

THERMO

R1	H	7C	4O	4	Og	300.00	5000.00	1000.00	1		
						1.45438553E+01	2.47475336E-02	-9.60865975E-06	1.71204029E-09	-1.14835302E-13	2
						-5.16877399E+04	-4.40275810E+01	4.63185053E+00	4.35242398E-02	-9.96605341E-06	3
						-1.63516981E-08	9.39190104E-12	-4.84466009E+04	9.46922357E+00		4
P1	H	7C	4O	4	Og	300.00	5000.00	1000.00	1		
						1.68961368E+01	2.24800929E-02	-8.72652917E-06	1.55613077E-09	-1.04492605E-13	2
						-4.53292595E+04	-5.72876592E+01	4.30245194E+00	4.55307634E-02	-4.34465410E-06	3
						-2.83814238E-08	1.49504893E-11	-4.12643020E+04	1.06608936E+01		4
R2	H	9C	5O	4	Og	300.00	5000.00	1000.00	1		
						1.66089567E+01	3.14976602E-02	-1.24588985E-05	2.24130122E-09	-1.51135136E-13	2
						-5.81594488E+04	-5.58374871E+01	4.79435249E+00	5.03695929E-02	-1.86002514E-06	3
						-3.11277412E-08	1.54972875E-11	-5.41224020E+04	8.78906042E+00		4
P2	H	9C	5O	4	Og	300.00	5000.00	1000.00	1		
						2.08002211E+01	2.71285440E-02	-1.07660234E-05	1.94056462E-09	-1.31037462E-13	2
						-5.06833446E+04	-7.91920513E+01	2.96137167E+00	6.40332894E-02	-1.67616881E-05	3
						-2.84556475E-08	1.71409785E-11	-4.51737899E+04	1.59173917E+01		4
R3	H	11C	6O	4	Og	300.00	5000.00	1000.00	1		
						1.89819174E+01	3.72334331E-02	-1.46878185E-05	2.63877335E-09	-1.77815569E-13	2
						-6.25042842E+04	-6.63154418E+01	4.70162094E+00	5.70742249E-02	8.65904676E-06	3
						-5.00561154E-08	2.35367736E-11	-5.75212053E+04	1.24211413E+01		4
P3	H	11C	6O	4	Og	300.00	5000.00	1000.00	1		
						2.06103488E+01	3.53902052E-02	-1.39044951E-05	2.49228866E-09	-1.67709512E-13	2
						-5.39316105E+04	-7.49888235E+01	4.79177362E+00	5.92321784E-02	7.83682941E-06	3
						-5.28915145E-08	2.53850065E-11	-4.85699927E+04	1.16134589E+01		4
R4	H	11C	6O	4	Og	300.00	5000.00	1000.00	1		
						1.91647846E+01	3.76284659E-02	-1.47899052E-05	2.64638594E-09	-1.77731742E-13	2
						-6.24911322E+04	-6.99526405E+01	5.30348321E+00	5.33264698E-02	1.82112542E-05	3
						-5.86206971E-08	2.61791522E-11	-5.74591708E+04	7.40205027E+00		4
P4	H	11C	6O	4	Og	300.00	5000.00	1000.00	1		
						2.09070526E+01	3.52467908E-02	-1.37188802E-05	2.44965839E-09	-1.64603418E-13	2
						-5.44799865E+04	-7.61307570E+01	5.65060071E+00	5.86883192E-02	3.77487705E-06	3
						-4.53028624E-08	2.18388710E-11	-4.92627441E+04	7.45579748E+00		4
R5	H	9C	5O	4	Og	300.00	5000.00	1000.00	1		
						1.70835452E+01	3.06678052E-02	-1.18729592E-05	2.11107221E-09	-1.41383331E-13	2
						-5.85850736E+04	-5.76054308E+01	4.32023653E+00	5.86621284E-02	-2.40924360E-05	3
						-8.80042870E-09	7.69737433E-12	-5.46051036E+04	1.03299506E+01		4
P5	H	9C	5O	4	Og	300.00	5000.00	1000.00	1		
						1.90484850E+01	2.87847950E-02	-1.12735008E-05	2.01287740E-09	-1.34976919E-13	2
						-5.09620504E+04	-6.85583419E+01	3.66815758E+00	6.47106090E-02	-3.02176786E-05	3
						-8.83137621E-09	9.05320474E-12	-4.63748035E+04	1.25272294E+01		4
R6	H	11C	6O	4	Og	300.00	5000.00	1000.00	1		
						1.98733709E+01	3.63117439E-02	-1.43094907E-05	2.56901667E-09	-1.73029273E-13	2
						-6.22995640E+04	-7.27430660E+01	4.02682957E+00	6.76276764E-02	-1.76439687E-05	3

-2.45475175E-08 1.47351676E-11-5.72262844E+04 1.23549943E+01	4
P6 H 11C 6O 4 0g 300.00 5000.00 1000.00 1	
2.16730637E+01 3.45372924E-02-1.35782174E-05 2.43262928E-09-1.63578084E-13	2
-5.50779664E+04-8.13435633E+01 4.32935353E+00 6.83496976E-02-1.44503489E-05	3
-3.11863188E-08 1.77915378E-11-4.95594440E+04 1.17757039E+01	4
R7 H 11C 6O 4 0g 300.00 5000.00 1000.00 1	
1.99004762E+01 3.62851928E-02-1.42647231E-05 2.55456520E-09-1.71691793E-13	2
-6.43800640E+04-7.32950747E+01 3.34247890E+00 7.07255201E-02-2.25784334E-05	3
-2.10697382E-08 1.38127608E-11-5.91854664E+04 1.51503760E+01	4
P7 H 11C 6O 4 0g 300.00 5000.00 1000.00 1	
2.13107610E+01 3.38025733E-02-1.29983783E-05 2.30143923E-09-1.53710124E-13	2
-5.53604418E+04-7.96553985E+01 3.31800226E+00 7.63847484E-02-3.70727386E-05	3
-8.21429890E-09 9.78352613E-12-5.00139259E+04 1.50844391E+01	4
R8 H 7C 4O 4 0g 300.00 5000.00 1000.00 1	
1.47181991E+01 2.58275626E-02-1.03727467E-05 1.88275323E-09-1.27692339E-13	2
-5.24939135E+04-4.59027540E+01 5.61916403E+00 2.83508948E-02 3.52028473E-05	3
-6.33851305E-08 2.60864179E-11-4.87939558E+04 6.81888395E+00	4
P8 H 7C 4O 4 0g 300.00 5000.00 1000.00 1	
1.63558602E+01 2.47798732E-02-1.00766025E-05 1.84217401E-09-1.25502017E-13	2
-4.76224675E+04-5.34075275E+01 5.55555139E+00 3.60646060E-02 1.85835942E-05	3
-4.89770258E-08 2.14939485E-11-4.36566958E+04 7.09482895E+00	4
R9 H 9C 5O 4 0g 300.00 5000.00 1000.00 1	
1.69543199E+01 3.14031361E-02-1.24598852E-05 2.24481005E-09-1.51500082E-13	2
-5.65197861E+04-5.64507305E+01 4.51138283E+00 4.35659774E-02 2.47511177E-05	3
-6.23135921E-08 2.74160549E-11-5.19581589E+04 1.33346003E+01	4
P9 H 9C 5O 4 0g 300.00 5000.00 1000.00 1	
1.73604133E+01 3.04123116E-02-1.17875750E-05 2.09874278E-09-1.40736876E-13	2
-4.89913605E+04-5.57597396E+01 7.57770710E+00 3.46392040E-02 3.29466455E-05	3
-6.40388601E-08 2.67619277E-11-4.51003867E+04 5.18181692E-01	4
R10 H 11C 6O 4 0g 300.00 5000.00 1000.00 1	
1.81911122E+01 3.87441391E-02-1.53597105E-05 2.76944863E-09-1.87118229E-13	2
-6.00706734E+04-6.02161781E+01 6.09479495E+00 4.17143718E-02 4.66983000E-05	3
-8.60242472E-08 3.55978612E-11-5.51318880E+04 9.96135231E+00	4
P10 H 11C 6O 4 0g 300.00 5000.00 1000.00 1	
2.00682198E+01 3.71904937E-02-1.46640171E-05 2.63280058E-09-1.77318484E-13	2
-5.32114927E+04-7.01933159E+01 5.61481102E+00 5.38401957E-02 1.94962133E-05	3
-6.15734085E-08 2.75998711E-11-4.79993539E+04 1.03443878E+01	4
R11 H 9C 5O 4 0g 300.00 5000.00 1000.00 1	
1.66089567E+01 3.14976602E-02-1.24588985E-05 2.24130122E-09-1.51135136E-13	2
-5.81594488E+04-5.58374871E+01 4.79435249E+00 5.03695929E-02-1.86002514E-06	3
-3.11277412E-08 1.54972875E-11-5.41224020E+04 8.78906042E+00	4
P11 H 9C 5O 4 0g 300.00 5000.00 1000.00 1	
1.86739486E+01 3.05570543E-02-1.23205924E-05 2.24228123E-09-1.52357569E-13	2
-5.35668655E+04-6.75300703E+01 4.45053912E+00 5.43856740E-02-3.15389655E-06	3

-3.37868948E-08	1.70355270E-11	-4.87669199E+04	9.99460036E+00		4
R12	H	11C	6O	4 Og	300.00 5000.00 1000.00 1
1.89819174E+01	3.72334331E-02	-1.46878185E-05	2.63877335E-09	-1.77815569E-13	2
-6.25042842E+04	-6.63154418E+01	4.70162094E+00	5.70742249E-02	8.65904676E-06	3
-5.00561154E-08	2.35367736E-11	-5.75212053E+04	1.24211413E+01		4
P12	H	11C	6O	4 Og	300.00 5000.00 1000.00 1
1.87628518E+01	3.84019840E-02	-1.49982477E-05	2.67461555E-09	-1.79242051E-13	2
-5.46793246E+04	-6.32324597E+01	6.40463852E+00	5.43865867E-02	8.25370890E-06	3
-4.56490061E-08	2.11950417E-11	-5.02818859E+04	5.26024271E+00		4
R13	H	11C	6O	4 Og	300.00 5000.00 1000.00 1
1.93703395E+01	3.74928189E-02	-1.48351994E-05	2.67123977E-09	-1.80303946E-13	2
-6.23952593E+04	-6.86013633E+01	3.84121075E+00	6.10138744E-02	4.37463208E-06	3
-4.79014780E-08	2.31149049E-11	-5.70720985E+04	1.65463819E+01		4
P13	H	11C	6O	4 Og	300.00 5000.00 1000.00 1
2.02281759E+01	3.65549085E-02	-1.45342993E-05	2.62398996E-09	-1.77405335E-13	2
-5.80240500E+04	-7.35228577E+01	3.19919418E+00	6.39007619E-02	1.40582617E-06	3
-4.69232642E-08	2.30360470E-11	-5.22640055E+04	1.94735880E+01		4
R14	H	11C	6O	4 Og	300.00 5000.00 1000.00 1
1.93703395E+01	3.74928189E-02	-1.48351994E-05	2.67123977E-09	-1.80303946E-13	2
-6.23952593E+04	-6.86013633E+01	3.84121075E+00	6.10138744E-02	4.37463208E-06	3
-4.79014780E-08	2.31149049E-11	-5.70720985E+04	1.65463819E+01		4
P14	H	11C	6O	4 Og	300.00 5000.00 1000.00 1
2.21640059E+01	3.35188779E-02	-1.30312268E-05	2.32559395E-09	-1.56228018E-13	2
-5.58753967E+04	-8.41287909E+01	4.09963320E+00	6.71992230E-02	-8.86273665E-06	3
-3.82815658E-08	2.06009752E-11	-5.00642014E+04	1.32087116E+01		4
R15	H	9C	5O	4 Og	300.00 5000.00 1000.00 1
1.68480510E+01	3.14020960E-02	-1.24673590E-05	2.24929609E-09	-1.52007358E-13	2
-5.56435659E+04	-5.62222685E+01	4.68828746E+00	4.97271883E-02	1.85566696E-06	3
-3.57002502E-08	1.72434055E-11	-5.14344122E+04	1.05624217E+01		4
P15	H	9C	5O	4 Og	300.00 5000.00 1000.00 1
1.72367026E+01	3.08671343E-02	-1.20528714E-05	2.14739597E-09	-1.43764239E-13	2
-4.78018332E+04	-5.61006660E+01	5.86947554E+00	5.09728342E-02	-6.61538062E-06	3
-2.61431697E-08	1.39149715E-11	-4.40577273E+04	5.49010635E+00		4
R16	H	11C	6O	4 Og	300.00 5000.00 1000.00 1
1.93110604E+01	3.70734317E-02	-1.46789139E-05	2.64478653E-09	-1.78612728E-13	2
-5.94535164E+04	-6.83023225E+01	4.77847225E+00	5.69256923E-02	9.58251572E-06	3
-5.09784121E-08	2.37878717E-11	-5.43478648E+04	1.19537296E+01		4
P16	H	11C	6O	4 Og	300.00 5000.00 1000.00 1
1.95995944E+01	3.76987868E-02	-1.47417019E-05	2.63073123E-09	-1.76383052E-13	2
-5.33793196E+04	-6.87440215E+01	4.71418611E+00	6.35130573E-02	-6.07342848E-06	3
-3.59183780E-08	1.87054491E-11	-4.84533900E+04	1.20330744E+01		4
R17	H	11C	6O	4 Og	300.00 5000.00 1000.00 1
1.98733709E+01	3.63117439E-02	-1.43094907E-05	2.56901667E-09	-1.73029273E-13	2
-6.22995640E+04	-7.27430660E+01	4.02682957E+00	6.76276764E-02	-1.76439687E-05	3

-2.45475175E-08 1.47351676E-11-5.72262844E+04 1.23549943E+01	4
P17 H 11C 6O 4 Og 300.00 5000.00 1000.00 1	
2.04872862E+01 3.62919630E-02-1.41734235E-05 2.52717497E-09-1.69337832E-13	2
-5.64574877E+04-7.47630021E+01 4.76412498E+00 6.99590813E-02-2.51734209E-05	3
-1.65392814E-08 1.18841198E-11-5.15678140E+04 8.99679790E+00	4
R18 H 11C 6O 4 Og 300.00 5000.00 1000.00 1	
1.99004762E+01 3.62851928E-02-1.42647231E-05 2.55456520E-09-1.71691793E-13	2
-6.43800640E+04-7.32950747E+01 3.34247890E+00 7.07255201E-02-2.25784334E-05	3
-2.10697382E-08 1.38127608E-11-5.91854664E+04 1.51503760E+01	4
P18 H 11C 6O 4 Og 300.00 5000.00 1000.00 1	
2.12649349E+01 3.49671989E-02-1.36155173E-05 2.43103842E-09-1.63314501E-13	2
-5.95551622E+04-8.06113930E+01 3.78677559E+00 7.39385686E-02-3.12196543E-05	3
-1.24368701E-08 1.07435585E-11-5.41827833E+04 1.21549270E+01	4
R19 H 9C 5O 4 Og 300.00 5000.00 1000.00 1	
1.68251623E+01 3.06486946E-02-1.19255438E-05 2.12834584E-09-1.42937752E-13	2
-5.68027010E+04-5.58790556E+01 5.11865303E+00 4.59126954E-02 9.85060595E-06	3
-4.33569580E-08 1.99490114E-11-5.26548973E+04 8.94829957E+00	4
P19 H 9C 5O 4 Og 300.00 5000.00 1000.00 1	
1.79301460E+01 3.10297693E-02-1.23115711E-05 2.22546365E-09-1.50768562E-13	2
-5.37359860E+04-6.21029942E+01 5.76754555E+00 4.59277403E-02 1.13527163E-05	3
-4.43013239E-08 1.99065685E-11-4.93138567E+04 5.64942239E+00	4
R20 H 11C 6O 4 Og 300.00 5000.00 1000.00 1	
1.78019148E+01 3.92679956E-02-1.54691252E-05 2.77628042E-09-1.86935372E-13	2
-6.06486913E+04-6.09731532E+01 4.40449043E+00 5.83149038E-02 3.71254728E-06	3
-4.26220324E-08 2.03019397E-11-5.59427658E+04 1.29147297E+01	4
P20 H 11C 6O 4 Og 300.00 5000.00 1000.00 1	
2.17449774E+01 3.50521430E-02-1.39275294E-05 2.52237135E-09-1.71193977E-13	2
-5.59877793E+04-8.31756428E+01 5.20371183E+00 5.47757149E-02 2.13973875E-05	3
-6.51931435E-08 2.89572347E-11-5.00087374E+04 8.95667209E+00	4
R21 H 11C 6O 4 Og 300.00 5000.00 1000.00 1	
1.94457910E+01 3.74546719E-02-1.48303847E-05 2.67176966E-09-1.80411942E-13	2
-6.06803883E+04-7.02000063E+01 4.14622193E+00 5.66955252E-02 1.69031588E-05	3
-6.12450775E-08 2.79873419E-11-5.52601414E+04 1.46097773E+01	4
P21 H 11C 6O 4 Og 300.00 5000.00 1000.00 1	
2.07972410E+01 3.59273965E-02-1.42599976E-05 2.57083919E-09-1.73618465E-13	2
-5.73681259E+04-7.67952907E+01 4.21355264E+00 6.32436371E-02-8.83125053E-08	3
-4.50449310E-08 2.24650141E-11-5.18159044E+04 1.35402196E+01	4
R22 H 11C 6O 4 Og 300.00 5000.00 1000.00 1	
1.91647846E+01 3.76284659E-02-1.47899052E-05 2.64638594E-09-1.77731742E-13	2
-6.24911322E+04-6.99526405E+01 5.30348321E+00 5.33264698E-02 1.82112542E-05	3
-5.86206971E-08 2.61791522E-11-5.74591708E+04 7.40205027E+00	4
P22 H 11C 6O 4 Og 300.00 5000.00 1000.00 1	
2.00915995E+01 3.74497799E-02-1.47096225E-05 2.63359051E-09-1.77001298E-13	2
-5.95331086E+04-6.97806457E+01 5.44038557E+00 6.21733776E-02-5.27950673E-06	3

-3.50805961E-08	1.79607688E-11	-5.46106260E+04	9.99525317E+00	4	
R23	H	11C	6O 4 0g 300.00 5000.00 1000.00	1	
1.97913970E+01	3.63405329E-02	-1.41496329E-05	2.52651687E-09	-1.69740836E-13	2
-6.06500214E+04	-7.18826025E+01	4.31876143E+00	6.06467588E-02	2.36507725E-06	3
-4.50789784E-08	2.20162604E-11	-5.53962556E+04	1.27270248E+01		4
P23	H	11C	6O 4 0g 300.00 5000.00 1000.00	1	
1.97687547E+01	3.70690253E-02	-1.46208942E-05	2.62437188E-09	-1.76671907E-13	2
-5.54877642E+04	-6.89715662E+01	4.64176590E+00	6.76370085E-02	-2.10948674E-05	3
-1.87160557E-08	1.21205714E-11	-5.06355266E+04	1.22008956E+01		4
R24	H	9C	5O 4 0g 300.00 5000.00 1000.00	1	
1.68480510E+01	3.14020960E-02	-1.24673590E-05	2.24929609E-09	-1.52007358E-13	2
-5.56435659E+04	-5.62222685E+01	4.68828746E+00	4.97271883E-02	1.85566696E-06	3
-3.57002502E-08	1.72434055E-11	-5.14344122E+04	1.05624217E+01		4
P24	H	9C	5O 4 0g 300.00 5000.00 1000.00	1	
1.82446180E+01	3.01755476E-02	-1.18594285E-05	2.12301245E-09	-1.42640469E-13	2
-4.86351185E+04	-6.36291996E+01	4.11021821E+00	5.51053427E-02	-3.88372376E-06	3
-3.50148582E-08	1.81678507E-11	-4.40218751E+04	1.28677989E+01		4
R25	H	9C	5O 4 0g 300.00 5000.00 1000.00	1	
1.68251623E+01	3.06486946E-02	-1.19255438E-05	2.12834584E-09	-1.42937752E-13	2
-5.68027010E+04	-5.58790556E+01	5.11865303E+00	4.59126954E-02	9.85060595E-06	3
-4.33569580E-08	1.99490114E-11	-5.26548973E+04	8.94829957E+00		4
P25	H	9C	5O 4 0g 300.00 5000.00 1000.00	1	
1.77514636E+01	3.12159105E-02	-1.24090921E-05	2.23826995E-09	-1.51174125E-13	2
-4.96452879E+04	-6.29247083E+01	3.89573743E+00	5.43284422E-02	-2.08393042E-06	3
-3.53777667E-08	1.78185696E-11	-4.49995472E+04	1.25319673E+01		4
R26	H	11C	6O 4 0g 300.00 5000.00 1000.00	1	
1.93703395E+01	3.74928189E-02	-1.48351994E-05	2.67123977E-09	-1.80303946E-13	2
-6.23952593E+04	-6.86013633E+01	3.84121075E+00	6.10138744E-02	4.37463208E-06	3
-4.79014780E-08	2.31149049E-11	-5.70720985E+04	1.65463819E+01		4
P26	H	11C	6O 4 0g 300.00 5000.00 1000.00	1	
1.87090745E+01	3.81406525E-02	-1.49414109E-05	2.67032766E-09	-1.79245830E-13	2
-5.42863992E+04	-6.48181944E+01	3.14248850E+00	6.42004010E-02	-2.69372008E-06	3
-4.12357565E-08	2.09145489E-11	-4.90991856E+04	1.98607565E+01		4
R27	H	11C	6O 4 0g 300.00 5000.00 1000.00	1	
1.98733709E+01	3.63117439E-02	-1.43094907E-05	2.56901667E-09	-1.73029273E-13	2
-6.22995640E+04	-7.27430660E+01	4.02682957E+00	6.76276764E-02	-1.76439687E-05	3
-2.45475175E-08	1.47351676E-11	-5.72262844E+04	1.23549943E+01		4
P27	H	11C	6O 4 0g 300.00 5000.00 1000.00	1	
2.06345010E+01	3.53067186E-02	-1.36929293E-05	2.43918332E-09	-1.63629813E-13	2
-5.57469720E+04	-7.58007403E+01	4.11035780E+00	6.38617598E-02	-3.79002450E-06	3
-4.03798384E-08	2.06529307E-11	-5.02837376E+04	1.38780494E+01		4
R28	H	11C	6O 4 0g 300.00 5000.00 1000.00	1	
1.91647846E+01	3.76284659E-02	-1.47899052E-05	2.64638594E-09	-1.77731742E-13	2
-6.24911322E+04	-6.99526405E+01	5.30348321E+00	5.33264698E-02	1.82112542E-05	3

-5.86206971E-08	2.61791522E-11	-5.74591708E+04	7.40205027E+00		4
P28	H	11C	6O	4 Og	300.00 5000.00 1000.00 1
2.07920690E+01	3.53276676E-02	-1.37444150E-05	2.45360274E-09	-1.64843695E-13	2
-5.49425267E+04	-7.86398799E+01	3.64503298E+00	6.68168431E-02	-9.57872831E-06	3
-3.51944841E-08	1.89045396E-11	-4.93552036E+04	1.39880240E+01		4
R29	H	11C	6O	4 Og	300.00 5000.00 1000.00 1
1.90028459E+01	3.69903792E-02	-1.43761430E-05	2.56344202E-09	-1.72044319E-13	2
-6.16418003E+04	-6.73714202E+01	5.28080837E+00	5.65479607E-02	5.27562954E-06	3
-4.39030050E-08	2.07340570E-11	-5.68385272E+04	8.26620829E+00		4
P29	H	11C	6O	4 Og	300.00 5000.00 1000.00 1
2.02226519E+01	3.53921713E-02	-1.36412180E-05	2.41895818E-09	-1.61727730E-13	2
-5.30006058E+04	-7.11179051E+01	7.14849104E+00	5.38452790E-02	6.49233116E-06	3
-4.41018468E-08	2.07809788E-11	-4.84452091E+04	9.19421984E-01		4
R30	H	11C	6O	4 Og	300.00 5000.00 1000.00 1
1.97913970E+01	3.63405329E-02	-1.41496329E-05	2.52651687E-09	-1.69740836E-13	2
-6.06500214E+04	-7.18826025E+01	4.31876143E+00	6.06467588E-02	2.36507725E-06	3
-4.50789784E-08	2.20162604E-11	-5.53962556E+04	1.27270248E+01		4
P30	H	11C	6O	4 Og	300.00 5000.00 1000.00 1
2.04644341E+01	3.59188039E-02	-1.40521773E-05	2.50889020E-09	-1.68284592E-13	2
-5.12325592E+04	-7.46563199E+01	4.92162674E+00	6.39352477E-02	-7.71853711E-06	3
-3.53091019E-08	1.87756745E-11	-4.61665773E+04	9.36870632E+00		4
R31	H	9C	5O	4 Og	300.00 5000.00 1000.00 1
1.69543199E+01	3.14031361E-02	-1.24598852E-05	2.24481005E-09	-1.51500082E-13	2
-5.65197861E+04	-5.64507305E+01	4.51138283E+00	4.35659774E-02	2.47511177E-05	3
-6.23135921E-08	2.74160549E-11	-5.19581589E+04	1.33346003E+01		4
P31	H	9C	5O	4 Og	300.00 5000.00 1000.00 1
1.81418035E+01	3.04715088E-02	-1.21248357E-05	2.19610118E-09	-1.48994649E-13	2
-5.22519824E+04	-6.38808149E+01	5.92002381E+00	3.96462460E-02	3.07460648E-05	3
-6.56887474E-08	2.78450407E-11	-4.75596645E+04	5.53483083E+00		4
R32	H	11C	6O	4 Og	300.00 5000.00 1000.00 1
1.81911122E+01	3.87441391E-02	-1.53597105E-05	2.76944863E-09	-1.87118229E-13	2
-6.00706734E+04	-6.02161781E+01	6.09479495E+00	4.17143718E-02	4.66983000E-05	3
-8.60242472E-08	3.55978612E-11	-5.51318880E+04	9.96135231E+00		4
P32	H	11C	6O	4 Og	300.00 5000.00 1000.00 1
1.92939812E+01	3.64610217E-02	-1.41078915E-05	2.50836690E-09	-1.68019056E-13	2
-5.23674597E+04	-6.38360505E+01	8.48643015E+00	4.15550179E-02	3.34740339E-05	3
-6.82147233E-08	2.86190506E-11	-4.80682399E+04	-1.71625913E+00		4
R33	H	11C	6O	4 Og	300.00 5000.00 1000.00 1
1.94457910E+01	3.74546719E-02	-1.48303847E-05	2.67176966E-09	-1.80411942E-13	2
-6.06803883E+04	-7.02000063E+01	4.14622193E+00	5.66955252E-02	1.69031588E-05	3
-6.12450775E-08	2.79873419E-11	-5.52601414E+04	1.46097773E+01		4
P33	H	11C	6O	4 Og	300.00 5000.00 1000.00 1
1.97051562E+01	3.73716872E-02	-1.46861257E-05	2.63019822E-09	-1.76810159E-13	2
-5.46033899E+04	-7.25513476E+01	3.53599283E+00	6.85982591E-02	-1.58422855E-05	3

-2.73533707E-08	1.58316840E-11	-4.93925231E+04	1.44557361E+01	4	
R34	H	11C	6O 4 Og 300.00 5000.00 1000.00	1	
1.89819174E+01	3.72334331E-02	-1.46878185E-05	2.63877335E-09	-1.77815569E-13	2
-6.25042842E+04	-6.63154418E+01	4.70162094E+00	5.70742249E-02	8.65904676E-06	3
-5.00561154E-08	2.35367736E-11	-5.75212053E+04	1.24211413E+01		4
P34	H	11C	6O 4 Og 300.00 5000.00 1000.00	1	
1.82956454E+01	4.04799205E-02	-1.62651664E-05	2.94923660E-09	-1.99734104E-13	2
-6.01515119E+04	-6.63571934E+01	2.40033505E+00	7.04307695E-02	-1.64911802E-05	3
-2.63921818E-08	1.52252816E-11	-5.49336442E+04	1.94969300E+01		4
R35	H	11C	6O 4 Og 300.00 5000.00 1000.00	1	
1.93110604E+01	3.70734317E-02	-1.46789139E-05	2.64478653E-09	-1.78612728E-13	2
-5.94535164E+04	-6.83023225E+01	4.77847225E+00	5.69256923E-02	9.58251572E-06	3
-5.09784121E-08	2.37878717E-11	-5.43478648E+04	1.19537296E+01		4
P35	H	11C	6O 4 Og 300.00 5000.00 1000.00	1	
2.05528910E+01	3.53899546E-02	-1.37242604E-05	2.44438292E-09	-1.63950782E-13	2
-5.43116234E+04	-7.43067434E+01	5.43889464E+00	5.76707961E-02	7.37207744E-06	3
-4.96441818E-08	2.35940719E-11	-4.91237744E+04	8.66246835E+00		4
R36	H	11C	6O 4 Og 300.00 5000.00 1000.00	1	
1.78019148E+01	3.92679956E-02	-1.54691252E-05	2.77628042E-09	-1.86935372E-13	2
-6.06486913E+04	-6.09731532E+01	4.40449043E+00	5.83149038E-02	3.71254728E-06	3
-4.26220324E-08	2.03019397E-11	-5.59427658E+04	1.29147297E+01		4
P36	H	11C	6O 4 Og 300.00 5000.00 1000.00	1	
2.05910811E+01	3.63629738E-02	-1.44745299E-05	2.61305382E-09	-1.76584426E-13	2
-5.66729889E+04	-7.56198536E+01	4.76719887E+00	6.29012838E-02	-2.93252001E-06	3
-4.03342541E-08	2.04395568E-11	-5.13775808E+04	1.05094499E+01		4
R37	H	11C	6O 4 Og 300.00 5000.00 1000.00	1	
1.90691874E+01	3.71652533E-02	-1.45114836E-05	2.59633407E-09	-1.74686431E-13	2
-6.08999812E+04	-6.71817050E+01	5.09649738E+00	4.98320650E-02	2.91199682E-05	3
-7.07013019E-08	3.07251077E-11	-5.56864827E+04	1.15316586E+01		4
P37	H	11C	6O 4 Og 300.00 5000.00 1000.00	1	
1.88969910E+01	3.88244258E-02	-1.55140403E-05	2.80657515E-09	-1.89891969E-13	2
-5.80370640E+04	-6.54461552E+01	6.93288567E+00	4.87456176E-02	2.24193897E-05	3
-5.86272890E-08	2.52717754E-11	-5.34390608E+04	2.39108246E+00		4
R38	H	11C	6O 4 Og 300.00 5000.00 1000.00	1	
1.93110604E+01	3.70734317E-02	-1.46789139E-05	2.64478653E-09	-1.78612728E-13	2
-5.94535164E+04	-6.83023225E+01	4.77847225E+00	5.69256923E-02	9.58251572E-06	3
-5.09784121E-08	2.37878717E-11	-5.43478648E+04	1.19537296E+01		4
P38	H	11C	6O 4 Og 300.00 5000.00 1000.00	1	
2.12367674E+01	3.50765326E-02	-1.37946810E-05	2.47912692E-09	-1.67288759E-13	2
-5.33003747E+04	-7.82011350E+01	4.07782552E+00	6.35137640E-02	6.99181711E-07	3
-4.69251578E-08	2.33935971E-11	-4.75781798E+04	1.51915208E+01		4
R39	H	11C	6O 4 Og 300.00 5000.00 1000.00	1	
1.94457910E+01	3.74546719E-02	-1.48303847E-05	2.67176966E-09	-1.80411942E-13	2
-6.06803883E+04	-7.02000063E+01	4.14622193E+00	5.66955252E-02	1.69031588E-05	3

-6.12450775E-08	2.79873419E-11	-5.52601414E+04	1.46097773E+01	4	
P39	H	11C	6O 4 0g 300.00 5000.00 1000.00	1	
1.95623308E+01	3.74008445E-02	-1.47991539E-05	2.66340814E-09	-1.79680452E-13	2
-5.09021373E+04	-7.05842584E+01	6.05751111E+00	4.94659462E-02	2.70732643E-05	3
-6.70679755E-08	2.90438881E-11	-4.58257227E+04	5.60858261E+00		4
R40	H	11C	6O 4 0g 300.00 5000.00 1000.00	1	
1.90691874E+01	3.71652533E-02	-1.45114836E-05	2.59633407E-09	-1.74686431E-13	2
-6.08999812E+04	-6.71817050E+01	5.09649738E+00	4.98320650E-02	2.91199682E-05	3
-7.07013019E-08	3.07251077E-11	-5.56864827E+04	1.15316586E+01		4
P40	H	11C	6O 4 0g 300.00 5000.00 1000.00	1	
2.02932905E+01	3.55526321E-02	-1.37688885E-05	2.45028979E-09	-1.64258202E-13	2
-5.21938156E+04	-7.19972723E+01	6.81377812E+00	4.78714180E-02	2.88080047E-05	3
-6.94551741E-08	3.02598422E-11	-4.71987749E+04	3.84203111E+00		4
R41	H	11C	6O 4 0g 300.00 5000.00 1000.00	1	
1.81911122E+01	3.87441391E-02	-1.53597105E-05	2.76944863E-09	-1.87118229E-13	2
-6.00706734E+04	-6.02161781E+01	6.09479495E+00	4.17143718E-02	4.66983000E-05	3
-8.60242472E-08	3.55978612E-11	-5.51318880E+04	9.96135231E+00		4
P41	H	11C	6O 4 0g 300.00 5000.00 1000.00	1	
2.00427165E+01	3.67075379E-02	-1.44272766E-05	2.59064477E-09	-1.74673053E-13	2
-5.57525496E+04	-7.20865743E+01	4.70093033E+00	5.85967748E-02	8.83935075E-06	3
-5.19848045E-08	2.45129622E-11	-5.04307000E+04	1.23568325E+01		4
R42	H	5C	3O 4 0g 300.00 5000.00 1000.00	1	
1.15583965E+01	2.09365671E-02	-8.37530526E-06	1.51430177E-09	-1.02359835E-13	2
-4.53768365E+04	-2.91510711E+01	4.80771275E+00	2.77857365E-02	9.42632110E-06	3
-2.95668834E-08	1.30355238E-11	-4.28562202E+04	8.78979902E+00		4
P42	H	5C	3O 4 0g 300.00 5000.00 1000.00	1	
1.53606133E+01	1.71468326E-02	-6.85136365E-06	1.23731396E-09	-8.35622855E-14	2
-4.06720594E+04	-4.96585334E+01	3.33211273E+00	4.57376607E-02	-2.27962532E-05	3
-6.26259872E-09	6.76369942E-12	-3.71308104E+04	1.35863926E+01		4
R43	H	7C	4O 4 0g 300.00 5000.00 1000.00	1	
1.45438553E+01	2.47475336E-02	-9.60865975E-06	1.71204029E-09	-1.14835302E-13	2
-5.16877399E+04	-4.40275810E+01	4.63185053E+00	4.35242398E-02	-9.96605341E-06	3
-1.63516981E-08	9.39190104E-12	-4.84466009E+04	9.46922357E+00		4
P43	H	7C	4O 4 0g 300.00 5000.00 1000.00	1	
1.58528024E+01	2.46285878E-02	-9.61924935E-06	1.71253562E-09	-1.14542395E-13	2
-4.44111543E+04	-4.97303205E+01	5.23447033E+00	4.93596183E-02	-2.30497054E-05	3
-4.99769172E-09	5.86801243E-12	-4.12149049E+04	6.32655584E+00		4
R44	H	9C	5O 4 0g 300.00 5000.00 1000.00	1	
1.68480510E+01	3.14020960E-02	-1.24673590E-05	2.24929609E-09	-1.52007358E-13	2
-5.56435659E+04	-5.62222685E+01	4.68828746E+00	4.97271883E-02	1.85566696E-06	3
-3.57002502E-08	1.72434055E-11	-5.14344122E+04	1.05624217E+01		4
P44	H	9C	5O 4 0g 300.00 5000.00 1000.00	1	
1.97939204E+01	2.83908717E-02	-1.09487299E-05	1.94284685E-09	-1.29982051E-13	2
-5.04647832E+04	-7.33458051E+01	2.51277119E+00	7.02312489E-02	-3.63834207E-05	3

-6.19246681E-09	8.82673508E-12	-4.54019194E+04	1.73551515E+01	4
R45	H	11C	6O 4 0g	300.00 5000.00 1000.00 1
1.93110604E+01	3.70734317E-02	-1.46789139E-05	2.64478653E-09	-1.78612728E-13 2
-5.94535164E+04	-6.83023225E+01	4.77847225E+00	5.69256923E-02	9.58251572E-06 3
-5.09784121E-08	2.37878717E-11	-5.43478648E+04	1.19537296E+01	4
P45	H	11C	6O 4 0g	300.00 5000.00 1000.00 1
2.13886795E+01	3.62947426E-02	-1.43881192E-05	2.59094597E-09	-1.74804361E-13 2
-5.42180912E+04	-8.09859087E+01	2.85613923E+00	7.67418890E-02	-2.92512316E-05 3
-1.82566313E-08	1.35468913E-11	-4.85121996E+04	1.75055767E+01	4
R46	H	9C	5O 4 0g	300.00 5000.00 1000.00 1
1.70835452E+01	3.06678052E-02	-1.18729592E-05	2.11107221E-09	-1.41383331E-13 2
-5.85850736E+04	-5.76054308E+01	4.32023653E+00	5.86621284E-02	-2.40924360E-05 3
-8.80042870E-09	7.69737433E-12	-5.46051036E+04	1.03299506E+01	4
P46	H	9C	5O 4 0g	300.00 5000.00 1000.00 1
1.98794051E+01	2.80011384E-02	-1.07101932E-05	1.88908095E-09	-1.25819474E-13 2
-5.27990524E+04	-7.32604413E+01	2.60984351E+00	7.81859080E-02	-6.27228883E-05 3
2.23951632E-08	-1.58751074E-12	-4.81352583E+04	1.53649901E+01	4
R47	H	11C	6O 4 0g	300.00 5000.00 1000.00 1
1.98733709E+01	3.63117439E-02	-1.43094907E-05	2.56901667E-09	-1.73029273E-13 2
-6.22995640E+04	-7.27430660E+01	4.02682957E+00	6.76276764E-02	-1.76439687E-05 3
-2.45475175E-08	1.47351676E-11	-5.72262844E+04	1.23549943E+01	4
P47	H	11C	6O 4 0g	300.00 5000.00 1000.00 1
2.23630256E+01	3.36746656E-02	-1.29268792E-05	2.28592166E-09	-1.52533762E-13 2
-5.65773131E+04	-8.57162970E+01	1.91766125E+00	8.90891008E-02	-6.16562294E-05 3
1.25638501E-08	3.26630371E-12	-5.08702425E+04	2.01597202E+01	4
R48	H	7C	4O 4 0g	300.00 5000.00 1000.00 1
1.47181991E+01	2.58275626E-02	-1.03727467E-05	1.88275323E-09	-1.27692339E-13 2
-5.24939135E+04	-4.59027540E+01	5.61916403E+00	2.83508948E-02	3.52028473E-05 3
-6.33851305E-08	2.60864179E-11	-4.87939558E+04	6.81888395E+00	4
P48	H	7C	4O 4 0g	300.00 5000.00 1000.00 1
1.59923214E+01	2.47067968E-02	-9.71053715E-06	1.73685860E-09	-1.16578437E-13 2
-4.49774004E+04	-5.15308540E+01	4.98383562E+00	4.41846600E-02	-3.86045593E-06 3
-2.66528077E-08	1.39080137E-11	-4.13812956E+04	8.04820284E+00	4
R49	H	9C	5O 4 0g	300.00 5000.00 1000.00 1
1.66089567E+01	3.14976602E-02	-1.24588985E-05	2.24130122E-09	-1.51135136E-13 2
-5.81594488E+04	-5.58374871E+01	4.79435249E+00	5.03695929E-02	-1.86002514E-06 3
-3.11277412E-08	1.54972875E-11	-5.41224020E+04	8.78906042E+00	4
P49	H	9C	5O 4 0g	300.00 5000.00 1000.00 1
1.95491447E+01	2.85906405E-02	-1.10159513E-05	1.95329575E-09	-1.30600454E-13 2
-5.18324823E+04	-7.08373249E+01	2.93495566E+00	7.11333349E-02	-4.35361668E-05 3
3.43080911E-09	4.92785133E-12	-4.70490712E+04	1.58676105E+01	4
R50	H	11C	6O 4 0g	300.00 5000.00 1000.00 1
1.93703395E+01	3.74928189E-02	-1.48351994E-05	2.67123977E-09	-1.80303946E-13 2
-6.23952593E+04	-6.86013633E+01	3.84121075E+00	6.10138744E-02	4.37463208E-06 3

-4.79014780E-08	2.31149049E-11	-5.70720985E+04	1.65463819E+01	4	
P50	H	11C	6O 4 Og 300.00 5000.00 1000.00	1	
2.19984856E+01	3.50753546E-02	-1.37603557E-05	2.46158557E-09	-1.65346712E-13	2
-5.60703023E+04	-8.47058817E+01	2.23972014E+00	7.95180134E-02	-3.20004271E-05	3
-1.86651220E-08	1.44509145E-11	-5.01177557E+04	1.98204418E+01		4
R51	H	9C	5O 4 Og 300.00 5000.00 1000.00	1	
1.68251623E+01	3.06486946E-02	-1.19255438E-05	2.12834584E-09	-1.42937752E-13	2
-5.68027010E+04	-5.58790556E+01	5.11865303E+00	4.59126954E-02	9.85060595E-06	3
-4.33569580E-08	1.99490114E-11	-5.26548973E+04	8.94829957E+00		4
P51	H	9C	5O 4 Og 300.00 5000.00 1000.00	1	
1.94006067E+01	2.82604049E-02	-1.08895144E-05	1.93119220E-09	-1.29145726E-13	2
-4.97852897E+04	-6.89962400E+01	4.87480096E+00	5.72859784E-02	-1.31901844E-05	3
-2.51485978E-08	1.46996376E-11	-4.52198273E+04	8.76631722E+00		4
R52	H	11C	6O 4 Og 300.00 5000.00 1000.00	1	
1.90028459E+01	3.69903792E-02	-1.43761430E-05	2.56344202E-09	-1.72044319E-13	2
-6.16418003E+04	-6.73714202E+01	5.28080837E+00	5.65479607E-02	5.27562954E-06	3
-4.39030050E-08	2.07340570E-11	-5.68385272E+04	8.26620829E+00		4
P52	H	11C	6O 4 Og 300.00 5000.00 1000.00	1	
2.11534571E+01	3.48609315E-02	-1.34011633E-05	2.37202984E-09	-1.58382262E-13	2
-5.45373684E+04	-7.89361844E+01	4.79445190E+00	7.13092164E-02	-2.91316972E-05	3
-1.29464020E-08	1.07354472E-11	-4.95299362E+04	7.84138714E+00		4
R53	H	11C	6O 4 Og 300.00 5000.00 1000.00	1	
1.91647846E+01	3.76284659E-02	-1.47899052E-05	2.64638594E-09	-1.77731742E-13	2
-6.24911322E+04	-6.99526405E+01	5.30348321E+00	5.33264698E-02	1.82112542E-05	3
-5.86206971E-08	2.61791522E-11	-5.74591708E+04	7.40205027E+00		4
P53	H	11C	6O 4 Og 300.00 5000.00 1000.00	1	
2.25576255E+01	3.42663453E-02	-1.34887547E-05	2.42738643E-09	-1.64009244E-13	2
-5.63826621E+04	-8.88312868E+01	3.04222624E+00	7.72753188E-02	-3.25024894E-05	3
-1.38069583E-08	1.15125611E-11	-5.03364087E+04	1.49354575E+01		4
R54	H	11C	6O 4 Og 300.00 5000.00 1000.00	1	
1.99004762E+01	3.62851928E-02	-1.42647231E-05	2.55456520E-09	-1.71691793E-13	2
-6.43800640E+04	-7.32950747E+01	3.34247890E+00	7.07255201E-02	-2.25784334E-05	3
-2.10697382E-08	1.38127608E-11	-5.91854664E+04	1.51503760E+01		4
P54	H	11C	6O 4 Og 300.00 5000.00 1000.00	1	
2.22628833E+01	3.39336355E-02	-1.31997401E-05	2.34678254E-09	-1.56918012E-13	2
-5.76968947E+04	-8.52637994E+01	1.80190171E+00	9.30199736E-02	-7.34517711E-05	3
2.49440371E-08	-1.19231641E-12	-5.21576325E+04	1.98174010E+01		4
R55	H	9C	5O 4 Og 300.00 5000.00 1000.00	1	
1.69543199E+01	3.14031361E-02	-1.24598852E-05	2.24481005E-09	-1.51500082E-13	2
-5.65197861E+04	-5.64507305E+01	4.51138283E+00	4.35659774E-02	2.47511177E-05	3
-6.23135921E-08	2.74160549E-11	-5.19581589E+04	1.33346003E+01		4
P55	H	9C	5O 4 Og 300.00 5000.00 1000.00	1	
1.84000170E+01	3.03699402E-02	-1.19004809E-05	2.12601897E-09	-1.42634205E-13	2
-4.88058474E+04	-6.35840190E+01	4.77881492E+00	5.32715171E-02	-2.79053681E-07	3

-3.82881656E-08	1.93152421E-11	-4.43169939E+04	1.03789767E+01	4	
R56	H	11C	6O 4 0g 300.00 5000.00 1000.00	1	
1.89819174E+01	3.72334331E-02	-1.46878185E-05	2.63877335E-09	-1.77815569E-13	2
-6.25042842E+04	-6.63154418E+01	4.70162094E+00	5.70742249E-02	8.65904676E-06	3
-5.00561154E-08	2.35367736E-11	-5.75212053E+04	1.24211413E+01		4
P56	H	11C	6O 4 0g 300.00 5000.00 1000.00	1	
2.18566299E+01	3.46265483E-02	-1.35570155E-05	2.42184836E-09	-1.62516719E-13	2
-5.58781359E+04	-8.11769399E+01	4.01379850E+00	7.10976211E-02	-1.86209209E-05	3
-2.87850090E-08	1.74158555E-11	-5.03195647E+04	1.41183469E+01		4
R57	H	11C	6O 4 0g 300.00 5000.00 1000.00	1	
1.90691874E+01	3.71652533E-02	-1.45114836E-05	2.59633407E-09	-1.74686431E-13	2
-6.08999812E+04	-6.71817050E+01	5.09649738E+00	4.98320650E-02	2.91199682E-05	3
-7.07013019E-08	3.07251077E-11	-5.56864827E+04	1.15316586E+01		4
P57	H	11C	6O 4 0g 300.00 5000.00 1000.00	1	
2.02536810E+01	3.59956212E-02	-1.40502263E-05	2.50462574E-09	-1.67811769E-13	2
-5.29368895E+04	-7.14679962E+01	4.83527165E+00	6.25802518E-02	-3.23379038E-06	3
-4.05616882E-08	2.08515915E-11	-4.78761116E+04	1.21196170E+01		4
R58	H	11C	6O 4 0g 300.00 5000.00 1000.00	1	
1.78019148E+01	3.92679956E-02	-1.54691252E-05	2.77628042E-09	-1.86935372E-13	2
-6.06486913E+04	-6.09731532E+01	4.40449043E+00	5.83149038E-02	3.71254728E-06	3
-4.26220324E-08	2.03019397E-11	-5.59427658E+04	1.29147297E+01		4
P58	H	11C	6O 4 0g 300.00 5000.00 1000.00	1	
2.19172814E+01	3.44651059E-02	-1.34639894E-05	2.40128209E-09	-1.60937695E-13	2
-5.42143270E+04	-8.16496677E+01	3.74655548E+00	7.48219074E-02	-2.83668487E-05	3
-1.93264920E-08	1.42207220E-11	-4.87207703E+04	1.45847491E+01		4
R59	H	5C	3O 4 0g 300.00 5000.00 1000.00	1	
1.25785211E+01	2.08419178E-02	-8.58894034E-06	1.58454173E-09	-1.08632860E-13	2
-4.97192475E+04	-3.46898356E+01	2.86274386E+00	3.99053326E-02	-1.19924294E-05	3
-1.20084753E-08	7.48669488E-12	-4.65384697E+04	1.76745132E+01		4
P59	H	5C	3O 4 0g 300.00 5000.00 1000.00	1	
1.35088808E+01	1.94392650E-02	-7.93702986E-06	1.45783556E-09	-9.97190030E-14	2
-4.23800135E+04	-3.96762309E+01	3.57115092E+00	3.95144832E-02	-1.26277632E-05	3
-1.16159993E-08	7.47839779E-12	-3.91793208E+04	1.36857292E+01		4
R60	H	7C	4O 4 0g 300.00 5000.00 1000.00	1	
1.48399283E+01	2.58765152E-02	-1.03653612E-05	1.88183678E-09	-1.27751002E-13	2
-5.36086612E+04	-4.52595237E+01	3.76032784E+00	4.25024355E-02	2.89518358E-06	3
-3.28535571E-08	1.57433357E-11	-4.97721083E+04	1.56067374E+01		4
P60	H	7C	4O 4 0g 300.00 5000.00 1000.00	1	
1.52939191E+01	2.69903167E-02	-1.11243849E-05	2.05063097E-09	-1.40444236E-13	2
-4.82411245E+04	-4.64658797E+01	4.78884888E+00	4.48595050E-02	-6.45998348E-06	3
-2.14651291E-08	1.12802312E-11	-4.46516472E+04	1.08574493E+01		4
R61	H	9C	5O 4 0g 300.00 5000.00 1000.00	1	
1.64140066E+01	3.27545084E-02	-1.30111461E-05	2.34966377E-09	-1.58941247E-13	2
-5.70047965E+04	-5.42606140E+01	3.40680892E+00	5.13803101E-02	5.75147459E-06	3

-4.22809439E-08	2.00218154E-11	-5.24667433E+04	1.73863174E+01		4
P61	H	9C	5O	4	0g
			300.00	5000.00	1000.00
					1
1.89115732E+01	2.98951368E-02	-1.19312463E-05	2.16463728E-09	-1.47003804E-13	2
-5.27491051E+04	-6.61025209E+01	4.78580482E+00	5.27649565E-02	-6.43817540E-07	3
-3.56649509E-08	1.75820062E-11	-4.79326606E+04	1.11106682E+01		4
R62	H	11C	6O	4	0g
			300.00	5000.00	1000.00
					1
1.89747222E+01	3.83851106E-02	-1.52203692E-05	2.74643171E-09	-1.85714675E-13	2
-6.09110782E+04	-6.75410064E+01	3.21236357E+00	5.95518223E-02	1.26212459E-05	3
-5.73813823E-08	2.66171853E-11	-5.53691321E+04	1.95624895E+01		4
P62	H	11C	6O	4	0g
			300.00	5000.00	1000.00
					1
2.02650890E+01	3.71226188E-02	-1.44723578E-05	2.57480122E-09	-1.72234267E-13	2
-5.61170300E+04	-7.36424485E+01	3.52537474E+00	6.60042241E-02	-3.57978294E-06	3
-4.24183310E-08	2.17188810E-11	-5.06031183E+04	1.71594655E+01		4
R63	H	11C	6O	4	0g
			300.00	5000.00	1000.00
					1
1.92044872E+01	3.79352120E-02	-1.49836260E-05	2.69650837E-09	-1.81991355E-13	2
-6.18756130E+04	-6.88908277E+01	2.07738579E+00	7.35960043E-02	-2.47818434E-05	3
-1.95787320E-08	1.32776882E-11	-5.64621855E+04	2.26860561E+01		4
P63	H	11C	6O	4	0g
			300.00	5000.00	1000.00
					1
2.08901807E+01	3.58986584E-02	-1.41277408E-05	2.54061486E-09	-1.71528437E-13	2
-5.69540271E+04	-7.57305938E+01	4.58963613E+00	6.68539283E-02	-1.54906149E-05	3
-2.57409181E-08	1.47389850E-11	-5.16146183E+04	1.22640060E+01		4
R64	H	9C	5O	4	0g
			300.00	5000.00	1000.00
					1
1.63579984E+01	3.25077720E-02	-1.30630331E-05	2.37524567E-09	-1.61367979E-13	2
-5.73903020E+04	-5.37408398E+01	3.98446040E+00	5.54621468E-02	-1.37380478E-05	3
-1.85031016E-08	1.07354266E-11	-5.32523717E+04	1.33225645E+01		4
P64	H	9C	5O	4	0g
			300.00	5000.00	1000.00
					1
1.80704197E+01	3.11516898E-02	-1.23631330E-05	2.23024578E-09	-1.50720586E-13	2
-5.51872630E+04	-6.01402960E+01	5.57747063E+00	5.16196749E-02	-3.14809711E-06	3
-3.05149873E-08	1.53378711E-11	-5.09333518E+04	8.09905678E+00		4
R65	H	11C	6O	4	0g
			300.00	5000.00	1000.00
					1
1.93780571E+01	3.74487285E-02	-1.47765093E-05	2.65354110E-09	-1.78713733E-13	2
-6.12704590E+04	-6.96972567E+01	2.96593535E+00	6.64015037E-02	-6.90782931E-06	3
-3.78325585E-08	1.98239142E-11	-5.58620661E+04	1.92507977E+01		4
P65	H	11C	6O	4	0g
			300.00	5000.00	1000.00
					1
2.04843024E+01	3.67208989E-02	-1.46223981E-05	2.64499518E-09	-1.79123288E-13	2
-5.88744067E+04	-7.20752029E+01	4.83713421E+00	6.53974265E-02	-1.23051989E-05	3
-2.88635444E-08	1.59020956E-11	-5.37034931E+04	1.26272874E+01		4
R66	H	7C	4O	4	0g
			300.00	5000.00	1000.00
					1
1.48399283E+01	2.58765152E-02	-1.03653612E-05	1.88183678E-09	-1.27751002E-13	2
-5.36086612E+04	-4.52595237E+01	3.76032784E+00	4.25024355E-02	2.89518358E-06	3
-3.28535571E-08	1.57433357E-11	-4.97721083E+04	1.56067374E+01		4
P66	H	7C	4O	4	0g
			300.00	5000.00	1000.00
					1
1.58369146E+01	2.56169195E-02	-1.03202000E-05	1.88065034E-09	-1.27995365E-13	2
-4.42789807E+04	-4.96154407E+01	5.63712739E+00	4.03653524E-02	2.67830093E-06	3

-3.01434340E-08	1.42893783E-11	-4.06834260E+04	6.64121626E+00		4
R67	H	9C	5O	4	0g
300.00	5000.00	1000.00	1		
1.63579984E+01	3.25077720E-02	-1.30630331E-05	2.37524567E-09	-1.61367979E-13	2
-5.73903020E+04	-5.37408398E+01	3.98446040E+00	5.54621468E-02	-1.37380478E-05	3
-1.85031016E-08	1.07354266E-11	-5.32523717E+04	1.33225645E+01		4
P67	H	9C	5O	4	0g
300.00	5000.00	1000.00	1		
1.87234573E+01	2.93095978E-02	-1.12797118E-05	1.99827243E-09	-1.33516391E-13	2
-4.84853482E+04	-6.42625447E+01	4.86095689E+00	5.75202685E-02	-1.56002212E-05	3
-2.11684028E-08	1.29514735E-11	-4.41320839E+04	9.87433750E+00		4
R68	H	11C	6O	4	0g
300.00	5000.00	1000.00	1		
1.84827149E+01	3.84164262E-02	-1.50384732E-05	2.68441779E-09	-1.79977926E-13	2
-6.23325620E+04	-6.47845198E+01	3.33578023E+00	7.12427997E-02	-2.79606458E-05	3
-1.23265683E-08	9.99895215E-12	-5.75980914E+04	1.59121520E+01		4
P68	H	11C	6O	4	0g
300.00	5000.00	1000.00	1		
2.10933730E+01	3.60275029E-02	-1.43047306E-05	2.58119212E-09	-1.74460994E-13	2
-5.34296079E+04	-7.71489894E+01	4.59559368E+00	7.23371164E-02	-3.02297939E-05	3
-1.16214485E-08	1.00632812E-11	-4.83000802E+04	1.06114765E+01		4
R69	H	11C	6O	4	0g
300.00	5000.00	1000.00	1		
1.93780571E+01	3.74487285E-02	-1.47765093E-05	2.65354110E-09	-1.78713733E-13	2
-6.12704590E+04	-6.96972567E+01	2.96593535E+00	6.64015037E-02	-6.90782931E-06	3
-3.78325585E-08	1.98239142E-11	-5.58620661E+04	1.92507977E+01		4
P69	H	11C	6O	4	0g
300.00	5000.00	1000.00	1		
2.10740845E+01	3.60244820E-02	-1.41413957E-05	2.53956657E-09	-1.71322661E-13	2
-5.25348548E+04	-7.72337610E+01	5.49340747E+00	6.05708537E-02	3.75353714E-07	3
-4.13439206E-08	2.01521713E-11	-4.71864688E+04	8.10432628E+00		4
R70	H	9C	5O	4	0g
300.00	5000.00	1000.00	1		
1.64140066E+01	3.27545084E-02	-1.30111461E-05	2.34966377E-09	-1.58941247E-13	2
-5.70047965E+04	-5.42606140E+01	3.40680892E+00	5.13803101E-02	5.75147459E-06	3
-4.22809439E-08	2.00218154E-11	-5.24667433E+04	1.73863174E+01		4
P70	H	9C	5O	4	0g
300.00	5000.00	1000.00	1		
1.79781318E+01	3.12460579E-02	-1.24372908E-05	2.25077134E-09	-1.52529845E-13	2
-4.94374385E+04	-5.92698862E+01	6.30352024E+00	4.48334427E-02	1.28460250E-05	3
-4.55422857E-08	2.03756928E-11	-4.51650238E+04	5.91741162E+00		4
R71	H	11C	6O	4	0g
300.00	5000.00	1000.00	1		
1.93780571E+01	3.74487285E-02	-1.47765093E-05	2.65354110E-09	-1.78713733E-13	2
-6.12704590E+04	-6.96972567E+01	2.96593535E+00	6.64015037E-02	-6.90782931E-06	3
-3.78325585E-08	1.98239142E-11	-5.58620661E+04	1.92507977E+01		4
P71	H	11C	6O	4	0g
300.00	5000.00	1000.00	1		
2.03319662E+01	3.56656692E-02	-1.38440840E-05	2.46678373E-09	-1.65483703E-13	2
-5.34044906E+04	-7.15754316E+01	6.55267580E+00	5.82879247E-02	-3.65308597E-06	3
-3.38140897E-08	1.70100968E-11	-4.87219859E+04	3.66203419E+00		4
R72	H	11C	6O	4	0g
300.00	5000.00	1000.00	1		
1.89747222E+01	3.83851106E-02	-1.52203692E-05	2.74643171E-09	-1.85714675E-13	2
-6.09110782E+04	-6.75410064E+01	3.21236357E+00	5.95518223E-02	1.26212459E-05	3

-5.73813823E-08 2.66171853E-11-5.53691321E+04 1.95624895E+01	4
P72 H 11C 6O 4 Og 300.00 5000.00 1000.00 1	
1.96108027E+01 3.71201149E-02-1.44916407E-05 2.59242737E-09-1.74402914E-13	2
-5.60079784E+04-7.00258305E+01 4.37308575E+00 6.18179970E-02-2.17715025E-06	3
-3.86458024E-08 1.92124584E-11-5.08177400E+04 1.32457809E+01	4
R73 H 11C 6O 4 Og 300.00 5000.00 1000.00 1	
1.92044872E+01 3.79352120E-02-1.49836260E-05 2.69650837E-09-1.81991355E-13	2
-6.18756130E+04-6.88908277E+01 2.07738579E+00 7.35960043E-02-2.47818434E-05	3
-1.95787320E-08 1.32776882E-11-5.64621855E+04 2.26860561E+01	4
P73 H 11C 6O 4 Og 300.00 5000.00 1000.00 1	
1.99530805E+01 3.65705599E-02-1.43934502E-05 2.58332597E-09-1.73999899E-13	2
-5.75377660E+04-7.18193904E+01 3.25943187E+00 7.39954742E-02-3.24021014E-05	3
-9.95944899E-09 9.56967730E-12-5.23911440E+04 1.67914106E+01	4
R74 H 9C 5O 4 Og 300.00 5000.00 1000.00 1	
1.64140066E+01 3.27545084E-02-1.30111461E-05 2.34966377E-09-1.58941247E-13	2
-5.70047965E+04-5.42606140E+01 3.40680892E+00 5.13803101E-02 5.75147459E-06	3
-4.22809439E-08 2.00218154E-11-5.24667433E+04 1.73863174E+01	4
P74 H 9C 5O 4 Og 300.00 5000.00 1000.00 1	
1.88593315E+01 3.01773111E-02-1.19775793E-05 2.16498650E-09-1.46646425E-13	2
-4.85411027E+04-6.35833956E+01 5.53937065E+00 4.88299527E-02 8.64810993E-06	3
-4.50101736E-08 2.10051075E-11-4.38822275E+04 9.87173444E+00	4
R75 H 11C 6O 4 Og 300.00 5000.00 1000.00 1	
1.93780571E+01 3.74487285E-02-1.47765093E-05 2.65354110E-09-1.78713733E-13	2
-6.12704590E+04-6.96972567E+01 2.96593535E+00 6.64015037E-02-6.90782931E-06	3
-3.78325585E-08 1.98239142E-11-5.58620661E+04 1.92507977E+01	4
P75 H 11C 6O 4 Og 300.00 5000.00 1000.00 1	
2.03988364E+01 3.62709646E-02-1.43353859E-05 2.58232974E-09-1.74449446E-13	2
-5.26341148E+04-7.31241448E+01 5.11149470E+00 5.99922738E-02 2.27448721E-06	3
-4.42706944E-08 2.15592012E-11-4.74036097E+04 1.06038502E+01	4
R76 H 11C 6O 4 Og 300.00 5000.00 1000.00 1	
1.92044872E+01 3.79352120E-02-1.49836260E-05 2.69650837E-09-1.81991355E-13	2
-6.18756130E+04-6.88908277E+01 2.07738579E+00 7.35960043E-02-2.47818434E-05	3
-1.95787320E-08 1.32776882E-11-5.64621855E+04 2.26860561E+01	4
P76 H 11C 6O 4 Og 300.00 5000.00 1000.00 1	
2.13957182E+01 3.64445245E-02-1.46617734E-05 2.66968798E-09-1.81610171E-13	2
-5.32530723E+04-7.87310714E+01 4.87147752E+00 6.53769369E-02-8.56176569E-06	3
-3.38729582E-08 1.77675330E-11-4.77106887E+04 1.10917611E+01	4
R77 H 11C 6O 4 Og 300.00 5000.00 1000.00 1	
1.89747222E+01 3.83851106E-02-1.52203692E-05 2.74643171E-09-1.85714675E-13	2
-6.09110782E+04-6.75410064E+01 3.21236357E+00 5.95518223E-02 1.26212459E-05	3
-5.73813823E-08 2.66171853E-11-5.53691321E+04 1.95624895E+01	4
P77 H 11C 6O 4 Og 300.00 5000.00 1000.00 1	
2.02121293E+01 3.70021270E-02-1.46449711E-05 2.64080378E-09-1.78533258E-13	2
-5.32802247E+04-7.14574729E+01 5.70176527E+00 5.80441356E-02 4.63286887E-06	3

-4.46124320E-08	2.11861751E-11	-4.82031997E+04	8.47349047E+00		4
R78	H	11C	6O	4 Og	300.00 5000.00 1000.00 1
1.89747222E+01	3.83851106E-02	-1.52203692E-05	2.74643171E-09	-1.85714675E-13	2
-6.09110782E+04	-6.75410064E+01	3.21236357E+00	5.95518223E-02	1.26212459E-05	3
-5.73813823E-08	2.66171853E-11	-5.53691321E+04	1.95624895E+01		4
P78	H	11C	6O	4 Og	300.00 5000.00 1000.00 1
2.08957929E+01	3.53893067E-02	-1.38114236E-05	2.47095907E-09	-1.66270019E-13	2
-5.21952231E+04	-7.44978319E+01	5.08598950E+00	5.58883664E-02	1.73995366E-05	3
-6.20736604E-08	2.84095704E-11	-4.66432245E+04	1.29481346E+01		4
END					