Electronic Supplementary Information for

Mechanisms and kinetics of the low-temperature oxidation of 2-methylfuran: Insight from DFT calculations and kinetic simulations

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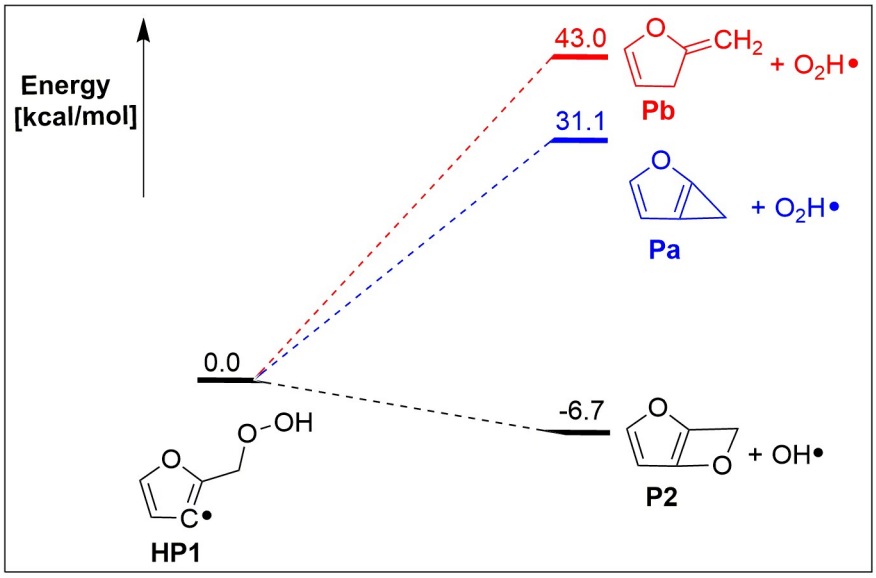

Fig. S1 Predicted relative free energies (in kcal/mol) for the decomposition processes of HP1 by the G4 method at 298 K and 1 atm.

Table S1 Arrhenius parameters for the O_2 addition to furylCH$_2$ obtained by fitting high-pressure limiting rate constants over the temperature range 300–1500 K, based on k=Aexp(-E_a/RT) (Activation energies are in kcal/mol, and A values are in s^{-1} and cm^3 mol^{-1} s^{-1} for unimolecular and bimolecular reactions, respectively)

	Reaction	forward		reverse	
		A	Ea	A	Ea
R1	furylCH$_2$ + O_2 → PO1	1.874E-12	8.7	2.558E14	25.5
R2	furylCH$_2$ + O_2 → PO2	4.254E-14	10.7	1.283E13	14.0
R3	furylCH$_2$ + O_2 → PO3	4.660E-13	13.5	9.313E13	22.3

Table S2 Arrhenius parameters for the decomposition of PO1 obtained by fitting high-pressure limiting rate constants over the temperature range 300–1500 K, based on $k=Aexp(-E_a/RT)$ (Activation energies are in kcal/mol, and A values are in s^{-1} and cm^3 mol^{-1} s^{-1} for unimolecular and bimolecular reactions, respectively)

	Reaction	forward		reverse	
		A	Ea	A	Ea
R4	PO1 → P1 + OH	1.119E12	38.1	7.034E-14	66.0
R5	PO1 → HP1	5.895E11	42.5	1.943E11	7.2
R6	PO1 → HP2	1.315E8	86.4	3.887E7	51.20
R7	PO1 → HP3	2.505E9	77.9	7.229E8	42.9
R8	HP1 → P2 + OH	5.286E12	36.9	4.380E-12	37.5
R9	HP1 → HP2	7.774E12	69.6	6.995E12	69.8
R10	HP2 → HP3	3.352E13	61.8	3.268E13	62.1
R11	HP3 → I1	1.827E14	32.22	2.218E12	25.2
R12	I1 → P3 + OH	7.466E13	20.6	1.363E-11	40.9
R13	I1 → P4 + O_2H	9.651E13	20.9	3.817E-13	16.1

Table S3 Arrhenius parameters for the decomposition of PO2 obtained by fitting high-pressure limiting rate constants over the temperature range 300–1500 K, based on $k=Aexp(-E_a/RT)$ (Activation energies are in kcal/mol, and A values are in s^{-1} and cm^3 mol^{-1} s^{-1} for unimolecular and bimolecular reactions, respectively)

	Reaction	forward		reverse	
		A	Ea	A	Ea
R14	PO2 → P5 + OH	5.377E12	33.7	1.505E-13	71.7
R15	PO2 → HP4	7.557E11	49.1	1.793E11	14.5
R16	PO2 → HP5	7.109E10	65.8	2.618E10	34.4
R17	HP4 → P6 + OH	9.191E13	42.1	7.636E-12	21.3

R18	HP4 → P5 + OH	3.679E12	28.3	4.337E-13	97.2
R19	HP4 → HP5	1.409E13	56.0	2.188E13	59.2
R20	HP5 → I2	1.022E14	28.0	5.000E11	30.4
R21	I2 → P7 + OH	3.400E12	35.4	6.567E-13	94.8
R22	I2 → P4 + O_2H	3.809E13	17.6	1.327E-13	13.3

Table S4 Arrhenius parameters for the decomposition of PO3 obtained by fitting high-pressure limiting rate constants over the temperature range 300–1500 K, based on $k=Aexp(-E_a/RT)$ (Activation energies are in kcal/mol, and A values are in s^{-1} and cm^3 mol^{-1} s^{-1} for unimolecular and bimolecular reactions, respectively)

	Reaction	**forward**		**reverse**	
		A	Ea	A	Ea
R23	PO3 → P8 + OH	2.159E12	37.1	1.134E-13	81.3
R24	PO3 → HP6	5.206E11	47.1	2.620E11	14.1
R25	PO3 → HP7	3.666E10	72.8	1.672E10	40.3
R26	HP6 → I3 + OH	1.602E14	40.5	8.970E-12	69.8
R27	I3 → P9	4.493E13	16.3	1.470E11	23.7
R28	HP6 → HP7	6.216E13	57.7	5.634E13	58.3
R29	HP6 → P8 + OH	4.239E12	31.0	4.422E-13	108.3

Table S5 Arrhenius coefficients for the decomposition of P1 obtained by fitting high-pressure limiting rate constants over the temperature range 300–1500K, based on $k=AT^nexp(-Ea/RT)$ (Activation energies are in kcal/mol, and A values are in s^{-1} and cm^3 mol^{-1} s^{-1} for unimolecular and bimolecular reactions, respectively)

	Reaction	**forward**			**reverse**		
		A	n	Ea	A	n	Ea
R31	P1 + OH → P31 + H_2O	7.546E-24	3.52	3.7	2.962E-26	3.93	0.4
R32	P1 + OH → P32 + H_2O	3.099E-24	3.91	5.3	1.442E-26	4.30	2.8
R33	P1 + OH → P33 + H_2O	1.576E-23	3.72	6.1	8.461E-26	4.08	4.3
R34	P30 → P34+CO	5.475E17	0.28	32.2	4.015E-16	1.79	0.4
R35	P34 → P35	9.367E10	1.03	33.1	3.018E11	0.17	25.5

R36	P35 → C_2H_2 + P36	1.937E12	0.70	34.0	1.247E-19	2.27	3.4
R37	P31 → P37	1.596E05	2.64	24.9	1.533E04	2.11	26.0
R38	P32 → P38	3.868E06	2.27	27.6	2.055E07	1.35	30.5
R39	P38 → P39 + HCO	1.382E13	0.55	34.6	1.992E-22	2.93	3.3
R40	P38 → P40	3.456E-05	5.20	37.7	3.008E-06	5.42	33.7
R41	P40 → P41 + CO	8.905E12	0.47	8.0	4.167E-22	2.85	5.9
R42	P41 → P42 + CO	1.039E11	0.97	8.6	1.400E-19	2.22	12.3
R43	P33 → P43	4.406E12	0.63	33.6	3.149E11	0.12	24.7
R44	P43 → P36 + P44	1.664E12	0.77	36.0	1.241E-21	2.84	0.8

Table S6 Arrhenius coefficients for the decomposition of P1 obtained by fitting high-pressure limiting rate constants over the temperature range 300–1500K, based on k=Aexp(-Ea/RT) (Activation energies are in kcal/mol, and A values are in s^{-1} and cm^3 mol^{-1} s^{-1} for unimolecular and bimolecular reactions, respectively)

	Reaction	**forward**		**reverse**	
		A	Ea	A	Ea
R31	P1 + OH → P31 + H_2O	2.960E-12	8.2	2.525E-13	5.5
R32	P1 + OH → P32 + H_2O	2.350E-11	10.3	2.122E-12	8.3
R33	P1 + OH → P33 + H_2O	2.766E-11	10.9	2.277E-12	9.5
R34	P30 → P34+CO	6.538E16	31.9	3.065E-10	2.7
R35	P34 → P35	2.253E14	34.4	1.111E12	25.7
R36	P35 → C_2H_2 + P36	3.776E14	34.9	3.821E-12	6.3
R37	P31 → P37	8.040E13	28.3	1.328E11	28.7
R38	P32 → P38	1.143E14	30.5	5.560E11	32.2
R39	P38 → P39 + HCO	8.931E14	35.4	9.223E-13	7.0

R40	P38 → P40	4.738E12	44.4	2.118E12	40.7
R41	P40 → P41 + CO	3.106E14	8.6	9.843E-13	9.5
R42	P41 → P42 + CO	1.650E14	9.9	2.874E-12	15.2
R43	P33 → P43	5.086E14	34.4	7.715E11	24.9
R44	P43 → P36 + P44	5.683E14	37.0	2.722E-12	4.5

Optimized geometries in Cartesian Coordinates (in Å), harmonic vibrational frequencies (in cm^{-1}, and the hindered rotor is labeled in red) and moment of inertia (in Amu.bohr**2) by the G4 method.

furylCH_2

0 2

O	-1.07550800	-0.13995900	0.00000000
C	0.79322500	-1.38913800	0.00000000
H	1.43456800	-2.25675100	0.00000000
C	0.00000000	0.73335000	0.00000000
C	1.18046900	-0.03468800	0.00000000
H	2.18177000	0.36626400	0.00000000
C	-0.23840400	2.08476800	0.00000000
H	-1.24815000	2.47039200	0.00000000
H	0.59045100	2.77852500	0.00000000
C	-0.57668700	-1.40157000	0.00000000
H	-1.30618900	-2.19509000	0.00000000

Freq: 251.34 356.26 524.68 591.50 659.51 702.47 708.65 715.14 749.93 856.74 888.66 903.16 955.87 1038.36 1121.80 1189.24 1238.70 1312.90 1393.54 1428.39 1509.18 1543.53 3185.61 3249.92 3262.80 3281.19 3287.07

MOMENT OF INERTIA: 203.21679 466.82581 670.04261

O_2

0 3

O	0.00000000	0.00000000	0.60319500
O	0.00000000	0.00000000	-0.60319500

Freq: 1664.1127

MOMENT OF INERTIA : 41.56479

TS1

0 2

O	-1.02775900	-1.05891400	0.25207100

C	-2.43412600	0.53647600	-0.45572400
H	-3.31289800	1.00658200	-0.86805500
C	-0.40985100	0.15651000	0.46105100
C	-1.26344300	1.16551500	0.02705000
H	-1.04983100	2.22238500	0.06205200
C	-2.23575100	-0.80767400	-0.29536200
H	-2.84260700	-1.67194800	-0.51220500
C	0.88187100	0.16326800	0.98398500
H	1.31836500	1.10434400	1.28599300
H	1.30355700	-0.74376800	1.39267000
O	2.26722700	0.04456800	-0.66969300
O	3.42943300	-0.13592500	-0.29318500

Freq: 263.27i 19.77 69.88 101.86 245.84 329.26 347.45 591.60 672.39 709.97 719.74 758.15 797.70 865.22 870.40 897.72 923.40 976.68 1047.30 1124.52 1195.68 1254.26 1305.59 1410.07 1427.82 1446.68 1501.35 1570.44 3190.90 3253.70 3264.66 3282.58 3294.02

MOMENT OF INERTIA : 317.15237 1800.96238 1891.19487

PO1

0 2

O	-0.90275900	-1.03735700	0.20554200
C	-2.42726100	0.51709900	-0.29226200
H	-3.36283900	0.97813300	-0.56591100
C	-0.29437100	0.18264200	0.29825700
C	-1.18885900	1.16730800	0.00202500
H	-0.98695300	2.22721100	-0.00550500
C	-2.18945200	-0.81464900	-0.15365200
H	-2.80252700	-1.69382200	-0.26553400
C	1.13293900	0.19332300	0.66164000
H	1.43781500	1.16729900	1.04884300
H	1.38923000	-0.59008400	1.37803400
O	1.94700300	-0.06148100	-0.54644300
O	3.22166800	-0.09654700	-0.24484600

Freq: 46.81 84.97 119.21 314.85 358.79 402.57 615.20 665.82 758.25 769.52
822.06 865.26 901.17 915.28 922.26 976.79 1041.60 1113.45 1185.32 1199.96 1205.81 1255.32 1278.81 1365.42 1424.32 1467.28 1527.02 1638.48 3076.59 3139.40 3253.94 3264.93 3286.45

MOMENT OF INERTIA : 263.12709 1581.63449 1720.88433

TS2

0 2

O	-1.31502700	0.88050900	-0.52800500
C	-1.26056900	-1.19359800	0.37980400

H	-1.55609700	-2.20286300	0.61535000
C	-0.18301600	0.82826000	0.28072800
C	-0.06146100	-0.51318700	0.80758700
H	0.46445100	-0.72267300	1.72766900
C	0.67631400	1.85012600	0.35667300
H	0.52308600	2.75960600	-0.21008700
H	1.53270100	1.78394900	1.01058700
C	-1.91871000	-0.33080000	-0.42414200
H	-2.83757000	-0.43022800	-0.98271400
O	2.22139300	-0.31269100	-0.55151500
O	1.38839400	-1.19689100	-0.24106800

Freq: 271.68i 101.71 146.96 177.33 268.84 361.21 463.54 558.64 663.95 702.23 718.91 781.46 876.20 886.31 893.13 896.75 936.88 993.95 1045.87 1112.56 1192.74 1230.54 1322.27 1341.14 1399.52 1438.53 1596.22 1697.65 3188.99 3231.06 3253.56 3278.63 3291.54
MOMENT OF INERTIA : 547.27376 894.73926 1229.54478

PO2
0 2

O	-1.63301400	0.61448200	-0.34731600
C	-0.85149000	-1.41151400	0.33522800
H	-0.82729000	-2.46730600	0.55011200
C	-0.34626900	0.85618000	0.12090000
C	0.28632500	-0.46222000	0.51133400
H	0.77978700	-0.44803600	1.48407000
C	0.16676100	2.07625200	0.17459100
H	-0.39146400	2.93765300	-0.16947700
H	1.17252600	2.21698900	0.54574600
C	-1.87166500	-0.72060500	-0.17643800
H	-2.86344700	-1.03484600	-0.46854900
O	2.48363800	-0.18732300	-0.17272400
O	1.37786600	-0.83128600	-0.44691000

Freq: 70.60 108.53 242.78 264.59 377.00 427.40 508.63 633.19 683.00 743.67 746.24 841.63 865.00 885.85 906.19 924.43 933.33 1035.37 1094.03 1191.15 1200.66 1221.87 1269.78 1303.98 1378.69 1423.67 1663.26 1751.45 3103.89 3180.58 3247.83 3277.03 3277.91
MOMENT OF INERTIA : 519.95885 895.02828 1314.94404

TS3
0 2

O	-0.48137300	-0.71868500	0.66674100
C	0.02673300	1.43469400	0.17662000
H	0.60025700	2.34760400	0.13269900
C	-1.55233900	-0.17487600	-0.03522700

C	-1.21914000	1.19403700	-0.32522600
H	-1.86373500	1.87422800	-0.86085000
C	-2.63347900	-0.92105100	-0.31873000
H	-2.69344000	-1.95780300	-0.01714800
H	-3.46239400	-0.48589600	-0.85961700
C	0.49620400	0.21018800	0.72797400
H	1.25491300	0.05055700	1.47947100
O	1.87954700	-0.41434100	-0.64654400
O	3.03389100	-0.40280400	-0.17357500

Freq: 402.31i 40.31 82.86 165.52 239.57 309.43 367.62 521.98 648.87 688.67 708.68 800.39 830.12 873.57 893.27 912.18 940.39 945.14 1049.58 1100.41 1196.80 1231.46 1321.38 1355.74 1419.87 1445.05 1519.06 1647.27 3186.07 3241.61 3251.92 3269.91 3283.47

MOMENT OF INERTIA : 380.97009 1400.54954 1587.99178

PO3

0 2

O	-0.44573600	-0.86773100	0.43127200
C	0.22195100	1.32818100	0.18366900
H	0.88205400	2.18262800	0.18819600
C	-1.51984400	-0.11831300	-0.02059600
C	-1.06967300	1.26190500	-0.15202100
H	-1.71223400	2.06703300	-0.47865500
C	-2.71537000	-0.65887700	-0.24738900
H	-2.89205400	-1.71700800	-0.10918500
H	-3.53411300	-0.03454400	-0.57773600
C	0.68180100	-0.05635200	0.52020600
H	1.20920100	-0.19569600	1.46679800
O	1.63966700	-0.54225500	-0.51187100
O	2.86281300	-0.19522400	-0.19348000

Freq: 42.58 102.13 240.45 305.61 355.78 429.97 494.50 655.69 710.49 713.25 801.67 844.10 858.35 884.14 914.24 932.35 956.87 990.32 1086.46 1158.79 1214.71 1234.07 1322.53 1348.00 1361.41 1435.01 1639.22 1733.19 3092.21 3184.61 3238.09 3261.78 3278.09

MOMENT OF INERTIA : 322.18825 1266.03502 1480.15922

TS4

0 2

O	-1.19369700	-1.11008100	0.00637300
C	-2.17408900	0.90075400	0.09763200
H	-2.93710200	1.65929800	0.17175500
C	-0.21706300	-0.16215900	-0.11447000
C	-0.77414400	1.09347000	-0.05556700
H	-0.22899900	2.02088400	-0.11924600

C	-2.37062700	-0.44920200	0.13242700
H	-3.24664200	-1.06918000	0.23075900
C	1.14722000	-0.61726500	-0.22407200
H	1.31499600	-1.60662500	-0.66135200
O	2.06570700	0.35242100	-0.59727700
O	2.83313000	0.14380900	0.64951700
H	1.78885000	-0.68715800	0.89347800

Freq: 1741.58i 101.18 109.50 186.89 273.10 430.87 586.59 602.52 664.15 762.56 770.55 819.60 872.15 877.35 898.08 935.41 964.65 1034.04 1111.49 1114.27 1174.17 1195.62 1215.52 1259.85 1363.56 1436.15 1496.32 1585.89 1984.27 3070.98 3259.35 3278.69 3287.58
MOMENT OF INERTIA : 283.45354 1451.20438 1628.13368

P1
0 1

O	1.24611200	-0.28144000	0.00000000
C	-0.26242900	-1.93199400	0.00000000
H	-0.68470400	-2.92434500	0.00000000
C	0.00000000	0.28853100	0.00000000
C	-0.95679300	-0.69250100	0.00000000
H	-2.02186100	-0.52408600	0.00000000
C	1.06690900	-1.61640000	0.00000000
H	1.96591400	-2.21168700	0.00000000
C	-0.06783600	1.74032600	0.00000000
H	0.92658800	2.23591500	0.00000000
O	-1.10424200	2.36849400	0.00000000

Freq: 161.74 202.23 259.46 497.36 612.22 652.27 759.71 784.37 842.73 894.74 900.82 964.37 1033.29 1037.17 1118.01 1189.15 1231.89 1266.29 1401.08 1448.83 1496.47 1610.62 1785.30 2906.67 3257.34 3272.70 3283.13
MOMENT OF INERTIA : 219.10687 881.49868 1100.60554

OH
0 2

O	0.00000000	0.00000000	0.10848300
H	0.00000000	0.00000000	-0.86786700

Freq: 3691.4816
MOMENT OF INERTIA : 3.22743

TS5
0 2

O	-1.32318400	-1.09383600	-0.00078200
C	-1.79097900	1.11674000	-0.02381800
H	-2.34187700	2.04059200	-0.09183200

C	-0.15047400	-0.41623900	0.11772300
C	-0.38049000	0.91668000	0.05704400
H	1.02708600	1.38697000	-0.02229800
C	-2.30742800	-0.14337700	-0.07461500
H	-3.30813800	-0.52643300	-0.19146200
C	1.18333200	-1.07684700	0.20497900
H	1.51820200	-1.23150600	1.23893300
H	1.22143900	-2.02495000	-0.33951800
O	2.08920200	-0.19913600	-0.47572800
O	2.05392100	1.03967000	0.19129800

Freq: 1360.90i 100.02 214.61 328.39 354.13 427.67 509.57 588.34 630.50 725.50 743.38 834.95 871.56 908.27 937.55 1007.17 1026.49 1067.97 1112.73 1158.28 1222.61 1267.70 1279.74 1354.75 1412.71 1472.79 1504.71 1568.91 1615.04 3020.07 3101.60 3263.30 3284.47

MOMENT OF INERTIA : 346.19312 1123.97836 1422.56415

HP1

0 2

O	0.98939900	0.98445600	0.19470900
C	2.53132400	-0.58661600	-0.27738300
H	3.46746100	-1.05386400	-0.53372300
C	0.35396600	-0.23606900	0.28326500
C	1.27515100	-1.18561500	-0.00050500
C	2.28168500	0.74742200	-0.14173800
H	2.90178000	1.62355300	-0.24601000
C	-1.08256400	-0.24442500	0.63417600
H	-1.36339400	-1.23779500	1.00576600
H	-1.30410600	0.50026000	1.40745400
O	-1.81995100	0.07180600	-0.55085800
O	-3.20571300	0.17146900	-0.15029300
H	-3.56899200	-0.62218000	-0.56884900

Freq: 64.21 97.09 116.86 228.69 318.57 349.86 376.13 591.96 640.27 738.50 756.26 844.56 881.25 929.91 941.48 987.15 1034.60 1094.81 1155.43 1184.33 1215.64 1253.79 1374.21 1378.11 1394.18 1497.55 1505.57 1618.59 3022.24 3069.69 3262.65 3284.89 3750.53

MOMENT OF INERTIA : 240.95614 1646.19773 1769.86017

TS6

0 2

O	1.21557900	0.96016000	-0.41683700
C	1.06969800	-1.17866100	0.25456500
H	-0.10541000	-1.61677600	-0.14355100
C	0.32173600	0.86870800	0.67104500
C	0.42196300	-0.37415400	1.24548600

H	-0.22661600	-0.74108200	2.02430300
C	1.59918500	-0.30372100	-0.67286000
H	2.22496200	-0.45183600	-1.53933000
C	-1.08182600	1.14678700	0.22392800
H	-1.79982300	1.08786600	1.04180200
H	-1.21167800	2.05347300	-0.36924900
O	-1.38110500	0.06610900	-0.77601600
O	-1.44272100	-1.18694500	-0.22551700

Freq: 2767.42i 194.03 223.48 320.78 369.85 431.88 505.69 608.39 642.00 672.34 712.73 800.93 833.09 863.11 897.64 936.69 1024.87 1068.69 1098.92 1143.85 1170.09 1198.47 1243.67 1289.24 1318.60 1435.39 1460.68 1476.61 1550.62 3089.81 3164.56 3268.68 3269.99
MOMENT OF INERTIA : 505.90832 754.39488 892.06083

HP2
0 2

O	-1.03240800	-0.99513600	0.21362400
C	-2.50603200	0.54839300	-0.32396600
C	-0.41398800	0.22285200	0.26767100
C	-1.28686300	1.22308700	-0.05777100
H	-1.07052000	2.27790700	-0.10141100
C	-2.33290900	-0.78002900	-0.15463600
H	-2.95781600	-1.65167200	-0.23625500
C	1.02343800	0.22482100	0.63272900
H	1.31419200	1.20896300	1.01721100
H	1.22824400	-0.53075800	1.40248300
O	1.76949900	-0.07287300	-0.55111800
O	3.16355800	-0.05032100	-0.16782000
H	3.37882400	-0.99255000	-0.22367400

Freq: 55.99 95.44 122.05 233.91 327.32 352.41 375.89 548.40 659.24 751.59 767.91 823.06 883.22 931.80 941.71 998.72 1034.60 1086.98 1118.92 1205.22 1225.49 1255.03 1370.44 1378.33 1390.07 1498.03 1511.08 1592.29 3016.60 3069.62 3273.26 3304.40 3749.19
MOMENT OF INERTIA : 261.16815 1583.6557 1727.98488

TS7
0 2

O	-0.29488600	-0.02029500	1.20611400
C	-1.83005500	-0.22298500	-0.40228800
H	-2.62135800	-0.63837500	-1.00977800
C	-0.11707600	0.99853800	0.30954000
C	-1.18990300	0.99178900	-0.59586700
H	-1.35308800	1.71295400	-1.38316700
C	-1.10428500	-0.96052700	0.61088000

H	-0.10443000	-1.65420400	0.10170200
C	1.32707700	1.02073300	-0.04014200
H	1.51193700	1.50023100	-1.00643200
H	1.99478900	1.42341300	0.72523500
O	1.72294000	-0.41132800	-0.05502200
O	0.82914600	-1.23204000	-0.74112900

Freq: 2424.91i 200.69 246.52 325.38 352.64 431.03 461.95 526.56 667.70 725.12 769.86 788.78 805.92 883.08 898.14 929.50 994.63 1012.14 1056.55 1068.05 1146.75 1219.76 1280.07 1317.81 1375.02 1404.91 1445.88 1464.02 1741.59 3054.95 3120.60 3240.26 3256.87

MOMENT OF INERTIA : 476.0496 773.53264 905.93731

HP3

0 2

O	-0.96963000	-1.10336700	0.18326100
C	-2.58047400	0.39671600	-0.28880700
H	-3.54032000	0.80832700	-0.54776200
C	-0.40191100	0.16181200	0.28156200
C	-1.35336600	1.09369700	-0.00039800
H	-1.20557300	2.16341300	-0.00687800
C	-2.23354700	-0.90829600	-0.15411400
C	1.03281100	0.22802600	0.63229500
H	1.27115700	1.22492400	1.02189500
H	1.28832600	-0.51816800	1.39558800
O	1.78634300	-0.02200900	-0.55844400
O	3.17995500	0.04712800	-0.17843300
H	3.43198400	-0.88424600	-0.25713100

Freq: 62.01 95.71 121.19 235.11 323.63 350.21 375.25 503.64 646.30 755.56 784.33 855.83 878.62 919.65 939.96 989.08 1027.63 1033.40 1121.83 1184.17 1236.52 1246.59 1356.07 1378.94 1393.19 1460.10 1496.07 1637.60 3017.14 3064.85 3249.01 3293.21 3750.00

MOMENT OF INERTIA : 252.53291 1607.49036 1742.97346

TS8

O	1.64413500	-1.05157300	0.03047400
C	1.70365900	1.23326000	0.01566100
H	2.09531400	2.23664400	0.05291500
C	0.40439900	-0.58136100	-0.24516600
C	0.38962200	0.76449200	-0.29421100
H	-3.31362500	1.06021900	0.46886300
C	2.42398100	0.07779000	0.14100200
H	3.48276000	-0.11084800	0.22466000

C	-0.99275500	-0.99458000	0.02439500
H	-1.54530800	-1.46432300	-0.79287800
H	-1.14249300	-1.55490700	0.95310000
O	-1.40298300	0.39110800	0.17852500
O	-3.13491200	0.26491600	-0.05359300

Freq: 754.97i 89.96 160.94 179.46 227.31 267.64 339.43 490.80 580.63 627.88 727.64 740.99 841.28 860.87 930.91 956.54 1013.53 1035.53 1063.23 1119.34 1138.52 1167.93 1269.50 1319.69 1414.82 1488.24 1502.67 1596.98 3051.80 3106.44 3260.49 3280.52 3780.73
MOMENT OF INERTIA : 277.20923 1388.31063 1634.13257

P2
0 1

O	1.03295400	-1.16477400	-0.00841400
C	1.09140700	1.13617000	0.04634900
H	1.49642700	2.13089000	0.13810900
C	-0.21532400	-0.67329600	-0.25650700
C	-0.23072400	0.66725100	-0.19064700
C	1.80903400	-0.03754600	0.10139200
H	2.87153000	-0.22158000	0.13564700
C	-1.69131800	-0.64410100	0.13785900
H	-2.43394900	-1.06154900	-0.54625300
H	-1.90704800	-0.90880600	1.17507800
O	-1.60863000	0.83604700	0.01675700

Freq: 159.36 348.82 445.83 588.23 655.64 699.28 744.85 794.84 816.99 872.38 935.27 978.64 1031.15 1061.93 1103.58 1149.78 1220.36 1273.73 1343.73 1429.61 1475.57 1490.79 1654.42 3067.17 3134.41 3257.41 3275.89
MOMENT OF INERTIA : 262.82191 612.61757 851.66428

TS9
0 2

O	-0.98262000	-0.96996600	0.25454900
C	-2.53484000	0.54091600	-0.26573700
C	-0.39008500	0.26361700	0.29898200
C	-1.35386200	1.21269400	0.02235100
H	-1.98804500	1.37852900	-1.09689300
C	-2.25993300	-0.80691100	-0.16493300
H	-2.82446000	-1.71601400	-0.29321100
C	1.05346600	0.30009800	0.63165000
H	1.33668500	1.31745000	0.91863700
H	1.28691800	-0.38428500	1.45825100
O	1.77054300	-0.09844400	-0.54163100
O	3.17410900	-0.01899100	-0.20617100

H 3.40417700 -0.95895800 -0.17464100
Freq: 1816.82i 57.12 94.77 117.08 233.24 324.85 354.54 378.29 436.38 555.09 648.92 702.32 759.44 805.60 938.20 942.33 1002.93 1030.52 1103.60 1165.31 1215.38 1263.05 1343.67 1369.41 1385.64 1400.01 1487.94 1506.29 2156.91 3014.93 3086.16 3278.97 3747.70
MOMENT OF INERTIA : 255.31854 1596.94188 1596.94188

TS10
0 2
O -0.96280500 -1.00971900 0.23081100
C -2.53397900 0.41217500 -0.25471800
C -0.42103800 0.24927700 0.23580000
C -1.33684900 1.19755400 -0.08394500
H -1.18242000 2.25753500 -0.19483100
C -2.35144200 -0.93605400 0.00656800
H -2.58227400 -0.44530400 -1.21804100
C 1.02337000 0.34803300 0.58786100
H 1.29258200 1.38793900 0.80508400
H 1.23343000 -0.26719000 1.47306400
O 1.75919200 -0.13233000 -0.53326900
O 3.15205700 -0.05350000 -0.16260400
H 3.37075800 -0.99450500 -0.09417700
Freq: 1266.42i 54.57 85.84 124.79 240.57 315.16 353.29 374.23 536.31 592.60 650.76 756.74 806.78 908.38 934.73 957.19 961.73 1004.88 1050.10 1055.75 1168.06 1219.65 1243.04 1321.08 1377.23 1396.63 1499.48 1613.87 2135.71 3015.69 3069.55 3281.11 3747.15
MOMENT OF INERTIA : 259.5199 1576.39931 1723.24583

TS11
0 2
C -2.26678000 0.84556400 -0.11333500
H -3.02785200 1.59505700 -0.21935800
C -0.05840600 0.06519100 0.53602800
C -0.92410500 1.05597400 0.43619800
H -0.65105200 2.05434600 0.77305500
H 1.77636100 0.84335800 -1.39272800
C 1.25162200 -0.46715300 0.87241300
H 1.69983700 0.16259600 1.66007200
H 1.18407000 -1.49142000 1.25899700
O 2.15965200 -0.58155700 -0.22206700
O 2.43742500 0.75087200 -0.68956600
C -2.30104200 -0.46253900 -0.42564200
O -1.49571400 -1.34258500 -0.32761900
Freq: 391.11i 39.12 71.10 127.48 218.77 271.37 343.56 422.91 497.19

504.04 614.40 622.13 695.54 818.91 862.04 907.91 971.21 994.32
1040.00 1108.42 1172.04 1253.98 1318.05 1349.03 1401.41 1411.06
1710.79 1839.70 2962.04 3060.19 3154.68 3315.53 3727.75
MOMENT OF INERTIA : 408.11621 1468.35056 1632.30914

I1
0 2

C	1.90847800	0.95711800	0.05331300
H	2.43234000	1.88560600	0.24751600
C	-0.29756400	-0.04658500	-0.58546500
C	0.49557700	0.97498100	-0.31719100
H	0.07182700	1.98416700	-0.37923800
H	-1.84433700	0.08289500	1.62413500
C	-1.70334300	-0.24677900	-0.97153100
H	-2.12769100	0.70148900	-1.34536600
H	-1.80694800	-1.00159700	-1.76124000
O	-2.52668200	-0.75558400	0.07716500
O	-2.62705800	0.26932100	1.08254400
C	2.63502500	-0.13951500	0.17147600
O	3.28446100	-1.09472100	0.27911400

Freq: 35.46 63.36 87.98 162.60 203.44 253.45 279.86 384.86 435.07
523.51 557.96 583.35 743.62 807.62 868.35 901.72 989.49 1018.16
1056.89 1161.02 1246.39 1297.71 1351.04 1403.18 1422.26 1430.73
1720.89 2223.57 2950.61 3040.74 3052.36 3200.36 3718.80
MOMENT OF INERTIA : 380.83035 2189.03078 2249.44384

TS12
0 2

C	-2.05767500	-0.40440300	-0.02015200
H	-3.12615300	-0.58404600	-0.03715800
C	0.16969700	-1.54192300	-0.01010700
C	-1.13645300	-1.53882900	-0.03627200
H	-1.63102300	-2.51143400	-0.07656400
H	2.13049600	1.76546100	-0.67621300
C	1.56509300	-1.16082800	0.01904400
H	2.12413900	-1.49342000	0.90488600
H	2.12925500	-1.39948400	-0.89334300
O	1.10394700	0.14970800	0.08492900
O	2.52508000	1.20829300	0.01065500
C	-1.70371000	0.87017500	0.00974700
O	-1.46008100	2.00172100	0.03002000

Freq: 731.85i 54.52 56.50 89.55 146.52 161.26 181.91 251.74 330.42
349.24 465.40 518.59 568.74 721.65 808.01 810.31 921.50 993.67
1040.42 1102.20 1152.76 1165.44 1292.82 1320.27 1420.92 1516.81

1838.77 2227.24 2991.89 3031.47 3095.74 3199.45 3777.57
MOMENT OF INERTIA : 671.46259 1124.85021 1780.30865

P3
0 1

C	1.20682200	1.06619500	-0.00028500
H	1.85803900	1.93306100	-0.00088000
C	-1.15710900	0.30807400	0.00023000
C	-0.24335400	1.26410500	0.00018200
H	-0.58813900	2.29038700	0.00063200
C	-2.46591300	-0.27077600	0.00022400
H	-3.03797700	-0.34961300	0.92238800
H	-3.03827100	-0.34886100	-0.92182100
O	-1.20770400	-1.05166200	-0.00028600
C	1.83804200	-0.09137700	-0.00010300
O	2.42463100	-1.09612700	0.00005900

Freq: 54.76 86.78 223.22 237.77 440.92 493.13 512.86 563.78 698.15 787.62 806.51 908.41 997.77 1028.15 1071.63 1093.65 1156.10 1214.65 1359.14 1424.97 1509.66 1888.86 2219.69 3097.38 3187.93 3190.45 3209.70
MOMENT OF INERTIA : 295.13509 1032.46204 1315.35648

TS13
0 2

C	-2.02677100	1.01756800	-0.08664000
H	-2.51963000	1.98102500	-0.14074700
C	0.19405100	-0.12153800	-0.22729600
C	-0.56840200	0.94040700	-0.24643000
H	-0.09604100	1.91310400	-0.40143500
H	3.11840200	1.14434100	0.83877300
C	1.19277200	-1.03232200	-0.25660600
H	1.50236500	-1.51211600	0.66880200
H	1.31374600	-1.64860500	-1.14582400
O	2.79873000	-0.11005500	-0.50374200
O	3.33132400	0.20359900	0.73979000
C	-2.81962200	-0.01486200	0.12225200
O	-3.52393100	-0.92020200	0.30754500

Freq: 568.11i 33.05 53.25 67.62 125.46 168.29 250.69 304.48 365.70 418.35 498.57 512.85 556.63 751.06 757.25 847.81 889.85 963.11 1054.63 1065.86 1072.24 1168.46 1328.86 1402.70 1417.61 1460.47 1906.13 2220.88 3083.82 3107.04 3179.50 3200.31 3702.85
MOMENT OF INERTIA : 298.95727 2525.04954 2685.61469

P4

0 1

C	-1.23190900	0.46005900	0.00000000
H	-2.19228400	0.96207400	0.00000000
C	1.23481200	0.82248200	0.00000000
C	0.00000000	1.25878500	0.00000000
H	-0.16584500	2.33397300	0.00000000
C	2.46171000	0.39035200	0.00000000
H	3.00378500	0.19972400	0.92422900
H	3.00378500	0.19972400	-0.92422900
C	-1.28401400	-0.85699100	0.00000000
O	-1.34163000	-2.01795100	0.00000000

Freq: 76.71 95.04 257.76 301.24 497.39 533.25 539.65 622.00 774.05 885.45 895.24 895.29 1021.11 1101.31 1186.34 1366.56 1421.03 1488.34 2060.44 2220.96 3108.27 3143.94 3174.11 3199.43
MOMENT OF INERTIA : 243.48659 813.28035 1044.46987

O_2H
0 2

O	0.05542300	0.71635300	0.00000000
O	0.05542300	-0.60794400	0.00000000
H	-0.88677600	-0.86726900	0.00000000

Freq: 1183.26 1448.59 3581.96
MOMENT OF INERTIA : 2.91436 53.23216 56.14652

TS14
0 2

O	1.81761100	0.23961700	-0.16307700
C	0.40196500	-1.51792100	0.12435300
H	0.03928000	-2.52607300	0.23950700
C	0.56315300	0.80443100	-0.02813300
C	-0.43119400	-0.30494200	0.01045100
H	-1.07336200	-0.33915600	-1.06104300
C	0.37241200	2.12014300	0.06232600
H	1.20118700	2.81531600	0.04422700
H	-0.63622100	2.49673200	0.16555500
C	1.67147200	-1.11762400	-0.03714700
H	2.59796300	-1.67063900	-0.08020100
O	-2.40281500	-0.19492100	-0.55242300
O	-1.61425800	-0.12978200	0.70310600

Freq: 1442.89i 97.99 146.55 247.69 283.21 416.95 488.71 539.04 639.17 710.79 718.99 772.89 841.58 874.95 882.25 897.52 907.53 913.82 979.02 1046.99 1121.95 1170.20 1243.30 1267.82 1392.22 1415.29 1611.66 1678.50 2041.03 3182.91 3253.84 3282.75 3283.26
MOMENT OF INERTIA : 519.68907 909.07086 1323.82166

P5
0 1

O	0.47268400	-1.37894700	0.00030500
C	1.37243000	0.72196700	-0.00033000
H	2.11247700	1.50541700	-0.00096800
C	-0.60720400	-0.51068900	0.00013500
C	-0.08417600	0.90371400	0.00056300
C	-1.86789800	-0.92196200	-0.00012200
H	-2.13744000	-1.97037700	-0.00026100
H	-2.64797300	-0.17080600	-0.00012800
C	1.59394300	-0.60342000	0.00009200
H	2.51632000	-1.16781700	-0.00010900
O	-0.75842900	1.91218700	-0.00037500

Freq: 161.28 279.39 321.34 502.39 514.52 627.81 750.00 766.48 769.15 829.78 837.47 905.23 937.31 944.93 1049.19 1096.78 1198.75 1268.31 1365.72 1412.11 1618.68 1729.31 1801.47 3174.58 3239.98 3273.19 3277.49
MOMENT OF INERTIA : 454.01309 492.36658 946.37961

TS15
0 2

O	1.49832000	0.87183800	-0.29411800
C	-0.64541600	1.12288800	0.41715300
H	-1.98261200	0.74033300	0.13372700
C	1.10272500	-0.40868900	0.07641400
C	-0.33425300	-0.36427200	0.53463700
H	-0.53586700	-0.81639800	1.50914800
C	1.93465800	-1.43919300	0.01481500
H	2.94416700	-1.32651200	-0.36020500
H	1.60578300	-2.42146100	0.32652100
C	0.43717400	1.72888400	-0.06052700
H	0.64250300	2.75781400	-0.31610100
O	-2.45878200	-0.30495800	-0.15323000
O	-1.24495000	-0.91331600	-0.45115800

Freq: 2149.23i 110.65 184.76 259.07 339.73 398.11 550.55 575.24 604.23 687.39 736.27 833.51 880.52 890.99 902.28 909.89 944.23 968.39 988.03 1030.24 1102.69 1210.18 1230.14 1292.02 1312.51 1429.22 1632.62 1741.62 1806.26 3074.59 3177.59 3260.28 3271.23
MOMENT OF INERTIA : 485.16245 911.09702 1301.78732

HP4
0 2

O	-1.83616000	-0.34387900	-0.24463600

C	0.05378300	-1.45070900	0.27492900
H	2.76299300	-0.80128400	-0.58892500
C	-0.90976300	0.63181400	0.09888800
C	0.42804200	-0.01384700	0.47617600
H	0.75281300	0.22324400	1.49498400
C	-1.19682000	1.92378000	0.04915900
H	-2.16669700	2.27121100	-0.28472000
H	-0.44933600	2.65379600	0.32804300
C	-1.21245500	-1.57419700	-0.08661300
H	-1.84453100	-2.42563500	-0.28566100
O	2.67901600	-0.02771100	-0.01090000
O	1.40314900	0.49379300	-0.43683300

Freq: 76.78 118.42 186.87 256.71 293.17 327.56 419.75 545.10 577.40 674.65 731.21 820.51 873.34 884.23 891.93 923.05 940.27 984.19 1043.70 1093.07 1196.39 1238.16 1294.08 1332.88 1389.77 1420.89 1648.99 1744.33 3046.73 3176.71 3271.32 3272.43 3732.23

MOMENT OF INERTIA : 498.29345 980.80082 1402.52682

TS16

0 2

O	0.68025300	1.08958800	-0.64026900
C	-0.80806500	0.82850300	1.08878600
H	-1.69674000	0.94622100	1.69008900
C	1.09727400	-0.02892800	0.07713000
C	-0.05419100	-0.41951700	0.94596600
H	0.11743300	-1.10143000	1.77277400
C	2.29386800	-0.58034900	-0.06061200
H	3.03362600	-0.16279100	-0.73114800
H	2.54359300	-1.47482000	0.49421700
C	-0.58246800	1.37585400	-0.16630300
H	-1.34788100	0.68972700	-0.92995200
O	-1.30597400	-0.67089600	-1.15251100
O	-1.16534700	-1.16247700	0.09205800

Freq: 2332.54i 134.43 220.88 284.94 321.83 385.79 475.54 544.50 642.59 667.14 702.17 703.86 728.32 835.77 883.11 898.30 917.13 1006.89 1022.24 1054.55 1154.79 1219.35 1250.25 1267.97 1310.19 1363.70 1432.98 1727.05 1757.58 3179.56 3182.94 3257.36 3272.35

MOMENT OF INERTIA : 535.92123 814.07131 915.17207

HP5

0 2

O	1.47703400	0.58495400	-0.58534600
C	-0.31118600	1.53823500	0.48733700
H	-0.98286400	2.29615200	0.85256200

C	0.88750800	-0.47415600	0.13665100
C	-0.37491100	0.05044600	0.81880300
H	-0.37852000	-0.14845300	1.89763500
C	1.42099000	-1.68225500	0.14769500
H	2.32086000	-1.91125900	-0.40822300
H	0.93726900	-2.47474000	0.70390100
C	0.74736000	1.66495800	-0.30352200
H	-2.06005000	0.31843500	-1.16025100
O	-1.66339900	-0.55650000	-1.02566500
O	-1.57054300	-0.61139200	0.41008500

Freq: 88.10 140.15 204.88 233.34 309.58 408.29 417.71 552.50 611.64 672.82 726.78 731.24 816.30 854.91 875.23 896.42 934.67 973.01 1011.97 1095.46 1171.96 1221.38 1282.01 1332.36 1403.88 1419.59 1618.14 1756.40 3043.07 3178.00 3270.27 3284.35 3719.44
MOMENT OF INERTIA : 613.71278 783.40363 1084.04031

TS17
0 2

O	-1.70171400	-0.37440100	-0.42646700
C	0.02983900	-1.35291500	0.67374400
H	3.31400400	-0.08995600	-0.59624900
C	-0.91503500	0.69457800	0.05026500
C	0.31656000	0.08458600	0.65510400
H	0.78571000	0.60516300	1.48626000
C	-1.36344300	1.93933500	0.00508700
H	-2.34114600	2.17801700	-0.39400000
H	-0.73803200	2.74716100	0.36109800
C	-1.04578400	-1.52685800	-0.15779800
H	-1.46548600	-2.40783300	-0.62162300
O	2.73432400	0.62030900	-0.28312200
O	1.25640600	-0.50402200	-0.23964800

Freq: 754.57i 91.29 112.79 125.52 211.83 231.63 340.73 361.15 429.26 632.25 667.63 739.08 781.12 822.69 851.24 858.41 904.03 920.92 940.25 1047.87 1119.42 1197.60 1211.13 1276.51 1321.59 1428.64 1451.75 1748.88 3153.54 3177.80 3254.49 3271.26 3774.61
MOMENT OF INERTIA : 539.72298 989.55673 1391.88512

P6
0 1

O	0.58161100	1.23665200	0.04269300
C	-1.35766000	0.12534500	0.28760100
C	0.91442100	-0.14142700	0.00068000
C	-0.32163500	-0.88858100	0.38344600
H	-0.27911100	-1.62624600	1.17737900

C	2.17347900	-0.53183600	-0.14551700
H	2.98287700	0.18126000	-0.23611100
H	2.40887600	-1.58720300	-0.17424100
C	-0.78198300	1.31025600	-0.04981300
H	-1.18077800	2.26897300	-0.34299600
O	-1.54306100	-1.04656800	-0.45299400

Freq: 156.58 277.23 350.11 450.50 551.30 648.48 674.37 724.70 735.48 821.40 837.43 889.88 924.02 950.30 953.84 1106.39 1163.65 1198.83 1286.32 1353.28 1424.94 1574.32 1737.96 3173.20 3178.52 3262.54 3271.29

MOMENT OF INERTIA : 335.03727 590.51313 869.32753

TS18

0 2

O	-1.80341400	-0.51635600	-0.05577800
C	0.37183900	-1.40680100	-0.00602400
H	2.25945400	-0.86213200	-0.25953300
C	-0.98679300	0.58647600	0.02203600
C	0.37010600	0.03776100	0.12278400
H	0.47629600	-0.65975400	1.17653800
C	-1.44204800	1.84605000	-0.01545600
H	-2.49669100	2.06072300	-0.12385900
H	-0.74187900	2.66697100	0.05488100
C	-1.01620400	-1.64173200	-0.05030800
H	-1.57825400	-2.56288500	-0.07062600
O	2.64299600	0.03215900	-0.06421400
O	1.44787700	0.83751700	-0.03195800

Freq: 929.78i 117.44 187.48 211.50 329.56 385.23 462.29 515.97 562.43 642.70 675.32 690.45 740.72 816.11 846.70 863.41 914.79 941.72 1074.72 1091.77 1144.17 1208.15 1265.38 1368.45 1387.22 1425.69 1562.49 1639.32 2014.64 3183.87 3263.66 3283.41 3318.03

MOMENT OF INERTIA : 491.01963 951.15532 1429.09379

TS19

0 2

O	-1.87074700	-0.47889700	-0.12897600
C	0.23361900	-1.52484500	-0.03584000
H	2.64048000	-0.75193400	-0.31140500
C	-0.97638000	0.58486000	0.09705100
C	0.39558800	-0.02248500	0.40136200
H	0.67772400	0.04032600	1.45832200
C	-1.34616000	1.85161500	0.03098100
H	-2.35970100	2.13370500	-0.22404700
H	-0.62160700	2.63132300	0.22496700

C	-1.09515300	-1.59417200	-0.18943400
H	-0.68655500	-2.21098000	0.80730900
O	2.64636000	0.15410200	0.04629300
O	1.35945900	0.62326100	-0.38980100

Freq: 1311.98i 79.33 120.43 191.86 289.12 320.15 389.51 464.19 532.34 573.10 651.28 715.64 745.02 824.43 852.20 892.60 903.52 921.37 952.02 1049.14 1092.04 1196.13 1221.85 1319.40 1415.63 1434.04 1533.51 1748.14 2221.52 3043.58 3178.22 3271.43 3665.12
MOMENT OF INERTIA : 495.55234 964.88298 1401.96906

TS20
0 2

O	1.56333000	-0.97305000	0.64890800
C	-0.30457500	-1.41717600	-0.68728900
H	-0.96517500	-2.10267200	-1.18705600
C	0.78257900	0.73931300	-0.21532700
C	-0.41186500	0.11027500	-0.82516700
H	-0.49006200	0.40284500	-1.88135800
C	1.48229800	1.82137000	-0.04920300
H	2.38715700	1.83302000	0.55091800
H	1.17330300	2.76566500	-0.50053800
C	0.72560200	-1.66232700	0.11649400
H	-1.76276300	-0.61351100	1.11900700
O	-1.67775500	0.35616500	1.12025500
O	-1.63391100	0.63762600	-0.28641500

Freq: 465.00i 81.62 127.19 180.27 227.03 294.15 365.99 374.72 479.02 512.71 560.13 628.27 675.85 731.70 833.34 909.51 916.35 944.83 958.85 997.12 1127.03 1138.09 1304.15 1349.29 1398.60 1428.99 1790.10 1818.52 3027.33 3094.65 3193.12 3295.25 3661.86
MOMENT OF INERTIA : 679.5607 834.20749 1160.4162

I2
0 2

O	2.62278600	0.40864800	0.60943200
C	0.92160600	-0.78457000	-0.73776300
H	1.22664700	-1.71776700	-1.19592600
C	-0.61161600	1.16870200	-0.65149000
C	-0.49065900	-0.27686400	-0.91391700
H	-0.81392900	-0.49423300	-1.94099900
C	-1.13239800	2.01340700	0.19728400
H	-1.02611200	3.08973500	0.08162200
H	-1.69902300	1.66795300	1.06487600
C	1.81755400	-0.14691600	-0.01397400
H	-0.48553300	-1.57054200	1.37126600

O -1.20411800 -0.93351200 1.23265300
O -1.44728800 -1.07734800 -0.17479500
Freq: 49.11 70.93 136.95 171.09 205.55 246.95 315.22 335.55 416.37 521.98 543.17 575.77 647.10 767.01 813.90 905.90 917.44 942.42 999.03 1024.84 1141.37 1273.42 1317.02 1398.04 1408.76 1412.45 1768.38 2232.44 3026.40 3076.93 3166.43 3201.64 3712.02
MOMENT OF INERTIA : 669.93901 1096.45931 1330.97302

TS21
0 2
O 2.95908800 0.28972400 0.55239100
C 1.01306800 -0.86590500 -0.46369600
H 1.15671300 -1.86379000 -0.85956000
C -0.43382300 1.20983100 -0.41286200
C -0.29782700 -0.20023200 -0.57169900
H -0.33428600 0.58890900 -1.60984100
C -1.22323200 2.10530600 0.16139000
H -1.34684500 3.10952700 -0.23162300
H -1.74248200 1.86891700 1.09062800
C 2.04769900 -0.24986600 0.07783800
H -1.48578800 -1.78279500 1.25770900
O -1.92196700 -0.99635400 0.89563600
O -1.39744800 -1.03281700 -0.49717100
Freq: 1846.03i 58.75 90.94 100.02 187.91 223.12 233.12 311.69 380.26 444.03 550.97 554.35 601.07 658.20 704.37 741.19 802.93 870.24 999.25 1033.90 1107.48 1118.75 1232.24 1321.42 1391.36 1437.11 1678.04 2094.52 2222.24 3096.53 3195.41 3200.38 3738.43
MOMENT OF INERTIA : 614.31619 1284.90077 1636.7609

P7
0 1
O -1.41730000 -2.40972500 0.00000000
C -1.27134000 0.06489200 0.00000000
H -2.19779200 0.62595400 0.00000000
C 0.00000000 0.81995200 0.00000000
C 2.45201300 0.62092600 0.00000000
H 3.37765800 0.05673300 0.00000000
H 2.51423500 1.70416000 0.00000000
C -1.35427900 -1.25327400 0.00000000
O -0.00827900 2.03590000 0.00000000
C 1.26202600 0.02475200 0.00000000
H 1.18000600 -1.05973100 0.00000000
Freq: 94.14 121.75 128.64 279.66 415.30 474.47 529.82 580.06 628.39 692.58 789.64 821.50 1002.60 1022.03 1074.96 1103.44 1189.55 1334.97

1370.69 1433.64 1679.94 1755.72 2222.23 3151.25 3164.00 3211.20 3251.02
MOMENT OF INERTIA : 348.96156 1022.00192 1370.96349

TS22
0 2

O	-2.55736600	0.48826400	-0.71948500
C	-0.95686900	-0.28188800	1.01141500
H	-1.35167500	-0.97334600	1.74604500
C	0.93262500	1.18587000	0.36424900
C	0.46552100	0.08956200	1.03798400
H	0.96290700	-0.15370400	1.97408900
C	1.51399500	1.91792800	-0.53677200
H	2.03981800	1.46149600	-1.37773200
H	1.51011000	3.00571800	-0.49970900
C	-1.79724100	0.12278300	0.07603500
H	-0.08864600	-2.05365700	-0.81075200
O	0.72306300	-1.57652400	-1.04965700
O	1.33171600	-1.34824400	0.17546500

Freq: 561.27i 45.13 79.50 93.80 133.71 220.16 243.42 283.97 406.24 441.43 449.54 525.53 542.87 596.03 773.90 863.52 901.49 938.29 966.20 1049.72 1072.75 1161.86 1339.23 1409.92 1415.69 1439.28 1898.21 2224.43 3080.44 3144.69 3155.52 3203.69 3671.39
MOMENT OF INERTIA : 774.81149 1099.93776 1401.50562

TS23
0 2

O	0.29524400	-0.84705500	0.10765000
C	-0.10059800	1.42103500	-0.01379000
H	-0.66722800	2.33952700	-0.03377500
C	1.49623000	-0.18943300	-0.00911600
C	1.23144200	1.23747300	-0.05533400
H	2.00567800	1.98924700	-0.10791600
C	2.66016600	-0.85304400	-0.06760000
H	2.69426300	-1.93323000	-0.02450500
H	3.58846800	-0.30454100	-0.15109300
C	-0.73417800	0.09029300	-0.01034500
H	-1.40682600	-0.11192400	-1.07575500
O	-1.85384300	-0.18944600	0.70877900
O	-2.63299300	-0.49062700	-0.52516000

Freq: -1561.39 104.03 142.80 256.36 311.87 441.45 462.35 559.29 657.76 696.43 711.47 804.75 849.82 852.99 882.89 916.06 923.25 941.59 956.80 1070.74 1083.71 1143.81 1242.01 1316.17 1380.40 1434.34 1584.21 1658.39 1991.53 3184.08 3240.72 3266.03 3281.26

MOMENT OF INERTIA : 339.15906 1229.31493 1469.10824

P8
0 1

O	0.00000000	0.94076400	0.00000000
C	-0.75147500	-1.23944700	0.00000000
H	-1.46217700	-2.05137100	0.00000000
C	1.08188400	0.09344200	0.00000000
C	0.58855200	-1.27770400	0.00000000
H	1.23742700	-2.14227500	0.00000000
C	2.33854700	0.53945300	0.00000000
H	2.56189300	1.59810200	0.00000000
H	3.16005200	-0.16466600	0.00000000
C	-1.16977700	0.17859500	0.00000000
O	-2.25294700	0.68350900	0.00000000

Freq: 169.27 283.66 322.05 518.04 610.56 648.70 728.16 735.15 762.42 847.65 882.04 891.89 918.12 960.73 994.07 1083.51 1114.93 1307.19 1352.88 1436.89 1619.11 1721.53 1882.38 3181.28 3236.79 3267.69 3276.34
MOMENT OF INERTIA : 267.36492 744.32859 1011.6935

TS24
0 2

O	-0.59854900	-0.99841000	0.33413300
C	0.47583200	1.06636500	0.41268700
H	1.83582700	1.09716700	0.00366700
C	-1.48053700	0.01360700	-0.03193600
C	-0.78059200	1.30184200	0.04391200
H	-1.25047100	2.23815700	-0.22238700
C	-2.74014400	-0.24962800	-0.37448400
H	-3.11490200	-1.26429900	-0.39990700
H	-3.41159000	0.55921200	-0.62750400
C	0.64810800	-0.43959100	0.58458300
H	1.06289700	-0.79664200	1.53124100
O	1.56555800	-0.73677100	-0.49167300
O	2.55077000	0.23653500	-0.35417100

Freq: 2032.49i 105.38 240.06 245.13 336.33 420.58 537.69 608.07 655.08 709.35 734.99 794.95 854.42 874.30 883.99 908.20 935.66 948.01 958.62 1026.92 1140.78 1201.52 1215.87 1275.22 1362.00 1426.20 1623.31 1714.58 1810.23 3080.28 3183.00 3239.61 3277.27
MOMENT OF INERTIA : 320.56928 1165.37755 1354.87043

HP6
0 2

O	-0.51150500	-0.88177900	0.38579400
C	0.21168500	1.27727600	0.26340100
H	2.86689400	0.67950800	-0.83589300
C	-1.55007000	-0.06375800	-0.03270200
C	-1.06641600	1.32219100	-0.08226800
H	-1.68319000	2.16311700	-0.36279100
C	-2.76146000	-0.54830600	-0.29748000
H	-2.97248500	-1.60631400	-0.21319500
H	-3.55722100	0.11795800	-0.60075000
C	0.67384400	-0.12813300	0.53644300
H	1.11566400	-0.29292200	1.52435200
O	1.56955700	-0.62935700	-0.45358800
O	2.84005300	-0.01598500	-0.16171800

Freq: 70.50 112.56 221.00 270.88 302.01 344.88 442.87 550.20 608.63 692.73 703.95 808.30 841.75 872.26 889.07 922.78 956.11 964.17 1053.99 1086.13 1197.85 1231.11 1335.87 1349.80 1398.01 1426.05 1633.87 1720.68 3062.72 3180.93 3250.53 3274.48 3738.74

MOMENT OF INERTIA : 307.59155 1291.18522 1491.24649

TS25

0 2

O	-0.46141100	-0.59054300	-0.98895800
C	0.68217600	-1.00095400	0.97764500
H	1.50687200	-1.29114700	1.61357500
C	-1.21462400	-0.04928500	0.06208300
C	-0.30539900	-0.07096400	1.23641400
C	-2.46459000	0.35898700	-0.08842200
H	-2.96760800	0.28932000	-1.04370200
H	-2.99792500	0.77541300	0.75467500
C	0.78645500	-0.88213700	-0.47605900
H	1.35582600	-1.55070500	-1.11565500
O	1.68332700	0.42315900	-0.44829200
O	1.01050300	1.49485300	-0.01075400
H	0.33937600	1.02348900	1.10517500

Freq: 2247.89i 143.64 240.58 318.88 359.46 409.43 435.18 502.62 608.94 694.95 710.14 743.18 763.70 840.58 864.68 872.54 902.89 1017.05 1045.04 1121.19 1152.94 1217.81 1245.39 1279.65 1348.95 1402.95 1427.36 1724.28 1755.23 3174.38 3184.40 3235.80 3278.50

MOMENT OF INERTIA : 467.46783 894.67267 946.42134

HP7

0 2

O	-0.57177400	-0.82819600	0.40303000
C	0.21775600	1.36527400	0.12131200

H	0.92158700	2.18232600	0.10365600
C	-1.62129600	-0.02851800	-0.03468800
C	-1.06983800	1.30578200	-0.16549900
C	-2.84769900	-0.50011200	-0.24153100
H	-3.07904600	-1.54699500	-0.09918500
H	-3.63204400	0.17226400	-0.55907300
C	0.61010900	-0.06094500	0.48652500
H	1.05311000	-0.15189300	1.48716000
O	1.49964900	-0.65891700	-0.45374400
O	2.78821800	-0.05434700	-0.20884900
H	3.27346800	-0.81290700	0.14722800

Freq: 72.32 109.67 231.26 264.18 287.62 344.48 447.45 489.96 658.50 694.57 719.63 776.30 822.25 852.79 896.49 918.42 943.35 962.55 1046.29 1109.28 1172.03 1241.10 1331.84 1348.60 1392.13 1423.61 1644.03 1733.84 3018.08 3187.10 3268.42 3282.82 3749.37

MOMENT OF INERTIA : 303.20308 1292.88142 1502.04253

TS26

0 2

O	-0.43544300	-0.82047700	0.63345200
C	0.09192800	1.40052500	0.30604200
H	2.90252300	-0.72130200	-1.33617600
C	-1.47035300	-0.19153400	-0.03095000
C	-1.14366100	1.19167400	-0.27201400
H	-1.74667400	1.86986100	-0.85635700
C	-2.58010600	-0.86494700	-0.40180400
H	-2.67784900	-1.92661200	-0.21756200
H	-3.39106400	-0.34209000	-0.89001500
C	0.60816000	0.12323500	0.78277300
H	1.17984400	-0.06468600	1.68717400
O	1.34971600	0.43072000	-0.35325400
O	2.92290400	-0.70635400	-0.36661700

Freq: 711.51i 65.50 115.94 137.41 175.54 250.34 358.30 368.98 478.42 572.13 671.91 702.53 749.92 788.66 795.68 835.88 884.96 920.16 937.61 1012.80 1080.29 1158.92 1262.10 1281.49 1350.41 1376.49 1416.79 1582.63 3170.93 3181.56 3256.39 3281.05 3763.87

MOMENT OF INERTIA : 385.1846 1266.5116 1451.19388

I3

0 1

O	0.67453200	1.14173100	-0.00015300
C	-1.23816000	-0.21440200	0.00036300
C	1.08468900	-0.24027200	0.00027500
C	-0.06863800	-1.03953000	-0.00040300

H	-0.05379300	-2.11817000	-0.00105100
C	2.41691200	-0.41378200	0.00047100
H	3.08106300	0.43979700	0.00076100
H	2.84143900	-1.40863500	0.00008400
C	-0.62112700	1.12643900	0.00011700
H	-1.11624800	2.09309000	-0.00017000
O	-2.44884700	-0.43133200	-0.00041800

Freq: 164.22 301.69 313.64 467.04 576.00 606.05 625.07 707.57 717.80 787.68 818.19 877.85 932.41 933.72 975.75 1141.26 1190.89 1267.41 1301.36 1442.86 1455.43 1685.72 1730.10 3186.01 3200.86 3260.16 3285.71

MOMENT OF INERTIA : 236.74342 819.10696 1055.85033

TS27

0 1

O	0.53752500	1.32746200	-0.13628100
C	-1.20518000	-0.25016700	0.02433800
C	1.16071300	-0.44420000	-0.05458000
C	-0.03905800	-1.07797800	-0.11543500
H	-0.11698100	-2.10616300	-0.44243300
C	2.46456800	-0.36023500	0.12618300
H	3.03485300	0.48716600	-0.22939800
H	2.98692300	-1.16357400	0.63383200
C	-0.66624000	1.16466400	0.06222700
H	-1.31093800	2.01494900	0.31255900
O	-2.39786000	-0.50557200	0.06991100

Freq: 509.73i 159.69 265.37 316.86 440.93 507.62 537.82 588.91 655.03 668.60 750.45 777.81 881.97 958.26 983.07 1081.70 1177.79 1268.44 1302.88 1425.43 1648.72 1743.59 1834.54 3084.96 3165.75 3224.12 3258.21

MOMENT OF INERTIA : 281.2915 821.03184 1091.18848

P9

0 1

O	-0.19053900	1.86202800	0.00008000
C	-1.02116300	-0.43295100	-0.00002700
C	1.46811800	-0.53636800	0.00002500
C	0.28646400	-1.11042100	0.00007500
H	0.21651000	-2.19643400	0.00015900
C	2.66690800	-0.04414900	-0.00005700
H	3.18216600	0.18608000	-0.92793200
H	3.18223500	0.18629800	0.92772000
C	-1.11812300	1.10007100	-0.00005600
H	-2.18041200	1.42550100	-0.00020600

O -2.07117700 -1.04434500 -0.00001700
Freq: 35.14 124.09 143.08 245.16 346.99 424.13 460.47 489.59 621.74 640.92 839.06 863.16 914.37 990.29 1028.22 1106.65 1275.45 1330.95 1373.39 1456.33 1753.45 1835.01 2044.82 2919.17 3139.81 3147.30 3215.21
MOMENT OF INERTIA : 416.4243 841.85886 1245.89017

TS28
0 2
O -0.51417700 -0.84857600 0.38494900
C 0.19218300 1.37728100 0.04869400
H -0.75157100 1.97890500 0.76172200
C -1.58804600 -0.07724800 -0.04448700
C -1.10025800 1.30251300 -0.24782100
C -2.80710000 -0.57681800 -0.21711000
H -3.02221000 -1.62300800 -0.04136900
H -3.60365200 0.07446800 -0.54745600
C 0.64568800 -0.03502800 0.48244500
H 1.07101200 -0.07425200 1.49034000
O 1.54787700 -0.59727500 -0.44547800
O 2.83089700 0.00576600 -0.17435000
H 3.33483400 -0.77963900 0.08547000
Freq: 1171.73i 65.61 102.74 197.41 225.19 294.46 346.78 384.50 479.73 528.43 642.07 733.88 742.53 771.67 868.79 889.55 902.45 912.64 964.42 1054.04 1080.08 1184.84 1309.38 1339.58 1401.65 1418.76 1621.23 1726.10 2246.71 3058.70 3183.10 3281.57 3748.50
MOMENT OF INERTIA : 303.18603 1299.63335 1508.38207

TS29
0 2
O -0.52847000 -0.92973600 0.06891700
C 0.39617600 1.26936300 -0.00411500
H 2.37589400 0.92684900 -0.29123000
C -1.56899300 -0.02442800 -0.02997200
C -1.04314200 1.28388300 -0.03777600
H -1.66083700 2.17038800 -0.08908600
C -2.86003400 -0.49077800 -0.06802600
H -3.07785900 -1.54959400 -0.03371200
H -3.67741300 0.21319400 -0.14430900
C 0.59750300 -0.14193700 0.15654600
H 0.67665900 0.45464800 1.23704500
O 1.72627500 -0.84595900 -0.10092200
O 2.83150700 0.07668100 -0.06532700
Freq: 852.92i 101.54 188.04 241.23 340.08 363.90 481.17 517.28

544.56 645.78 696.90 721.79 780.67 782.41 815.96 937.37 951.48
970.63 1021.12 1104.57 1160.33 1209.90 1288.03 1328.00 1383.14
1413.25 1505.28 1558.99 2055.15 3182.84 3226.39 3287.44 3359.55
MOMENT OF INERTIA : 279.17306 1291.00393 1553.49123

TS30
0 2

O	0.80143200	-1.10105800	0.00000400
C	2.57058800	0.26654600	-0.00001700
H	3.59458400	0.60468900	-0.00002500
C	0.33762200	0.18666300	-0.00000300
C	1.39472100	1.06114700	-0.00001600
H	1.31513600	2.13653300	-0.00002400
C	2.14486600	-1.03296100	-0.00000400
H	2.66362400	-1.97820300	0.00000000
C	-1.09778300	0.37386500	0.00000300
H	-1.69148600	-0.58403400	0.00001400
O	-1.65454000	1.45029600	-0.00000200
O	-3.44687200	-1.00792600	0.00002800
H	-3.58209800	-0.04103300	0.00002100

Freq: -107.32 15.63 141.05 161.38 182.17 251.68 300.76 490.48 575.51
610.56 649.20 778.27 789.78 847.95 897.88 900.87 967.08 1004.54
1039.63 1119.14 1188.11 1231.79 1268.83 1378.10 1435.20 1491.43
1605.84 1782.07 2637.92 3259.01 3273.28 3284.43 3680.79
MOMENT OF INERTIA : 384.97593 1626.4581 2011.43403

P30
0 2

O	0.60998600	-1.11772300	0.00003700
C	1.73162600	0.81787600	-0.00011600
H	2.55321000	1.51669200	-0.00023900
C	-0.31012200	-0.10095500	-0.00003200
C	0.34349800	1.10840500	0.00010600
H	-0.13507700	2.07512200	0.00013500
C	1.82484900	-0.54686100	0.00013800
H	2.66305500	-1.22531900	0.00019300
C	-1.70023700	-0.48044500	-0.00003300
O	-2.66234500	0.22339600	-0.00009600

Freq: 168.07 197.48 258.12 494.57 613.69 648.70 704.21 789.08 848.73
894.53 900.35 957.42 1039.18 1113.71 1197.72 1227.70 1260.80 1420.74
1469.42 1583.07 1883.86 3255.19 3268.75 3281.54
MOMENT OF INERTIA : 207.63587 878.47424 1086.1101

H_2O

0 1

H	0.75662200	-0.47546400	0.00000000
O	0.00000000	0.11886600	0.00000000
H	-0.75662200	-0.47546400	0.00000000

Freq: 1671.71 3803.51 3907.34
MOMENT OF INERTIA : 2.25799 4.1207 6.37869

TS31
0 2

O	-1.41995300	-1.05214800	-0.02239400
C	-1.61478400	1.18910700	0.01689600
H	-2.05941900	2.17089800	0.02784900
C	-0.15033100	-0.52204600	0.01208600
C	-0.24419800	0.84162500	0.04258300
H	0.87293800	1.61274300	0.13445800
C	-2.27516500	-0.01091500	-0.01939400
H	-3.32315200	-0.26628800	-0.04312100
C	0.97209300	-1.43324400	0.00340700
H	0.69663100	-2.50562200	-0.01587200
O	2.13744700	-1.07604400	0.01481600
O	1.95321900	1.83700700	-0.04263600
H	2.32161000	0.93058700	-0.03506600

Freq: -1310.66 97.45 154.98 164.19 251.17 262.57 345.95 462.62 506.51 568.09 616.01 649.84 775.75 778.84 847.47 857.51 916.74 1025.92 1052.22 1103.42 1186.88 1195.68 1244.67 1386.53 1434.16 1483.57 1553.29 1645.35 1750.06 2949.65 3260.54 3280.61 3604.60
MOMENT OF INERTIA : 565.20734 1050.86254 1615.39894

P31
0 2

O	0.62545700	-1.06660500	-0.00016800
C	1.79734800	0.85861600	-0.00013900
H	2.62815500	1.54463900	-0.00021700
C	-0.29410700	-0.03352800	0.00000500
C	0.41443200	1.13027900	-0.00001500
C	1.85397300	-0.51069600	0.00017900
H	2.68017800	-1.20466600	0.00029900
C	-1.70263300	-0.38870100	0.00005000
H	-1.88196100	-1.48497400	0.00002400
O	-2.60551300	0.41775200	0.00009500

Freq: 160.18 196.76 247.71 488.23 596.02 631.52 761.52 763.86 861.17 878.95 961.01 1029.58 1086.30 1136.67 1186.94 1229.29 1377.65 1430.59 1479.86 1573.18 1787.59 2909.04 3260.63 3283.31
MOMENT OF INERTIA : 200.45232 894.38964 1094.84195

TS32
0 2

O	-0.42492100	1.40204400	0.02664100
C	1.27034800	-0.02175100	-0.08868900
H	2.51165800	-0.46394000	-0.22018300
C	-0.93370400	0.12845800	-0.00311300
C	0.08308000	-0.79079000	-0.06911300
H	-0.03650000	-1.86120500	-0.10843700
C	0.92130200	1.29328800	-0.01997800
H	1.47986500	2.21409800	-0.00153600
C	-2.38295500	-0.00439200	0.03675400
H	-2.91702000	0.96851200	0.08741700
O	-2.96556100	-1.06539200	0.01877000
O	3.59345000	-0.78322500	-0.02401300
H	3.58982200	-0.91376400	0.93638900

Freq: -1376.71 67.82 93.29 152.25 169.76 203.48 267.06 374.71 503.50 567.89 646.95 711.40 760.21 803.32 830.99 863.07 939.66 967.38 1029.44 1098.67 1159.22 1210.19 1242.18 1356.73 1428.61 1430.97 1500.15 1582.12 1786.75 2908.27 3278.31 3289.04 3772.51
MOMENT OF INERTIA : 352.529 1747.89334 2092.34458

P32
0 2

O	1.19582100	-0.45093900	0.00000000
C	-0.43999900	-1.92684000	0.00000000
C	0.00000000	0.22183000	0.00000000
C	-1.05463900	-0.66010300	0.00000000
H	-2.09928600	-0.39647500	0.00000000
C	0.90925500	-1.77869200	0.00000000
H	1.74800200	-2.45312700	0.00000000
C	0.06780900	1.67516500	0.00000000
H	1.10645100	2.06918700	0.00000000
O	-0.90203700	2.39997100	0.00000000

Freq: 161.17 201.56 262.98 495.69 552.73 643.79 746.19 791.71 854.28 879.03 957.98 1027.11 1084.23 1130.65 1208.19 1230.51 1358.57 1428.40 1477.71 1562.08 1785.80 2908.99 3282.65 3299.64
MOMENT OF INERTIA : 210.20434 854.7106 1064.91494

TS33
0 2

O	-0.30019300	-0.74221400	-0.08223700
C	-0.80441500	1.44675200	-0.01022500
H	-1.38964200	2.35106600	0.00631400

C	0.88398600	-0.03591500	-0.00983800
C	0.61130700	1.30750800	0.03286400
H	1.35191200	2.09030900	0.08633700
C	-1.27369400	0.16534600	-0.10479200
H	-2.51488500	-0.29924300	-0.22876500
C	2.11966900	-0.80098300	-0.00330600
H	1.97430800	-1.89985300	-0.06035200
O	3.21695400	-0.29133500	0.06271900
O	-3.55720100	-0.70068800	-0.00334800
H	-3.51929200	-0.86463500	0.95118600

Freq: -1385.35 71.83 79.03 114.28 179.76 206.23 257.85 369.24 501.91 539.16 639.21 736.58 755.38 811.69 859.25 890.18 926.82 978.25 1029.18 1032.61 1142.00 1193.47 1248.76 1350.53 1412.52 1430.53 1486.65 1597.94 1781.29 2919.84 3263.74 3282.90 3773.23

MOMENT OF INERTIA : 312.14224 1757.27920 2060.34123

P33

0 2

O	0.65726400	-1.17308400	0.00025800
C	1.86946800	0.72848400	-0.00018100
H	2.72477300	1.38159700	-0.00038800
C	-0.23266800	-0.09983300	0.00012000
C	0.48353400	1.06975300	0.00014800
H	0.05147800	2.05899300	0.00018500
C	1.85723600	-0.63747900	0.00001200
C	-1.64974700	-0.40827600	0.00017300
H	-1.87816100	-1.49465800	-0.00030600
O	-2.51539200	0.44035600	-0.00039900

Freq: 166.45 199.30 257.53 491.74 525.39 631.30 754.28 799.52 874.25 893.95 939.14 1025.00 1028.10 1127.38 1171.67 1256.98 1355.92 1413.63 1432.31 1601.42 1779.01 2917.05 3260.02 3293.77

MOMENT OF INERTIA : 215.59101 852.90535 1068.49633

TS34

0 2

O	-0.78474500	-1.09647000	-0.00004700
C	-2.09070700	0.72235600	0.00002200
H	-2.96258300	1.35879600	0.00004400
C	-0.01900700	-0.01193700	-0.00000200
C	-0.71230600	1.15339800	0.00004300
H	-0.32502100	2.15761500	0.00008400
C	-2.08433100	-0.63500500	-0.00003200
H	-2.84554000	-1.39625800	-0.00006500
C	2.61530200	-0.57982200	-0.00001400

O 3.26967500 0.34470900 0.00002700
Freq: -60.64 15.59 28.11 32.21 131.03 487.74 609.78 714.09 778.13 850.13 862.09 874.94 1009.21 1034.81 1103.62 1176.86 1237.22 1359.21 1461.71 1575.81 2183.34 3249.86 3288.28 3294.76
MOMENT OF INERTIA : 216.76119 1393.89803 1610.65922

P34
0 2
O -1.00794200 -0.63292800 -0.00004300
C 0.50147800 1.02013700 0.00002500
H 0.94400600 2.00467500 0.00004700
C 0.21129300 -1.15780500 0.00000200
C 1.20832000 -0.23989400 0.00004700
H 2.27060000 -0.41111400 0.00008800
C -0.82503100 0.73548600 -0.00002900
H -1.72743500 1.32231800 -0.00006100
Freq: 480.87 609.63 712.44 782.47 856.35 866.45 873.83 1008.45 1034.61 1104.58 1176.23 1239.06 1361.12 1462.08 1577.69 3250.76 3291.65 3296.37
MOMENT OF INERTIA : 170.66701 195.66362 366.33062

CO
0 1
C 0.00000000 0.00000000 -0.64623600
O 0.00000000 0.00000000 0.48467700
Freq: 2205.05
MOMENT OF INERTIA : 0
31.31409
31.31409

TS35
0 2
O -1.20864600 -0.75747300 0.00000700
C 1.14851200 0.25545000 0.00000300
H 2.16577500 0.64094100 -0.00000500
C -1.05935100 0.43220800 -0.00001000
C 0.02830200 1.21521100 -0.00001800
H 0.11086300 2.28517600 -0.00001800
C 0.91127700 -1.03705300 0.00001200
H 1.22008400 -2.06123000 0.00004400
Freq: -493.30 337.73 451.17 501.00 587.28 620.08 639.64 782.40 810.49 974.08 1092.06 1161.15 1313.35 1599.37 1831.24 3160.20 3318.75 3386.61
MOMENT OF INERTIA : 188.31897 245.47144 433.79041

P35
0 2
O -2.06053900 -0.55056700 -0.00020300
C 1.34864700 0.36248300 0.00015200
H 2.10030300 1.15954800 0.00020300
C -1.10419700 0.10791000 -0.00013000
C -0.02622400 0.86851300 0.00001800
H -0.21073800 1.93621700 0.00002500
C 1.76311700 -0.88615600 0.00015700
H 2.70669400 -1.40773200 0.00021500
Freq: 126.87 146.51 426.34 517.07 550.40 610.89 671.90 793.83 877.03 948.95 1147.25 1267.19 1421.13 1655.35 2224.11 3046.61 3200.88 3275.61
MOMENT OF INERTIA : 114.65375 547.3286 661.98235

TS36
0 2
O 2.03696600 -0.64836500 0.15932800
C 0.28908000 1.04153800 -0.22444500
H -0.07534900 1.61758800 -1.05180000
C -1.60113200 0.12566000 0.56476700
H -1.56969000 0.66434200 1.48223500
C 1.21474300 0.14451300 -0.11383100
C -1.98239500 -0.62192000 -0.31644000
H -2.17247000 -1.23376300 -1.16536800
Freq: -358.78 75.67 117.96 217.47 438.62 573.79 586.03 604.86 633.72 707.26 799.03 801.43 1260.28 1955.26 2150.31 3352.44 3435.79 3520.48
MOMENT OF INERTIA : 143.88793 646.02079 712.36267

C_2H_2
0 1
C 0.00000000 0.00000000 0.59945800
H 0.00000000 0.00000000 1.66160100
C 0.00000000 0.00000000 -0.59945800
H 0.00000000 0.00000000 -1.66160100
Freq: 550.30 550.30 795.66 795.66 2078.97 3455.38 3557.59
MOMENT OF INERTIA : 50.67144

P36
0 2
C 1.07070100 -0.67492500 0.00000000
H 2.12585100 -0.47977100 0.00000000

C 0.00000000 0.04592700 0.00000000
O -1.06875700 0.53172000 0.00000000
Freq: 491.85 516.76 575.47 1266.98 2109.21 3353.56
MOMENT OF INERTIA : 1.65057 165.16751 166.81807

TS37
0 2
O -0.83944700 1.20847200 -0.06278800
C -1.75428900 -0.90634500 0.03216600
H -2.59910800 -1.57384800 -0.06641300
C 0.41387700 -0.20545400 -0.10267500
C -0.40491300 -1.21712200 -0.05874200
C -1.87920100 0.51834900 0.10038900
H -2.82658500 1.04092400 0.24202000
C 1.71975200 0.39268800 -0.03405400
H 1.71974800 1.49570000 -0.09945100
O 2.73127100 -0.26540600 0.10045600
Freq: -1485.33 123.44 178.19 212.54 289.35 475.82 522.25 687.41 759.36 809.93 889.28 960.63 996.99 1001.17 1205.88 1244.96 1334.05 1402.86 1473.52 1637.39 1728.65 2970.95 3133.15 3232.80
MOMENT OF INERTIA : 228.83532 956.28988 1180.76359

P37
0 2
O -2.54002800 1.09866200 -0.00045100
C -2.56991300 -0.11624900 -0.00044900
H -3.52962700 -0.67116700 -0.00103900
C 2.36269500 0.51688400 0.00060200
H 2.40410500 1.62242500 0.00220700
O 3.36901200 -0.16165500 -0.00135100
C 1.03469700 -0.02888000 0.00091200
C -0.10903600 -0.46875800 0.00087200
C -1.38158900 -0.96968500 0.00026300
H -1.52746600 -2.04719300 0.00005100
Freq: 45.76 80.83 147.43 169.52 255.73 385.56 467.00 551.34 679.84 762.81 859.25 982.43 1001.40 1008.76 1221.19 1399.22 1417.72 1429.75 1687.47 1706.48 2133.54 2931.31 2951.86 3163.03
MOMENT OF INERTIA : 157.64491 1741.72964 1899.37409

TS38
0 2
O -0.57811700 -1.19895300 -0.09060700
C -1.76784600 0.96737100 0.02195800
C 0.20910800 -0.20903200 0.01078100

C	-0.37552400	1.09810900	0.01035900
H	0.21740500	1.99639500	-0.08884000
C	-2.17549500	-0.26039400	0.02098600
H	-2.94473600	-1.00427500	0.07798100
C	1.67922800	-0.46220800	0.08007000
H	1.95158300	-1.52192800	0.25153000
O	2.49798200	0.41479400	-0.04759200

Freq: -1359.03 113.45 194.99 223.01 393.54 448.99 511.40 609.71 638.29 710.31 834.14 929.35 989.13 1026.10 1131.55 1219.42 1296.53 1388.19 1465.77 1601.74 1790.76 2949.34 3241.84 3381.14
MOMENT OF INERTIA : 225.13715 887.24301 1110.03178

P38
0 2

O	0.15708300	1.67781500	-0.00013100
C	-1.85701800	-0.42821900	-0.00000400
C	0.44650200	0.48740000	-0.00006000
C	-0.49480300	-0.61273000	-0.00009700
H	-0.08146400	-1.61672500	0.00013800
C	-3.06381700	-0.27059300	0.00009000
H	-4.11675500	-0.12602300	0.00013500
C	1.92621000	0.09755200	0.00002300
H	2.59585000	0.98266000	0.00007300
O	2.32540800	-1.03786200	0.00012300

Freq: 103.76 126.29 140.50 238.18 395.00 408.91 522.10 531.61 570.56 603.71 657.76 762.06 891.50 1022.44 1094.02 1166.63 1363.78 1424.83 1637.03 1819.40 2082.83 2932.63 3184.26 3489.18
MOMENT OF INERTIA : 272.75827 1123.67674 1396.43501

TS39
0 2

O	-0.50378200	1.65399200	-0.07838800
C	2.09932300	-0.34084600	0.01159900
C	-0.08473200	0.57702100	-0.25465000
C	0.75899000	-0.45781200	-0.41468400
H	0.40346500	-1.37834600	-0.85435100
C	3.24713700	-0.25560200	0.37277000
H	4.25641600	-0.17992500	0.69248500
C	-1.97956000	-0.72787100	-0.14559700
H	-1.85495700	-1.75170700	-0.57996700
O	-2.87770200	-0.33641200	0.49403900

Freq: -282.20 37.28 84.48 127.31 168.83 238.00 386.50 397.15 462.25 495.35 549.13 608.73 621.03 682.69 986.11 1079.00 1156.05 1371.50 1941.59 2107.30 2209.82 2751.96 3214.80 3505.66

MOMENT OF INERTIA : 270.74266 1435.6113 1633.46095

P39
0 1

O	-2.18170600	-0.43154700	0.00000000
C	1.23575600	0.06685600	0.00000000
C	-1.15883000	0.11274000	0.00000000
C	0.00000000	0.75155300	0.00000000
H	-0.05001600	1.83628500	0.00000000
C	2.30079500	-0.49589500	0.00000000
H	3.23733800	-0.99543500	0.00000000

Freq: 133.51 366.29 392.42 481.17 524.84 596.18 661.51 684.62 978.53 1144.39 1401.02 2222.99 2241.91 3166.59 3506.20
MOMENT OF INERTIA : 61.63765 659.04526 720.68291

HCO
0 2

C	0.06232000	0.58516700	0.00000000
H	-0.87248000	1.21718900	0.00000000
O	0.06232000	-0.59102400	0.00000000

Freq: 1116.16 1947.24 2637.94
MOMENT OF INERTIA : 2.55396 40.26102 42.81497

TS40
0 2

O	0.54540500	1.74877700	-0.14021100
C	-1.88014300	-0.30260000	0.06803400
C	0.50791400	0.60064200	0.18459700
C	-0.60953700	-0.29379000	0.66611900
H	-0.59213500	-0.44712000	1.74977200
C	-2.95716600	-0.35327800	-0.47762200
H	-3.90500800	-0.39040400	-0.95623600
C	1.57052300	-0.52392200	0.18509400
H	0.48463000	-1.29108900	0.57610800
O	2.48246500	-0.82798900	-0.50066100

Freq: -1714.87 68.83 137.81 253.62 281.80 369.75 449.40 507.11 554.92 609.67 617.40 642.85 775.24 866.92 931.61 1086.33 1217.79 1362.86 1636.99 1857.52 1906.39 2175.74 3077.13 3497.43
MOMENT OF INERTIA : 323.79926 1147.01837 1345.61396

P40
0 2

O	-0.13478100	2.21301100	0.00000000
C	1.18562500	-1.20064700	0.00000000

C	0.00000000	0.97485200	0.00000000
C	1.34182500	0.24632100	0.00000000
H	1.90689100	0.58312900	0.87825300
C	0.98554400	-2.38576800	0.00000000
H	0.82876500	-3.43651500	0.00000000
C	-1.16392800	0.19750900	0.00000000
H	1.90689100	0.58312900	-0.87825300
O	-2.20733700	-0.30342900	0.00000000

Freq: 64.12 102.90 194.34 218.21 331.52 356.39 419.63 472.97 638.50 674.70 688.60 733.73 928.75 978.20 1191.95 1192.54 1303.62 1456.21 1524.20 2158.29 2240.38 3027.67 3059.74 3502.76
MOMENT OF INERTIA : 463.94216 771.8652 1224.7033

TS41
0 2

O	1.59987800	-1.55076900	-0.21943600
C	-1.71894800	-0.10925400	0.00533800
C	0.68234700	-0.81283300	-0.13565800
C	-0.76301700	-1.17806500	0.22989700
H	-0.74508700	-1.47600600	1.28686700
C	-2.51175500	0.77184100	-0.18663900
H	-3.21137500	1.55323000	-0.35486100
C	1.02955800	1.14022200	0.51037100
H	-1.01317200	-2.07526900	-0.34861600
O	1.48268700	1.94159100	-0.17096900

Freq: -231.43 35.96 66.74 147.01 177.69 246.18 316.25 357.37 455.27 516.20 638.52 668.59 803.52 907.06 988.60 1175.59 1272.87 1424.28 1906.22 2061.98 2248.46 3024.99 3072.46 3504.14
MOMENT OF INERTIA : 580.92588 828.00848 1355.15142

P41
0 2

O	-2.29067800	-0.23767900	-0.09186400
C	1.31274300	0.10873300	-0.00547200
C	-1.15093400	-0.41152500	0.15574900
C	-0.03314600	0.65081700	0.01450200
H	-0.17430400	1.32153700	0.87331200
C	2.42750200	-0.33572900	-0.03136700
H	3.41306100	-0.73087200	-0.05127800
H	-0.25032300	1.23698900	-0.88759100

Freq: 40.09 175.18 324.03 421.20 497.09 634.21 659.39 759.70 858.84 986.93 1168.05 1261.32 1422.95 1931.28 2251.00 3015.58 3059.90 3505.99
MOMENT OF INERTIA : 54.51343 732.01305 772.20541

TS42
0 2
O -2.40993800 -0.14386200 -0.00020900
C 1.41163600 0.15116000 -0.00001400
C -1.34869300 -0.58952500 0.00030800
C 0.14742800 0.76100000 0.00006500
H -0.16031700 1.26866700 0.91155500
C 2.48415500 -0.40653700 -0.00007700
H 3.43314400 -0.88291800 -0.00013700
H -0.16048000 1.26855900 -0.91143100
Freq: -433.61 18.30 141.04 309.53 339.03 468.26 579.51 615.70 642.93 951.49 1029.65 1075.90 1450.35 2016.67 2158.99 3113.95 3191.54 3502.34
MOMENT OF INERTIA : 68.98876 808.72624 865.75448

P42
0 2
C 0.00000000 0.00000000 0.11459400
C 0.00000000 0.00000000 -1.24937600
H 0.00000000 0.92954100 -1.80784500
C 0.00000000 0.00000000 1.33753800
H 0.00000000 0.00000000 2.39915300
H 0.00000000 -0.92954100 -1.80784500
Freq: 356.58 359.79 428.80 592.77 679.27 1034.23 1098.14 1462.44 2025.59 3147.29 3237.21 3496.97
MOMENT OF INERTIA : 6.21942 188.22492 194.44435

TS43
0 2
O -1.26039100 -1.36175700 0.00008200
C -1.79547200 0.91415100 -0.00007400
H -2.52426800 1.70269500 -0.00013500
C 0.46047900 0.02741900 0.00000600
C -0.36060900 1.07784900 -0.00007200
H 0.05437500 2.08371600 -0.00013600
C -1.99465700 -0.42663500 0.00001300
C 1.79153000 -0.48770100 0.00004400
H 1.88882900 -1.58848000 0.00011500
O 2.75707100 0.25820500 0.00000100
Freq: -367.28 84.11 118.44 176.86 407.15 420.98 522.01 627.73 651.08 750.46 851.20 895.16 1003.82 1053.27 1099.82 1199.75 1308.27 1409.22 1632.14 1700.82 1862.98 2960.57 3163.83 3314.32
MOMENT OF INERTIA : 247.47523 1022.37299 1269.84822

P43
0 2
O -2.97559200 -0.86822100 -0.00032600
C -1.30742000 0.97037300 0.00001900
H -1.72463500 1.97055900 0.00011200
C 0.79541500 -0.38342800 0.00009200
C 0.12296800 0.76734200 0.00013400
H 0.71412000 1.68791600 0.00028000
C -2.19212400 -0.01773800 -0.00018800
C 2.20976900 -0.70249300 0.00019800
H 2.46989000 -1.77822500 0.00046900
O 3.07171400 0.15764800 0.00002700
Freq: 35.58 91.15 173.37 191.90 226.02 380.61 546.23 590.22 652.78 798.84 856.76 886.41 1016.13 1052.30 1165.37 1287.07 1421.18 1426.94 1642.50 1721.79 2225.40 2941.51 3077.42 3200.69
MOMENT OF INERTIA : 172.62255 1595.66326 1768.28581

TS44
0 2
O -2.42841600 -1.21530800 -0.37701200
C -1.60929900 0.84752100 0.68707500
H -1.24703300 1.12448300 1.65917200
C 1.12924300 0.74557500 -0.24225100
C 0.25099800 1.47442300 -0.66247000
H -0.35027000 2.18565600 -1.17596100
C -2.00615600 -0.29159100 0.20459300
C 2.12872100 -0.11781400 0.33108700
H 2.67501000 0.32912400 1.18529200
O 2.37357200 -1.23318600 -0.07007600
Freq: -253.31 36.31 51.05 100.00 116.09 225.90 317.36 453.90 557.58 577.06 636.34 649.44 675.38 743.53 955.33 1009.01 1252.07 1419.06 1747.09 2110.31 2143.56 2930.32 3338.68 3481.21
MOMENT OF INERTIA : 421.104 1301.66812 1570.27035

P44
0 1
O -1.60996300 -0.41563800 -0.00001400
C 1.86497700 -0.13469500 -0.00030100
H 2.90643400 -0.34913600 0.00087300
C 0.68195300 0.08911000 0.00016500
C -0.72731300 0.40870500 0.00002500
H -0.94442400 1.49552500 -0.00009000
Freq: 217.36 285.95 634.04 658.42 720.52 958.37 1021.67 1422.12

1777.04 2212.91 2929.45 3494.78
MOMENT OF INERTIA : 26.34091 373.26586 399.60675