668.17	668.70
CBr_4	668.17	668.70
CH_2O_2	629.02	634.08
CH_2O_2	683.34	663.26
CH_2O_2	1060.10	1044.93
CH_2O_2	1127.30	1120.30
CH_2O_2	1309.67	1307.61
CH_2O_2	1413.80	1404.08
CH_2O_2	1805.62	1806.65

Table S5: Harmonic frequencies/cm^{-1} calculated using B2PLYP and ANN potentials (Continued)

Molecule	B2PLYP	ANN
CH_2O_2	3093.40	3090.35
CH_2O_2	3751.28	3757.61
CH_2NH	1077.99	1061.66
CH_2NH	1103.38	1092.38
CH_2NH	1170.18	1177.80
CH_2NH	1378.55	1386.05
CH_2NH	1498.00	1504.33
CH_2NH	1696.58	1697.64
CH_2NH	3054.84	3065.27
CH_2NH	3155.89	3142.07
CH_2NH	3463.14	3461.26
CH_3OH	295.32	297.74
CH_3OH	1054.79	1044.24
CH_3OH	1090.13	1086.31
CH_3OH	1182.42	1192.05
CH_3OH	1381.96	1391.95
CH_3OH	1494.35	1487.65
CH_3OH	1512.14	1504.40
CH_3OH	1526.14	1519.28
CH_3OH	3025.91	3016.27
CH_3OH	3078.45	3080.84
CH_3OH	3147.19	3152.54
CH_3OH	3865.85	3875.54
CH_3SeH	198.32	163.24
CH_3SeH	597.13	599.39
CH_3SeH	721.18	747.36
CH_3SeH	926.87	949.99
CH_3SeH	1013.69	1008.41
CH_3SeH	1329.16	1334.25
CH_3SeH	1484.05	1473.75
CH_3SeH	1496.57	1474.36
CH_3SeH	2453.11	2429.60
CH_3SeH	3088.51	3094.45
CH_3SeH	3181.80	3174.28
CH_3SeH	3189.97	3183.75
C_2H_3Br	349.19	337.83
C_2H_3Br	605.19	560.91
C_2H_3Br	616.99	610.03
C_2H_3Br	938.68	923.37
C_2H_3Br	985.53	957.57
C_2H_3Br	1029.11	995.03

Table S5: Harmonic frequencies/cm^{-1} calculated using B2PLYP and ANN potentials (Continued)

Molecule	B2PLYP	ANN
C_2H_3Br	1293.32	1281.28
C_2H_3Br	1417.89	1439.85
C_2H_3Br	1656.11	1662.41
C_2H_3Br	3172.11	3165.60
C_2H_3Br	3236.74	3229.66
C_2H_3Br	3269.51	3280.90
CH_2CHCl	400.89	391.19
CH_2CHCl	641.57	611.59
CH_2CHCl	722.63	721.49
CH_2CHCl	930.48	920.23
CH_2CHCl	986.03	961.34
CH_2CHCl	1051.51	1041.58
CH_2CHCl	1315.34	1318.93
CH_2CHCl	1418.43	1448.66
CH_2CHCl	1663.26	1666.71
CH_2CHCl	3179.56	3179.01
CH_2CHCl	3232.99	3231.76
CH_2CHCl	3276.88	3278.96
SeF_6	260.61	268.98
SeF_6	260.61	268.98
SeF_6	260.61	268.98
SeF_6	397.40	405.88
SeF_6	397.40	405.88
SeF_6	397.40	405.88
SeF_6	431.95	431.07
SeF_6	431.95	431.07
SeF_6	431.95	431.07
SeF_6	653.38	656.31
SeF_6	653.38	656.31
SeF_6	704.87	706.03
SeF_6	776.48	777.70
SeF_6	776.48	777.70
SeF_6	776.48	777.70
$C_2H_4Br_2$	103.36	128.36
$C_2H_4Br_2$	180.28	188.99
$C_2H_4Br_2$	190.87	190.61
$C_2H_4Br_2$	604.72	608.98
$C_2H_4Br_2$	676.96	675.82
$C_2H_4Br_2$	763.19	783.20
$C_2H_4Br_2$	954.73	951.97
$C_2H_4Br_2$	1074.95	1070.96

Table S5: Harmonic frequencies/cm^{-1} calculated using B2PLYP and ANN potentials (Continued)

Molecule	B2PLYP	ANN
$C_2H_4Br_2$	1112.19	1130.82
$C_2H_4Br_2$	1219.48	1221.65
$C_2H_4Br_2$	1292.42	1262.06
$C_2H_4Br_2$	1298.15	1291.07
$C_2H_4Br_2$	1496.44	1531.67
$C_2H_4Br_2$	1499.05	1544.12
$C_2H_4Br_2$	3129.47	3120.09
$C_2H_4Br_2$	3137.96	3123.64
$C_2H_4Br_2$	3190.96	3175.41
$C_2H_4Br_2$	3213.62	3194.14
GeH_3CH_3	167.82	183.75
GeH_3CH_3	498.00	544.28
GeH_3CH_3	498.14	544.29
GeH_3CH_3	604.23	604.39
GeH_3CH_3	859.06	871.80
GeH_3CH_3	861.82	872.34
GeH_3CH_3	861.89	872.52
GeH_3CH_3	917.61	888.20
GeH_3CH_3	917.65	888.25
GeH_3CH_3	1291.37	1324.15
GeH_3CH_3	1481.98	1504.70
GeH_3CH_3	1481.98	1505.29
GeH_3CH_3	2154.99	2150.02
GeH_3CH_3	2155.16	2159.94
GeH_3CH_3	2157.39	2160.03
GeH_3CH_3	3069.36	3075.16
GeH_3CH_3	3155.29	3135.75
GeH_3CH_3	3155.31	3136.03
C_2H_5Br	260.52	290.64
C_2H_5Br	287.93	307.00
C_2H_5Br	577.00	580.30
C_2H_5Br	779.42	802.11
C_2H_5Br	984.12	975.86
C_2H_5Br	1044.22	1076.63
C_2H_5Br	1087.94	1082.19
C_2H_5Br	1277.64	1247.65
C_2H_5Br	1289.47	1284.71
C_2H_5Br	1425.09	1424.59
C_2H_5Br	1498.14	1495.29
C_2H_5Br	1499.56	1497.33
C_2H_5Br	1512.19	1538.59

Table S5: Harmonic frequencies/cm^{-1} calculated using B2PLYP and ANN potentials (Continued)

Molecule	B2PLYP	ANN
C_2H_5Br	3055.49	3035.10
C_2H_5Br	3116.27	3094.87
C_2H_5Br	3130.70	3123.64
C_2H_5Br	3145.81	3140.82
C_2H_5Br	3184.74	3172.60
C_3H_6	747.53	740.26
C_3H_6	747.75	740.36
C_3H_6	868.09	821.99
C_3H_6	890.49	883.23
C_3H_6	890.50	883.30
C_3H_6	1060.26	1063.18
C_3H_6	1061.49	1063.31
C_3H_6	1100.44	1103.13
C_3H_6	1164.18	1104.13
C_3H_6	1220.29	1226.04
C_3H_6	1221.98	1231.39
C_3H_6	1222.45	1231.40
C_3H_6	1487.75	1497.04
C_3H_6	1488.85	1497.07
C_3H_6	1533.35	1575.15
C_3H_6	3158.66	3153.98
C_3H_6	3159.21	3153.98
C_3H_6	3167.64	3159.28
C_3H_6	3238.87	3230.93
C_3H_6	3239.32	3230.93
C_3H_6	3260.21	3252.58
C_3H_6O	213.84	202.81
C_3H_6O	368.52	392.33
C_3H_6O	410.85	424.53
C_3H_6O	772.81	773.09
C_3H_6O	850.12	850.58
C_3H_6O	913.18	938.45
C_3H_6O	976.41	986.81
C_3H_6O	1050.40	1035.40
C_3H_6O	1135.32	1135.99
C_3H_6O	1165.72	1152.94
C_3H_6O	1175.06	1174.73
C_3H_6O	1197.19	1197.70
C_3H_6O	1300.91	1296.25
C_3H_6O	1415.38	1432.28
C_3H_6O	1452.55	1456.75

Table S5: Harmonic frequencies/cm^{-1} calculated using B2PLYP and ANN potentials (Continued)

Molecule	B2PLYP	ANN
C_3H_6O	1495.99	1492.38
C_3H_6O	1510.25	1532.52
C_3H_6O	1543.05	1554.21
C_3H_6O	3056.38	3056.22
C_3H_6O	3115.99	3099.46
C_3H_6O	3123.21	3104.36
C_3H_6O	3127.25	3119.89
C_3H_6O	3146.78	3132.44
C_3H_6O	3206.73	3208.75
$C_3H_4O_3$	89.59	80.13
$C_3H_4O_3$	123.73	206.00
$C_3H_4O_3$	253.69	256.99
$C_3H_4O_3$	393.82	388.56
$C_3H_4O_3$	396.26	410.00
$C_3H_4O_3$	528.12	541.35
$C_3H_4O_3$	610.09	620.12
$C_3H_4O_3$	704.30	702.35
$C_3H_4O_3$	744.32	747.40
$C_3H_4O_3$	770.81	763.11
$C_3H_4O_3$	985.93	1010.37
$C_3H_4O_3$	1044.27	1038.95
$C_3H_4O_3$	1161.16	1162.82
$C_3H_4O_3$	1256.15	1259.04
$C_3H_4O_3$	1388.36	1378.99
$C_3H_4O_3$	1414.64	1424.83
$C_3H_4O_3$	1466.63	1475.15
$C_3H_4O_3$	1472.30	1490.92
$C_3H_4O_3$	1759.17	1757.94
$C_3H_4O_3$	1829.15	1829.09
$C_3H_4O_3$	3071.15	3043.83
$C_3H_4O_3$	3133.34	3115.82
$C_3H_4O_3$	3186.99	3177.73
$C_3H_4O_3$	3649.41	3663.24
C_6H_6	411.46	489.49
C_6H_6	411.49	489.49
C_6H_6	620.11	606.31
C_6H_6	620.14	606.39
C_6H_6	692.36	657.37
C_6H_6	694.80	671.43
C_6H_6	867.32	864.71
C_6H_6	867.32	864.71

Table S5: Harmonic frequencies/cm^{-1} calculated using B2PLYP and ANN potentials (Continued)

Molecule	B2PLYP	ANN
C_6H_6	979.84	982.27
C_6H_6	979.86	982.27
C_6H_6	989.96	1019.27
C_6H_6	1014.48	1022.32
C_6H_6	1028.49	1039.72
C_6H_6	1063.24	1060.65
C_6H_6	1063.26	1060.68
C_6H_6	1178.11	1184.21
C_6H_6	1202.86	1238.58
C_6H_6	1202.87	1238.61
C_6H_6	1361.25	1364.42
C_6H_6	1387.56	1387.12
C_6H_6	1519.95	1526.19
C_6H_6	1519.96	1526.28
C_6H_6	1640.18	1639.79
C_6H_6	1640.19	1639.84
C_6H_6	3185.69	3192.04
C_6H_6	3195.67	3200.41
C_6H_6	3195.68	3200.81
C_6H_6	3211.38	3207.66
C_6H_6	3211.39	3208.07
C_6H_6	3221.14	3216.27
C_4H_8S	116.25	171.38
C_4H_8S	285.50	383.97
C_4H_8S	478.98	495.74
C_4H_8S	518.99	534.36
C_4H_8S	686.95	686.12
C_4H_8S	693.26	706.85
C_4H_8S	839.43	840.87
C_4H_8S	899.87	885.39
C_4H_8S	900.35	891.90
C_4H_8S	903.71	901.60
C_4H_8S	980.26	986.05
C_4H_8S	1051.67	1031.25
C_4H_8S	1055.03	1062.86
C_4H_8S	1079.72	1128.84
C_4H_8S	1159.98	1177.14
C_4H_8S	1226.49	1204.58
C_4H_8S	1250.11	1234.30
C_4H_8S	1297.34	1272.25
C_4H_8S	1315.16	1295.74

Table S5: Harmonic frequencies/cm^{-1} calculated using B2PLYP and ANN potentials (Continued)

Molecule	B2PLYP	ANN
C_4H_8S	1348.41	1341.27
C_4H_8S	1368.03	1361.82
C_4H_8S	1494.08	1494.66
C_4H_8S	1496.76	1505.67
C_4H_8S	1505.42	1527.22
C_4H_8S	1518.76	1535.37
C_4H_8S	3057.49	3057.90
C_4H_8S	3058.15	3064.39
C_4H_8S	3075.81	3065.63
C_4H_8S	3076.05	3074.01
C_4H_8S	3101.96	3111.73
C_4H_8S	3110.22	3120.14
C_4H_8S	3134.54	3140.69
C_4H_8S	3135.59	3145.97
$C_2H_6O_4S$	85.66	127.18
$C_2H_6O_4S$	102.51	160.80
$C_2H_6O_4S$	126.72	186.36
$C_2H_6O_4S$	165.26	227.16
$C_2H_6O_4S$	254.83	284.06
$C_2H_6O_4S$	257.84	306.79
$C_2H_6O_4S$	395.87	412.99
$C_2H_6O_4S$	420.77	464.47
$C_2H_6O_4S$	500.34	496.16
$C_2H_6O_4S$	561.86	583.28
$C_2H_6O_4S$	594.39	592.07
$C_2H_6O_4S$	750.90	788.00
$C_2H_6O_4S$	816.95	834.06
$C_2H_6O_4S$	1030.08	1022.75
$C_2H_6O_4S$	1044.09	1081.57
$C_2H_6O_4S$	1188.02	1161.87
$C_2H_6O_4S$	1189.31	1193.09
$C_2H_6O_4S$	1202.77	1201.07
$C_2H_6O_4S$	1206.19	1210.13
$C_2H_6O_4S$	1217.61	1215.30
$C_2H_6O_4S$	1437.67	1425.52
$C_2H_6O_4S$	1482.53	1463.09
$C_2H_6O_4S$	1487.69	1489.22
$C_2H_6O_4S$	1504.65	1506.59
$C_2H_6O_4S$	1505.48	1512.18
$C_2H_6O_4S$	1518.18	1528.16
$C_2H_6O_4S$	1521.80	1560.72

Table S5: Harmonic frequencies/cm^{-1} calculated using B2PLYP and ANN potentials (Continued)

Molecule	B2PLYP	ANN
$C_2H_6O_4S$	3083.03	3074.41
$C_2H_6O_4S$	3083.40	3085.62
$C_2H_6O_4S$	3171.86	3139.36
$C_2H_6O_4S$	3172.45	3147.35
$C_2H_6O_4S$	3197.76	3175.46
$C_2H_6O_4S$	3197.81	3175.59
$C_{10}H_8$	178.00	174.45
$C_{10}H_8$	187.00	188.06
$C_{10}H_8$	371.00	345.85
$C_{10}H_8$	401.00	426.99
$C_{10}H_8$	488.00	507.03
$C_{10}H_8$	494.00	513.39
$C_{10}H_8$	512.00	516.93
$C_{10}H_8$	520.00	546.86
$C_{10}H_8$	632.00	613.49
$C_{10}H_8$	645.00	631.50
$C_{10}H_8$	724.00	732.46
$C_{10}H_8$	772.00	748.01
$C_{10}H_8$	797.00	757.65
$C_{10}H_8$	801.00	773.30
$C_{10}H_8$	808.00	809.21
$C_{10}H_8$	846.00	888.76
$C_{10}H_8$	922.00	904.52
$C_{10}H_8$	940.00	950.84
$C_{10}H_8$	957.00	973.83
$C_{10}H_8$	980.00	973.91
$C_{10}H_8$	996.00	996.44
$C_{10}H_8$	1005.00	1014.31
$C_{10}H_8$	1034.00	1047.87
$C_{10}H_8$	1046.00	1048.73
$C_{10}H_8$	1149.00	1150.77
$C_{10}H_8$	1162.00	1169.29
$C_{10}H_8$	1162.00	1190.53
$C_{10}H_8$	1174.00	1197.35
$C_{10}H_8$	1229.00	1245.50
$C_{10}H_8$	1256.00	1295.18
$C_{10}H_8$	1280.00	1324.01
$C_{10}H_8$	1399.00	1407.13
$C_{10}H_8$	1405.00	1417.46
$C_{10}H_8$	1411.00	1436.84
$C_{10}H_8$	1477.00	1489.29

Table S5: Harmonic frequencies/cm^{-1} calculated using B2PLYP and ANN potentials (Continued)

Molecule	B2PLYP	ANN
$C_{10}H_8$	1480.00	1502.09
$C_{10}H_8$	1544.00	1564.10
$C_{10}H_8$	1619.00	1609.97
$C_{10}H_8$	1637.00	1627.29
$C_{10}H_8$	1668.00	1663.51
$C_{10}H_8$	3164.00	3173.74
$C_{10}H_8$	3165.00	3180.56
$C_{10}H_8$	3168.00	3201.24
$C_{10}H_8$	3170.00	3203.09
$C_{10}H_8$	3182.00	3210.90
$C_{10}H_8$	3182.00	3219.14
$C_{10}H_8$	3194.00	3223.21
$C_{10}H_8$	3195.00	3223.39