

OTHE MOLECULE IS A PROLATE ROTOR KAPPA = -.7743778 AND THE FOLLOWING TRANSFORMATIONS ARE VALID : A = Z B = X C = Y

HOWARD WILSON PARAMETERS
 0 DJ = .103097E-02 DJK = .103079E-01 DK = .238698E-01 R5 = -.187912E-02 R6 = -.276995E-04
 OWATSON'S FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
 0 DJ = -.213370E-02 DJK = -.758252E-01 DK = -.163608E+00 DEJ = .795539E-06 DEK = .192840E-04
 OCENTRIFUGAL DISTORTION CONSTANTS VIA REDUCED HAMILTON
 0 DELJ = .108637E-02 DELJK = .997555E-02 DELK = .241468E-01 DELTAJ = .231506E-03 DELTAK = .561175E-02

OCENTRIFUGAL DISTORTION CORRECTED ROTATIONAL CONSTANTS : 13783.93611 4629.65433 3465.66085
 0 NO. FREQUENCY PARAMETER CLASSICAL VALUE FREQUENCY IN CM-1
 1 .000000 .000000 761.820
 2 .031515 .000000 534.897
 3 .051394 .000000 328.006
 4 .050793 .000000 331.886
 5 .023621 .000000 713.669
 6 .038662 .000000 436.019

OU VALUES CALCULATED FOR TEMP = .0 DEGREES KELVIN

0	NO.	ATOMS	DISTANCE	U-VALUE	K-VALUE	U**2/R-K
	1	2	1.596700	.042695	.000867	.000275
	2	3	1.696640	.046079	.001627	-.000376
	3	1 3	2.277486	.063015	.000736	.001007
	4	3 4	3.389918	.057551	.000150	.000827

OU VALUES CALCULATED FOR TEMP = 300.0 DEGREES KELVIN

0	NO.	ATOMS	DISTANCE	U-VALUE	K-VALUE	U**2/R-K
	1	2	1.596700	.043934	.001124	.000085
	2	3	1.696640	.048469	.002416	-.001031
	3	1 3	2.277486	.072509	.001009	.001300
	4	3 4	3.389918	.062273	.000192	.000952

OMATRIX OF THE A COMPONENT OF ZETA

761.82	1/CM	.0000	.0000	.0000	.0000	.0000
534.90	1/CM	.0000	.0000	.0000	.0000	.0000
328.01	1/CM	.0000	.0000	.0000	.0000	.0000
331.89	1/CM	-.4155	-.0257	.9092	.0000	.0000
713.67	1/CM	.0000	.0000	.0000	.0000	.0000
436.02	1/CM	.0000	.0000	.0000	.0000	.0000

OMATRIX OF THE B COMPONENT OF ZETA

761.82	1/CM	.0000	.0000	.0000	.0000	.0000
534.90	1/CM	.0000	.0000	.0000	.0000	.0000
328.01	1/CM	.0000	.0000	.0000	.0000	.0000
331.89	1/CM	.0000	.0000	.0000	.9903	-.1392
713.67	1/CM	.0000	.0000	.0000	.0000	.0000
436.02	1/CM	.0000	.0000	.0000	.0000	.0000

OMATRIX OF THE C COMPONENT OF ZETA

761.82	1/CM	.0000	.0000	.0000	-.5070	-.6221
534.90	1/CM	.0000	.0000	.0000	.0670	.6616
328.01	1/CM	.0000	.0000	.0000	.8593	-.4186
331.89	1/CM	.0000	.0000	.0000	.0000	.0000
713.67	1/CM	.5070	-.0670	-.8593	.0000	.0000
436.02	1/CM	.6221	-.6616	.4186	.0000	.0000

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OINERTIAL DEFECT      DELTA (CENT) = .914012E-03
ODELTA (VIB) = .199842 V = 0 0 0 0 0 0
ODELTA (VIB) = -13.869901 V = 0 0 1 0 0 0
ODELTA (VIB) = 14.308976 V = 0 0 0 1 0 0
ODELTA (VIB) = .718962 V = 0 0 0 0 1 0
ODELTA (VIB) = -.016025 V = 0 1 0 0 0 0
ODELTA (VIB) = .609305 V = 0 0 0 0 1 0
ODELTA (VIB) = -.152583 V = 1 0 0 0 0 0

OCORRECTIONS OF THE MOMENTS OF INERTIA - ACCORDING TO: AA, AB, BB, AC, BC, CC
-.136002 -.007827 14.315779 -14.331521 -.000690 -.057194
.000000 .000000 -.000013 .000013 .000000 .000000
-.003923 -.181369 -.003483 .222384 -.192168 -.183033
.000000 .000000 .000000 .000000 .000000 .000000
.000000 .000000 .000000 .000000 .000000 .000000
-.492350 -.405064 .242550 .000000 .216605 .278893

OSUM OF THE CORRECTIONS FOR THE GROUND STATE : -.108728 .000000 -.170796 .000000 .000000 -.079683

OCOORDINATES IN CENTER OF MASS SYSTEM FOR ISOTOPE 2
O
I MASS X Y Z
1 18.998405 .000000 .000000 -1.243326
2 36.965898 .000000 .000000 .353374
3 18.998405 .000000 1.694959 .277876
4 18.998405 .000000 -1.694959 .277876

OFREQUENCIES IN CM-1 : 754.215 534.855 325.744 327.414 703.063 435.503
OMOMENTS OF INERTIA : 36.91884 109.16050 146.07935
OTRANSFORMATION MATRIX :
A .00000000E+00 .10000000E+01 .00000000E+00 Z INPUT SYSTEM
B .00000000E+00 .00000000E+00 .10000000E+01
C .10000000E+01 .00000000E+00 .00000000E+00

OTAU VALUES : TAAA = -.135445E+00 TBBB = -.619747E-02 TCCC = -.246357E-02
TAAB = .301688E-03 TABB = -.203455E-01 TAAC = -.848285E-02
TAC = -.793484E-32 TBCC = -.344146E-02 TBCB = -.113627E-16
ISOTOPE 2
OROTATIONAL CONSTANTS : 13688.80984 4629.65067 3459.59245
OTHE MOLECULE IS A PROLATE ROTOR KAPPA = -.7712321 AND THE FOLLOWING TRANSFORMATIONS ARE VALID : A = Z B = X C = Y
OHOWARD WILSON PARAMETERS
O DJ = .102706E-02 DJK = .101639E-01 DK = .226703E-01 R5 = -.187747E-02 R6 = -.277831E-04
OWATSON'S FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
O DJ = -.214417E-02 DJK = -.751150E-01 DK = -.161254E+00 DEJ = .797801E-06 DEK = .190998E-04
OCENTRIFUGAL DISTORTION CONSTANTS VIA REDUCED HAMILTON
ODELJ = .108263E-02 DELJK = .983053E-02 DELK = .229482E-01 DELTAJ = .233368E-03 DELTAK = .558696E-02
OCENTRIFUGAL DISTORTION CORRECTED ROTATIONAL CONSTANTS : 13688.79967 4629.64050 3459.60771
O
NO. FREQUENCY PARAMETER CLASSICAL VALUE FREQUENCY IN CM-1
1 .022351 .000000 754.215
2 .031518 .000000 534.855
3 .051751 .000000 325.744
4 .051487 .000000 327.414
5 .023977 .000000 703.063
6 .038708 .000000 435.503

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OU VALUES CALCULATED FOR TEMP = .0 DEGREES KELVIN

0	NO.	ATOMS	DISTANCE	U-VALUE	K-VALUE	U**2/R-K
	1	2	1.596700	.042495	.000844	.000287
	2	3	1.696640	.045881	.001607	-.000366
	3	1 3	2.277486	.062997	.000744	.000999
	4	3 4	3.389918	.057550	.000151	.000826

OU VALUES CALCULATED FOR TEMP = 300.0 DEGREES KELVIN

0	NO.	ATOMS	DISTANCE	U-VALUE	K-VALUE	U**2/R-K
	1	2	1.596700	.043768	.001096	.000103
	2	3	1.696640	.048313	.002404	-.001028
	3	1 3	2.277486	.072508	.001023	.001286
	4	3 4	3.389918	.062273	.000193	.000951

OMATRIX OF THE A COMPONENT OF ZETA

754.21	1/CM	.0000	.0000	.0000	-.3983	.0000	.0000
534.86	1/CM	.0000	.0000	.0000	-.0275	.0000	.0000
325.74	1/CM	.0000	.0000	.0000	-.9168	.0000	.0000
327.41	1/CM	.3983	.0275	.9168	.0000	.0000	.0000
703.06	1/CM	.0000	.0000	.0000	.0000	.0000	.0000
435.50	1/CM	.0000	.0000	.0000	.0000	.0000	.0000

OMATRIX OF THE B COMPONENT OF ZETA

754.21	1/CM	.0000	.0000	.0000	.0000	.0000	.0000
534.86	1/CM	.0000	.0000	.0000	.0000	.0000	.0000
325.74	1/CM	.0000	.0000	.0000	.0000	.0000	.0000
327.41	1/CM	.0000	.0000	.0000	.0000	-.9907	.1358
703.06	1/CM	.0000	.0000	.0000	.9907	.0000	.0000
435.50	1/CM	.0000	.0000	.0000	-.1358	.0000	.0000

OMATRIX OF THE C COMPONENT OF ZETA

754.21	1/CM	.0000	.0000	.0000	.0000	-.4883	-.6294
534.86	1/CM	.0000	.0000	.0000	.0000	.0634	.6653
325.74	1/CM	.0000	.0000	.0000	.0000	-.8704	.4016
327.41	1/CM	.0000	.0000	.0000	.0000	.0000	.0000
703.06	1/CM	.4883	-.0634	.8704	.0000	.0000	.0000
435.50	1/CM	.6294	-.6653	-.4016	.0000	.0000	.0000

0INERTIAL DEFECT DELTA (CENT) = .911602E-03

O DELTA (VIB) =	199915	V =	0	0	0	0	0
O DELTA (VIB) =	-33.443929	V =	0	0	1	0	0
O DELTA (VIB) =	33.877071	V =	0	0	0	1	0
O DELTA (VIB) =	.734634	V =	0	0	0	0	1
O DELTA (VIB) =	-.017113	V =	0	1	0	0	0
O DELTA (VIB) =	.560319	V =	0	0	0	0	1
O DELTA (VIB) =	-.111659	V =	1	0	0	0	0

OCORRECTIONS OF THE MOMENTS OF INERTIA - ACCORDING TO: AA, AB, BB, AC, BC, CC

-.136552	-.008069	33.887729	-33.901977	-.000671	-.057614
.000000	.000000	.000000	.000000	.000000	.000000
-.004142	-.181152	-.003471	.224813	-.195333	-.182060
.000000	.000000	.000000	.000000	.000000	.000000
.000000	.000000	.000000	.000000	.000000	.000000
-.452268	-.406250	.240404	.000000	.164401	.295045

OSUM OF THE CORRECTIONS FOR THE GROUND STATE : -.108577 .000000 .000000 .000000 .000000 -.079334

1	NUMBER OF PARAMETERS= 10	NUMBER OF DATA BLOCKS = 2	NUMBER OF DATA PER BLOCK 11	11
0 NR.	MEASURED	SCALING OF DATA PER BLOCK 1.000	WEIGHT	1.000
	ONUMBER HELD FIXED = 0	CALC - OBS		
	FREQUENCIES	CALCTD.		
1	.7619000000E+03	.7618197716E+03	-.8023835455E-01	.1000000000E+01
2	.5362000000E+03	.5348970187E+03	-.1302981304E+01	.1000000000E+01
3	.3280000000E+03	.3280055239E+03	.523890844E-02	.1000000000E+01
4	.3320000000E+03	.3318861323E+03	-.1138676980E+00	.1000000000E+01
5	.7131000000E+03	.7136694067E+03	.5694066604E+00	.1000000000E+01
6	.4360000000E+03	.4360189689E+03	-.5981031055E+01	.1000000000E+01
7	.1086501000E+01	.1086365484E+01	-.1355164088E-03	.6944444444E+04
8	.9968660000E+01	.9975545869E+01	.6885868771E-02	.2687449610E+03
9	.2421190000E+02	.2414680247E+02	-.6509753185E-01	.9182736455E+01
10	.2315010000E+00	.2315056153E+00	.4615336548E-05	.5948839976E+05
11	.5687440000E+01	.5611745870E+01	-.7569412955E-01	.1234567901E+03
12	-.7600000000E+01	-.7604947810E+01	-.4947809854E-02	.2500000000E+02
13	-.9180000000E-01	-.4197401739E-01	.4982598261E-01	.1020304051E-03
14	-.2086600000E+01	-.2261565434E+01	-.1749654343E+00	.1020304051E-03
15	-.4410000000E+01	-.4471821974E+01	.6182197441E-01	.1020304051E-03
16	-.1067000000E+02	-.1060596586E+02	.6403413537E-01	.2500000000E+02
17	-.4428000000E+00	-.5156168608E+00	-.72816866075E-01	.1020304051E-03
18	.1082635000E+01	.1082630489E+01	-.45111069669E-05	.1467976101E+04
19	.9818860000E+01	.9830529499E+01	.1166949912E-01	.6830134554E+02
20	.2301170000E+02	.2294815524E+02	-.6354476130E-01	.1291322314E+01
21	.2333620000E+00	.2333684641E+00	.6464145860E-05	.5165289256E+05
22	.5661120000E+01	.5586963611E+01	-.7415638936E-01	.5486968450E+02

DERIVATIVES OF THE MEASURED DATA WITH RESPECT TO THE PARAMETERS

1	.8763E+02	.2380E+01	.8864E+01	.0000E+00	.4089E+02	-.7881E+02	.2380E+01	-.9182E+01	.8864E+01
2	.3976E+01	.8010E+02	.1388E-01	.0000E+00	-.5056E+02	-.6628E+00	.8010E+02	.2128E+01	.1388E-01
3	.1570E+00	.3293E+00	.7800E+02	.1137E-09	.6431E+00	.9854E+01	.3293E+00	.1010E+02	.7800E+02
4	.5684E-10	.0000E+00	.5684E-10	.2273E+05	.1137E-09	.1137E-09	.1137E-09	.5684E-10	.0000E+00
5	.6821E-09	.1297E+03	.1822E+02	.0000E+00	-.2046E-08	-.4547E-09	-.1297E+03	.9724E+02	-.1821E+02
6	.0000E+00	.1300E+01	.1262E+03	.0000E+00	-.5684E-10	.1705E-09	-.1302E+01	.2556E+02	-.1263E+03
7	-.7466E-02	-.3057E+00	-.3294E-01	-.2220E-11	.1513E-01	-.1143E+01	.3057E+00	-.1738E+00	-.3294E-01
8	-.3786E-01	.8620E+00	.6911E+01	-.3553E-11	.3405E+01	-.1299E+02	.8620E+00	-.1609E+01	.5456E+01
9	-.4818E+01	-.5947E+00	.1797E+01	-.2487E-10	.4616E+01	-.1299E+02	-.6079E+00	.2674E+01	-.1057E+02
10	.1297E-02	-.8336E-01	.7445E-02	.4996E-12	.6042E-01	.2215E-01	-.8336E-01	.5374E-02	.7445E-02
11	.6526E-01	-.3029E+00	.3031E+01	.4441E-11	.5859E-01	.2126E+00	-.2963E+00	.6541E-01	.3152E+01
12	-.8925E+00	.8163E-01	.7775E+00	-.1137E-09	.4834E+00	.3921E+01	.8163E-01	.2628E+00	-.7775E+00
13	.7998E-01	-.8281E-01	-.2266E-02	.1137E-09	-.4803E+00	.5061E-01	-.8281E-01	-.1810E+00	-.2266E-02
14	-.4234E-01	-.1190E-02	.2388E+00	.0000E+00	.9452E-01	-.1453E+01	-.1190E-02	.3344E-01	-.2388E+00
15	.5684E-10	.5684E-10	.5684E-10	-.3062E+03	-.5684E-10	-.1137E-09	.5684E-10	.0000E+00	-.1137E-09
16	-.7958E-09	-.1663E+01	.1265E+01	-.1137E-09	.2160E-08	.3411E-09	.1663E+01	.4036E+01	.1265E+01
17	.5684E-10	-.1650E+00	.4666E+00	.5684E-10	.5684E-10	-.1137E-09	.1652E+00	.1635E+01	-.4662E+00
18	-.7579E-02	-.3051E+00	.3171E-01	.4441E-12	.1476E-01	-.1727E-01	-.3051E+00	-.1713E+00	-.3171E-01
19	-.3969E-01	.8644E+00	.6847E+01	-.7105E-11	-.3389E+01	-.1123E+01	.8733E+00	-.1567E+01	.5488E+01
20	-.4784E+01	-.5982E+00	.2214E+01	.3553E-11	.4604E+01	-.1229E+02	-.6071E+00	.2592E+01	-.1012E+02
21	.1354E-02	-.8365E-01	.6828E-02	.0000E+00	.6060E-01	.2191E-01	-.8365E-01	-.6605E-02	.6828E-02
22	.6601E-01	-.2992E+00	-.3029E+01	.2665E-11	.5529E-01	.2049E+00	-.2948E+00	-.3021E+00	.3138E+01

