Runge-Kutta

range:	-90...90	checked between +/-80...100							
BB	Qmin = [-56 -54 -53 -52], Qmax = [59 55 53 46]								
harm mode	v0	v1	anharm freq	polynomial					
1357.395292	652.606492745	1959.697304279	1307.090811534	-0.0000000048*t^6 + 0.0000000161*t^5 + 0.0000515888*t^4 - 0.0033339994*t^3 + 3.8703709911*t^2 - 0.6533683387*t					
1375.256965	688.3636407906	2066.3341806298	1377.9705398392	-0.0000000079*t^6 + 0.0000001505*t^5 + 0.0000396802*t^4 - 0.0017345305*t^3 + 4.3092894130*t^2 + 0.3042117826*t					
1455.68963	711.1396997993	2134.167677595	1423.0279777957	0.0000000031*t^6 - 0.0000001660*t^5 + 0.0000155540*t^4 - 0.0001608530*t^3 + 4.6052030374*t^2 + 0.9920357346*t					
1527.756431	756.6118084573	2273.2676313737	1516.6558229164	0.0000000177*t^6 + 0.0000011092*t^5 + 0.0001538325*t^4 + 0.0134007233*t^3 + 5.1932729150*t^2 + 0.9181879869*t					
anharm levels									
zpe	2808.7216417922								
zpe+mode1	4115.8124533262								
zpe+mode2	5493.7829931654								
zpe+mode3	6916.8109709611								
zpe+mode4	8433.4667938775								
M1	Qmin = [-56 -58 -52 -56], Qmax = [60 54 50 40]								
harm mode	v0	v1	anharm freq	polynomial					
1242.407205	645.0662792049	1937.8312264069	1292.764947202	-0.0000000104*t^6 + 0.0000003532*t^5 + 0.0000745800*t^4 - 0.0049143390*t^3 + 3.7782458423*t^2 - 1.0656853787*t					
1327.805934	660.6006925293	1984.2872427384	1323.6865502091	-0.0000000060*t^6 - 0.0000001432*t^5 + 0.0000752572*t^4 + 0.0055098336*t^3 + 3.9618966683*t^2 + 0.6375630000*t					
1469.237692	734.3831573145	2205.1359694129	1470.7528120984	-0.0000000006*t^6 - 0.0000001386*t^5 + 0.0000469033*t^4 + 0.0056535196*t^3 + 4.9151023548*t^2 + 2.7149755735*t					
1626.513751	800.9958513216	2398.3114191156	1597.315567794	0.0000000168*t^6 + 0.0000025042*t^5 + 0.0002828106*t^4 + 0.0406707061*t^3 + 5.8286447475*t^2 - 1.4136251494*t					
anharm levels									
zpe	2841.0459803703								
zpe+mode1	1292.764947202								
zpe+mode2	1323.6865502091								
zpe+mode3	1470.7528120984								
zpe+mode4	1597.315567794								
M2	Qmin = [-59 -56 -54 -56 -41], Qmax = [54 54 55 49 53]								
harm mode	v0	v1	anharm freq	polynomial					
1306.614543	656.3846590723	1971.9037064044	1315.5190473321	-0.0000000073*t^6 - 0.0000001308*t^5 + 0.0000881504*t^4 + 0.0065208304*t^3 +3.9067630299*t^2 -0.1991252463*t					
1358.326996	687.8837828256	2064.1729478007	1376.2891649751	-0.0000000062*t^6 - 0.0000008339*t^5 + 0.0000218864*t^4 + 0.0049116284*t^3 + 4.3104720418*t^2 + 0.9303850886*t					
1381.603402	690.9100735913	2073.8664710975	1382.9563975062	-0.0000000070*t^6 + 0.0000001438*t^5 + 0.0000335066*t^4 - 0.0025569502*t^3 + 4.3429990330*t^2 + 1.2022792436*t					
1473.003021	728.9861452872	2185.932843001	1456.9466977138	-0.0000000011*t^6 - 0.0000000997*t^5 + 0.0000082652*t^4 + 0.0125377866*t^3 + 4.8584565025*t^2 + 2.0680927695*t					
1646.607061	815.5538709435	2443.1363101095	1627.582439166	0.0000000118*t^6 - 0.0000017156*t^5 + 0.0001833556*t^4 - 0.0345096090*t^3 + 6.0526346165*t^2 + 1.0004572683*t					
anharm levels	5d	4d							
zpe	3579.7185317199	2888.8084581286							
zpe+mode1	4895.237579052	4204.3275054607							
zpe+mode2	6271.5267440271	5580.6166704358							
zpe+mode3	7654.4831415333	4345.7551558424							
zpe+mode4	9111.4298392471	5831.9099446267							
zpe+mode5	10739.0122784131								
Fits	1/3 of pts for test								
BB				harmonic=	1357.395292	1375.256965	1455.68963	1527.756431	
				anharm uncoupled=	1307.09	1377.97	1423.03	1516.66	
npts (2/3 of)	N	1000*Rfit	1000*Rtest	ZPE, cm-1	v1	v2	v3	v4	

10000	35	18.01	18.16	2826.67	1300.48	1376.83	1432.92	1469.32	
10000	70	3.02	3.04	2811.04	1297.97	1375.49	1430.25	1497.69	
10000	126	1.84	1.87	2812.21	1297.97	1375.44	1430.11	1497.9	
10000	210	1.03	1.09	2813.89	1297.98	1375.4	1430.12	1497.78	
7000	35	15.49	15.13	2815.8	1299.49	1375.4	1434.23	1494.16	
7000	70	3.1	3	2810.58	1297.79	1375.3	1430.04	1497.73	
7000	126	1.9	1.83	2813.74	1298.04	1375.47	1430.03	1498.01	
7000	210	1.05	1.06	2813.66	1297.99	1375.37	1430.07	1497.73	
4000	35	15.54	15.65	2816.81	1301.36	1375.22	1436.76	1495.64	
4000	70	3.1	3.21	2811.05	1297.85	1375.25	1430.52	1497.42	
4000	**126**	**1.89**	**2**	**2812.7**	**1297.97**	**1375.4**	**1430.19**	**1497.79**	122.39
4000	210	1.03	1.12	2813.16	1297.97	1375.37	1430.11	1497.78	
2500	35	15.26	16.71	2818.51	1297.96	1373.91	1430.05	1492.93	
2500	70	2.99	3.39	2810.82	1297.95	1375.39	1430.59	1497.52	
2500	126	1.8	2.08	2812.26	1297.92	1375.33	1430.35	1497.88	
2500	210	0.99	1.19	2813.72	1298.03	1375.21	1430.24	1497.81	
1500	35	14.63	15.99	2820.06	1292.55	1368.44	1437.75	1492.74	
1500	70	2.93	3.15	2811.06	1298.43	1375.1	1429.96	1498.39	
1500	126	1.76	2.15	2814.41	1297.79	1375.18	1430.51	1498.11	
1500	210	1.04	1.48	2808.9	1297.96	1375.33	1430.68	1497.73	
1000	35	14.01	16.79	2821.22	1291.8	1372.27	1439.01	1490.01	
1000	70	2.76	3.56	2810.95	1299.1	1376.21	1431.05	1497.65	
1000	126	1.6	2.4	2813.12	1297.82	1375.26	1430.01	1497.43	
1000	210	0.89	1.86	2811.74	1297.25	1375.32	1430.43	1497.17	
700	35	12.63	20.57	2822.79	1304.02	1372.51	1443.82	1487.05	
700	70	2.4	4.85	2812.2	1299.48	1376.03	1429.59	1496.09	
700	126	1.35	3.4	2812.41	1298.17	1375.23	1430.98	1496.39	
700	210	0.66	3	2810.91	1297.8	1375.22	1430.54	1495.62	
500	35	11.64	18.05	2822.47	1297.81	1370.89	1449.76	1481.81	
500	70	2.27	3.75	2811.17	1299.93	1374.66	1425.96	1496.65	
500	126	1.21	3.32	2811.37	1300.56	1374.82	1430.36	1493.24	
500	210	0.42	6.58	2817.83	1297.09	1375.08	1424.44	1493.48	
300	35	11.35	18.08	2829.51	1299.83	1362.61	1434.74	1485.44	
300	70	1.98	6.17	2809.08	1301.67	1371.997	1434.53	1494.87	
300	126	0.72	8.7	2805.96	1302.13	1378.95	1420.98	1491.66	
300	210	0	107.23	2808.72	1307.09	1377.97	1423.03	1516.66	
M1				harmonic=	1242.407205	1327.805934	1469.237692	1626.513751	
				anharm uncoupled=	1292.764947202	1323.6865502091	1470.7528120984	1597.315567794	
npts (2/3 of)	N	1000*Rfit	1000*Rtest	ZPE, cm-1	v1	v2	v3	v4	
4000	35	15.52	16.19	2850.32	1290.82	1321.51	1464.72	1597.2	
4000	70	2.98	3.18	2846.24	1286.25	1320.31	1465.73	1595.35	
4000	**126**	**1.76**	**1.95**	**2849.38**	**1286.39**	**1320.48**	**1465.09**	**1595.35**	**130.26**
4000	210	1.03	1	2847.71	1286.42	1320.62	1465.43	1595.3	
2500	35	15.43	16.48	2849.96	1290.39	1323.94	1463.73	1596.78	
2500	70	2.91	3.27	2846.28	1285.86	1320.36	1466.03	1595.09	
2500	126	1.71	1.98	2849.13	1286.37	1320.61	1465.64	1595.31	
2500	210	0.72	0.9	2846.61	1286.59	1320.8	1465.45	1595.68	
1500	35	14.35	16.82	2848.62	1293.13	1324.32	1463.47	1596.31	
1500	70	2.77	3.29	2846.27	1286.33	1320.05	1465.36	1595.08	
1500	126	1.58	2.14	2849.21	1286.76	1320.51	1465.53	1595.44	
1500	210	0.66	1.02	2846.46	1286.86	1320.73	1465.61	1596.04	

1000	35	14.52	18.44	2847.37	1305.86	1322.59	1460.41	1602.08	
1000	70	2.58	3.57	2846.53	1286.31	1319.69	1465.3	1595.25	
1000	126	1.47	2.28	2848.81	1286.2	1320.68	1465.66	1596.19	
1000	210	0.59	1.21	2846.79	1287.38	1320.89	1466.21	1596.51	
700	35	14.19	20.64	2857.62	1303.5	1338.09	1453.29	1598.65	
700	70	2.38	4.36	2847.24	1288.47	1319.8	1466.29	1595.92	
700	126	1.27	3.58	2846.9	1289.31	1319.03	1467.88	1596.72	
700	210	0.48	2.47	2846.14	1288.49	1320.74	1468.35	1596.66	
500	35	11.22	15.23	2846.5	1330.68	1330.89	1459.4	1595.38	
500	70	2.09	4.45	2847.47	1287.84	1319.59	1464.95	1594.6	
500	126	0.97	3.79	2847.13	1288.95	1318.5	1467.49	1596.13	
500	210	0.3	4.06	2847.77	1289.84	1318.79	1466.42	1598.21	
300	35	8.32	16.78	2858.74	1321.69	1325.86	1427.7	1558.2	
300	70	1.64	5	2847.14	1285.02	1319.33	1466.77	1595.26	
300	126	0.52	5.07	2847.08	1285	1322.51	1461.42	1590.47	
300	210	0	101.98	2841.05	1292.77	1323.69	1470.75	1597.32	
M2 4d				harmonic=	1306.614543	1358.326996	1473.003021	1646.607061	
				anharm uncoupled=	1315.5190473321	1376.2891649751	1456.9466977138	1627.582439166	
npts (2/3 of)	N	1000*Rfit	1000*Rtest	ZPE, cm-1	v1	v2	v3	v4	
4000	35	12.21	12.51	2899.72	1313.01	1370.3	1456.47	1636.23	
4000	70	3.06	3.15	2895.63	1310.84	1370.25	1452.7	1635.75	
4000	**126**	**1.7**	**1.75**	**2895.72**	**1311.03**	**1370.02**	**1452.39**	**1635.76**	**265.74**
4000	210	0.9	0.96	2895.62	1311.01	1370.02	1452.34	1635.72	
2500	35	11.91	12.73	2899.52	1313.67	1370.49	1454.71	1636.5	
2500	70	3.06	3.15	2895.79	1311.32	1370.69	1452.62	1635.97	
2500	126	1.69	1.79	2895.62	1311.15	1370.26	1451.92	1635.61	
2500	210	0.89	1	2895.77	1311.14	1370.24	1452.23	1635.61	
1500	35	11.26	13.21	2899.73	1314.58	1373.84	1454.2	1640.5	
1500	70	2.96	3.29	2895.88	1311.78	1370.88	1452.26	1636.21	
1500	126	1.59	2.02	2895.34	1311.57	1370.6	1451.85	1635.93	
1500	210	0.82	1.16	2895.58	1311.33	1370.54	1452.02	1635.62	
1000	35	12.92	13.01	2903.32	1312.07	1369.03	1455.19	1638.67	
1000	70	2.93	3.34	2896.6	1311.06	1370.66	1451.95	1636.83	
1000	126	1.52	2.09	2895.28	1311.29	1370.75	1451.87	1636.45	
1000	210	0.75	1.31	2895.89	1311.09	1370.55	1452.12	1635.43	
700	35	10.21	15.56	2903.88	1313.7	1370.45	1451.55	1639.12	
700	70	2.69	4.67	2897.06	1311.7	1371.19	1450.94	1637.58	
700	126	1.33	2.92	2896.1	1310.74	1370.93	1451.47	1636.28	
700	210	0.59	2.4	2896.04	1311.62	1371.22	1453.07	1635.46	
500	35	9.41	15.36	2907.48	1311.47	1363.99	1457.03	1637.35	
500	70	2.32	4.83	2897.59	1311.17	1372.06	1453.86	1636.56	
500	126	1.05	3.4	2895.23	1309.86	1371.23	1452.83	1636.34	
500	210	0.37	4.34	2892.52	1308.41	1374.4	1456.06	1633.64	
300	35	8.77	13.64	2905.86	1318.25	1397.39	1435.78	1644.24	
300	70	1.89	5.76	2898.81	1308.91	1370	1451.06	1637.87	
300	126	0.53	5.43	2893.99	1308.09	1373.52	1458.25	1638.42	
300	210	0	110.18	2888.88	1315.52	1376.29	1456.95	1627.58	
M2 5d				harmonic=	1306.614543	1358.326996	1381.603402	1473.003021	1646.607061

				anharm uncoupled=	1315.5190473321	1376.2891649751	1382.9563975062	1456.9466977138	1627.582439166
npts (2/3 of)	N	1000*Rfit	1000*Rtest	ZPE, cm-1	v1	v2	v3	v4	v5
4000	56	11.64	12.33	3591.06	1314.9	1360.96	1391.31	1452.31	1633.07
4000	126	2.65	3.04	3585.88	1311.9	1363.5	1387.6	1452.09	1632.57
4000	**252**	**1.39**	**1.72**	**3586.54**	**1311.48**	**1363.07**	**1387.3**	**1452.47**	**1632.26**
4000	462	0.77	1.13	3585.97	1312.27	1363.46	1387.65	1452.69	1632.28
2500	56	11.85	11.97	3589.67	1314.15	1359.77	1392.63	1448.24	1632.95
2500	126	2.63	3.11	3585.33	1311.95	1363.61	1388.35	1453.22	1632.42
2500	252	1.33	1.83	3586.32	1311.34	1363.74	1388.01	1453.38	1632.05
2500	462	0.69	1.29	3585.67	1312.56	1363.58	1387.93	1452.87	1632.09
1500	56	10.78	12.82	3589.47	1311.78	1389.77	1389.77	1443.82	1638.67
1500	126	2.39	3.32	3585.06	1311.64	1363.21	1387.25	1452.27	1632.22
1500	252	1.17	2.28	3586.23	1311.65	1363.99	1387.89	1454.51	1631.69
1500	462	0.52	2.01	3586.35	1313.01	1362.96	1387.64	1452.82	1633.31
1000	56	10.22	14.3	3585.39	1322.99	1390.1	1390.1	1455.75	1633.72
1000	126	2.04	4.44	3584.8	1311.73	1360.1	1389.27	1452.47	1629.36
1000	252	0.94	3.25	3585.61	1311.46	1361.6	1388.15	1455.21	1630.54
1000	462	0.28	5.53	3581.24	1315.43	1369.12	1390.04	1455.48	1629.39
700	56	10.46	19.04	3598.79	1315.31	1351.53	1378.2	1450.46	1617.84
700	126	1.63	5.75	3584.3	1314.44	1365.32	1387.79	1453.69	1628.25
700	252	0.63	5.64	3584.82	1310.69	1363.99	1386.72	1456.67	1632.97
700	462	0	1162.47	3579.58	1315.59	1376.35	1383.14	1457.09	1627.76