

SUMMARY OF PM5 CALCULATION

MOPAC 2002 Version 2.5.2

EMPIRICAL FORMULA: C222 H182 N2 O48

HERBERTS TEST WAS SATISFIED IN BFGS
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION = -1228.573638 KCAL = -5140.35210 KJ
ELECTRONIC ENERGY = -1380359.553309 EV
CORE-CORE REPULSION = 1337061.118253 EV
DIPOLE = 11.69120 DEBYE
NO. OF FILLED LEVELS = 684
IONIZATION POTENTIAL = 8.304389 EV
HOMO LUMO ENERGIES (EV) = -8.304 -0.860
MOLECULAR WEIGHT = 3645.864
SCF CALCULATIONS = 176
COMPUTATION TIME = 5 HOURS 9 MINUTES AND 14 SECONDS

FINAL GEOMETRY OBTAINED

0.1951	H(1)	-6.743955242	1	-9.910962833	1	9.933246366	1	
0.3786	O(2)	-2.174298844	1	7.749728617	1	-3.774739486	1	-
0.1093	C(3)	0.608559157	1	8.065739814	1	-3.864057408	1	
0.0409	C(4)	-2.558425349	1	9.898533934	1	-2.717793684	1	
0.0704	C(5)	-2.026550667	1	11.102018866	1	-2.240320765	1	-
0.1074	C(6)	-1.702078191	1	8.909583859	1	-3.276177309	1	
0.1469	C(7)	-0.642766105	1	11.248613734	1	-2.178084960	1	-
0.1688	C(8)	-0.315427115	1	9.118229257	1	-3.275968242	1	-
0.1449	C(9)	0.192507175	1	10.260819394	1	-2.659074712	1	-
0.4415	O(10)	1.047249694	1	7.192969797	1	-2.868729931	1	-
0.3751	O(11)	-3.870336500	1	9.587841102	1	-2.707519600	1	-
0.1678	C(12)	-2.910285430	1	12.198031222	1	-1.831319739	1	-
0.1278	C(13)	-3.793396175	1	12.750480497	1	-2.651812669	1	-
0.1139	H(14)	5.661185096	1	2.201389971	1	-9.083332279	1	

0.1473	H(15)	6.696762621	1	1.079425292	1	-8.149850606	1	
0.3705	O(16)	4.789279919	1	4.454993821	1	-8.713237011	1	-
0.1652	C(17)	6.935304855	1	3.078309204	1	-3.304487508	1	-
0.1177	C(18)	6.228443753	1	2.792866450	1	-4.389373174	1	-
0.1853	C(19)	4.866650353	1	4.826963030	1	-4.584204222	1	-
0.0116	C(20)	4.081069963	1	5.743719309	1	-5.328379758	1	
0.0091	C(21)	5.529367102	1	3.798902723	1	-5.189098870	1	
0.0731	C(22)	3.970326037	1	5.598641479	1	-6.721929919	1	-
0.0701	C(23)	5.483560332	1	3.674285630	1	-6.617241787	1	
0.0809	C(24)	4.736247750	1	4.569150643	1	-7.368574277	1	
0.1536	C(25)	3.381044712	1	6.793388316	1	-4.677277992	1	-
0.0387	C(26)	2.541514286	1	7.622248644	1	-5.371545104	1	-
0.1393	C(27)	2.383277739	1	7.426602576	1	-6.766345567	1	-
0.1535	C(28)	3.092799661	1	6.465674999	1	-7.420891639	1	-
0.1556	C(29)	1.805124742	1	8.712364358	1	-4.632832407	1	-
0.3850	O(30)	-7.580598770	1	-2.206593695	1	0.157230621	1	-
0.3946	O(31)	-4.939867336	1	-2.500596214	1	0.198046118	1	-
0.0728	C(32)	9.296543006	1	-1.163342161	1	-0.184952599	1	-
0.1093	C(33)	7.035143404	1	-1.979309508	1	4.223316470	1	
0.3340	O(34)	11.082572170	1	0.787247891	1	3.958104876	1	-
0.1258	C(35)	10.160292782	1	-0.090248329	1	1.933175008	1	
0.0924	C(36)	9.239937484	1	-0.949226175	1	1.297585843	1	-
0.0940	C(37)	8.273647061	1	-1.581927433	1	2.064416479	1	-
0.1698	C(38)	8.185764587	1	-1.381035193	1	3.438240257	1	-
0.1005	C(39)	9.101527749	1	-0.560326519	1	4.081474732	1	-
0.0167	C(40)	10.098408148	1	0.065387557	1	3.336183842	1	-
0.1263	C(41)	9.468786692	1	0.831717748	1	-1.701969328	1	-
0.1939	C(42)	8.897250566	1	1.835843051	1	-2.464467280	1	-
0.0028	C(43)	7.519567536	1	2.027468552	1	-2.459124642	1	

0.1481	C(44)	6.699680411	1	1.240084478	1	-1.646090853	1	-
0.1054	C(45)	7.294446130	1	0.206693989	1	-0.897530559	1	
0.0868	C(46)	8.683475397	1	-0.019169519	1	-0.934231537	1	-
0.1524	C(47)	5.230507771	1	1.506697103	1	-1.531017892	1	-
0.1565	C(48)	4.388247076	1	0.531226224	1	-2.354287838	1	-
0.1166	H(49)	4.992952109	1	2.541537629	1	-1.859574313	1	
0.1879	C(50)	2.403137253	1	0.029966296	1	-0.906471681	1	-
0.1509	C(51)	1.059829298	1	0.161985033	1	-0.594643430	1	-
0.0583	C(52)	0.235690612	1	0.977175270	1	-1.366239948	1	-
0.1578	C(53)	0.780838426	1	1.668799871	1	-2.445280651	1	-
0.1529	C(54)	2.121073863	1	1.527741534	1	-2.763610845	1	-
0.0737	C(55)	2.940770267	1	0.695610756	1	-2.005725673	1	-
0.1533	C(56)	-1.223389597	1	1.096977895	1	-1.053795983	1	-
0.1674	C(57)	-2.068073255	1	0.609167310	1	-2.234174010	1	-
0.3047	C(58)	-3.558453255	1	-0.969588045	1	-0.994000084	1	-
0.0019	C(59)	-3.437776793	1	0.194918609	1	-1.792650430	1	
0.2389	C(60)	-4.554564977	1	0.887866750	1	-2.152508316	1	-
0.1476	C(61)	-4.793790151	1	-1.398638344	1	-0.571717308	1	
0.1511	C(62)	-5.994099662	1	-0.696827382	1	-0.939754146	1	-
0.0513	C(63)	-5.846504559	1	0.453257717	1	-1.745948994	1	
0.2053	C(64)	-6.994942526	1	1.172485610	1	-2.164937123	1	-
0.1586	C(65)	-7.318254115	1	-1.092880258	1	-0.557497619	1	
0.2253	C(66)	-8.414839162	1	-0.369866556	1	-0.981948705	1	-
0.0908	C(67)	-8.238358743	1	0.759906288	1	-1.797335779	1	-
0.2161	H(68)	0.510944727	1	3.671688444	1	-5.416590798	1	
0.2041	H(69)	-0.901619402	1	5.117435613	1	-3.614996313	1	
0.1069	H(70)	-1.466480421	1	2.156284269	1	-0.823453963	1	
0.1987	N(71)	-1.443128759	1	3.095478149	1	-6.212877494	1	-
0.2073	C(72)	-1.298371119	1	4.455482497	1	-4.380823039	1	-

0.1423	C(73)	-0.572501239	1	3.734246473	1	-5.288784822	1	-
0.1706	C(74)	-2.693249502	1	4.211825730	1	-4.658578589	1	-
0.0244	C(75)	-2.759265012	1	3.323776579	1	-5.769547179	1	
0.1907	C(76)	-3.971572275	1	2.903464461	1	-6.320515476	1	-
0.0854	C(77)	-5.131128927	1	3.374276535	1	-5.754904991	1	-
0.0075	C(78)	-5.092903671	1	4.225146031	1	-4.630063501	1	
0.1540	C(79)	-3.882943131	1	4.675610029	1	-4.080442649	1	
0.2082	C(80)	6.961715591	1	-3.522717135	1	4.080668524	1	-
0.1851	H(81)	-6.103116892	1	3.073700256	1	-6.165454788	1	
0.1650	C(82)	6.521005031	1	-4.551933294	1	1.844474122	1	-
0.0816	C(83)	6.022342135	1	-3.995536106	1	3.017715470	1	-
0.0347	C(84)	4.631685061	1	-3.901784161	1	3.188056710	1	
0.0687	C(85)	3.767213970	1	-4.304464197	1	2.139989540	1	
0.1657	C(86)	4.291738409	1	-4.858665824	1	0.972606055	1	-
0.0151	C(87)	5.669970322	1	-4.985303127	1	0.832750717	1	-
0.1400	C(88)	6.234877696	1	-5.570683709	1	-0.387356742	1	-
0.2737	C(89)	5.756925606	1	-6.653369379	1	-0.966969582	1	-
0.3646	O(90)	-3.933541403	1	5.538326457	1	-3.050250403	1	-
0.4098	O(91)	4.042542309	1	-3.541046221	1	4.351120717	1	-
0.3189	O(92)	6.307423374	1	2.739234723	1	-7.165312545	1	-
0.0345	C(93)	1.356690417	1	9.882599204	1	-5.536191532	1	-
0.4600	O(94)	5.829185595	1	-1.355316466	1	3.894261956	1	-
0.1181	C(95)	10.737276403	1	2.084383053	1	4.396512815	1	-
0.3695	O(96)	11.059150871	1	0.532905754	1	1.152921350	1	-
0.3891	O(97)	6.577163781	1	-0.589042748	1	-0.067808987	1	-
0.2664	O(98)	-6.295775275	1	4.532571077	1	-4.039992099	1	-
0.3827	O(99)	2.429086382	1	-4.101795611	1	2.201024596	1	-
0.4457	O(100)	0.201778838	1	9.652864893	1	-6.272704663	1	-
0.3332	H(101)	-3.059288862	1	7.821712716	1	-4.138403962	1	

0.1805	H(102)	0.065049134	1	7.396726558	1	-4.588231724	1
0.1775	H(103)	-0.212852393	1	12.164689264	1	-1.753925810	1
0.1749	H(104)	1.276614118	1	10.400178790	1	-2.557131226	1
0.2738	H(105)	1.397085523	1	7.651945995	1	-2.108238365	1
0.3234	H(106)	-4.398793936	1	10.198495301	1	-2.196800429	1
0.1709	H(107)	-2.781561142	1	12.554445295	1	-0.801336180	1
0.1736	H(108)	-4.448777791	1	13.569538275	1	-2.329113702	1
0.2984	H(109)	4.005344663	1	4.798772492	1	-9.135886319	1
0.1592	H(110)	7.135874838	1	4.105163180	1	-2.972410584	1
0.1732	H(111)	6.103123486	1	1.755513599	1	-4.730167799	1
0.1699	H(112)	4.895969604	1	4.933245123	1	-3.493219459	1
0.1645	H(113)	3.529509958	1	6.909125434	1	-3.597193774	1
0.1861	H(114)	1.679182749	1	8.034100039	1	-7.345838440	1
0.1523	H(115)	2.960987155	1	6.371513299	1	-8.504475343	1
0.1210	H(116)	2.526965919	1	9.162401655	1	-3.905291524	1
0.3173	H(117)	-7.000829266	1	-2.319883292	1	0.906527119	1
0.3170	H(118)	-4.138068466	1	-3.023571248	1	0.243863675	1
0.1135	H(119)	8.763576922	1	-2.100314254	1	-0.457886198	1
0.1248	H(120)	10.349738905	1	-1.318399261	1	-0.504592314	1
0.1400	H(121)	7.168449217	1	-1.751063962	1	5.317045155	1
0.1772	H(122)	7.562755332	1	-2.254882347	1	1.569910530	1
0.1744	H(123)	9.053603919	1	-0.401888000	1	5.165508159	1
0.1822	H(124)	10.558143401	1	0.696410428	1	-1.716482562	1
0.1780	H(125)	9.533762494	1	2.471638695	1	-3.091434218	1
0.1051	H(126)	4.698238290	1	-0.522745286	1	-2.195236126	1
0.1204	H(127)	4.548633972	1	0.712285075	1	-3.438357624	1
0.1566	H(128)	3.038534720	1	-0.602177084	1	-0.275503771	1
0.1692	H(129)	0.149709408	1	2.333083162	1	-3.048558365	1
0.1641	H(130)	2.532588153	1	2.072123395	1	-3.621348710	1

0.1319	H(131)	-1.581612667	1	-0.259116707	1	-2.731897615	1
0.1192	H(132)	-2.132135256	1	1.404213410	1	-3.006911952	1
0.1957	H(133)	-2.644264194	1	-1.518431664	1	-0.728509690	1
0.1907	H(134)	-4.482533212	1	1.789702409	1	-2.775414528	1
0.1868	H(135)	-6.861718129	1	2.064174331	1	-2.790535726	1
0.1622	H(136)	-9.127889869	1	1.308460709	1	-2.127620821	1
0.1846	H(137)	-9.430700149	1	-0.676130916	1	-0.703795706	1
0.2611	H(138)	-1.187670259	1	2.242189617	1	-6.667240045	1
0.1787	H(139)	-4.003402066	1	2.229197151	1	-7.181878858	1
0.1260	H(140)	6.648978334	1	-3.958301244	1	5.054543404	1
0.1370	H(141)	7.986234067	1	-3.910843514	1	3.895110058	1
0.3165	H(142)	-3.081766475	1	5.650751327	1	-2.630026478	1
0.1744	H(143)	7.605581511	1	-4.666913961	1	1.721267535	1
0.1918	H(144)	3.618702670	1	-5.165812477	1	0.161890376	1
0.1567	H(145)	7.103919897	1	-5.036798919	1	-0.795163738	1
0.1490	H(146)	6.202184202	1	-7.063999728	1	-1.875334760	1
0.1441	H(147)	4.903116920	1	-7.216928156	1	-0.586083286	1
0.3294	H(148)	4.378343906	1	-2.716969212	1	4.705049342	1
0.1396	H(149)	2.150795456	1	10.097268462	1	-6.294528234	1
0.1027	H(150)	1.266987573	1	10.803364745	1	-4.906853172	1
0.2918	H(151)	5.718726809	1	-1.245198040	1	2.951362686	1
0.1078	H(152)	10.488138500	1	2.761308572	1	3.552392151	1
0.1366	H(153)	11.656923112	1	2.440954745	1	4.905545911	1
0.0992	H(154)	9.888387953	1	2.081802291	1	5.110449418	1
0.3293	H(155)	11.722785454	1	1.025036523	1	1.637635665	1
0.2986	H(156)	5.697992155	1	-0.762737956	1	-0.397226323	1
0.3092	H(157)	2.043423644	1	-4.488333772	1	2.986291690	1
0.2830	H(158)	-0.574725225	1	9.609470340	1	-5.719272580	1
0.1111	H(159)	4.929057820	1	1.478197869	1	-0.460445563	1

0.1166	H(160)	-1.462563218	1	0.527473394	1	-0.130034819	1	
0.2419	O(161)	-1.459754720	1	-10.404575434	1	-2.541451957	1	-
0.2268	C(162)	0.090637967	1	-10.206302982	1	-0.865141699	1	-
0.1412	C(163)	-0.354337102	1	-8.982734547	1	-4.250368836	1	
0.1890	C(164)	0.782915123	1	-8.197202729	1	-4.483238529	1	-
0.0556	C(165)	-0.441560795	1	-9.591644556	1	-2.995380463	1	-
0.1263	C(166)	1.760387609	1	-8.048754787	1	-3.503412501	1	-
0.0222	C(167)	0.555784130	1	-9.428099792	1	-1.996988659	1	-
0.1569	C(168)	1.668087687	1	-8.649362894	1	-2.258445702	1	-
0.3517	O(169)	-1.257646474	1	-9.119419623	1	-5.237048479	1	-
0.1899	H(170)	0.902779478	1	-7.698102643	1	-5.452741440	1	
0.3649	O(171)	-5.215658128	1	-15.193079019	1	0.939788739	1	-
0.1115	C(172)	-4.176806794	1	-12.811759107	1	5.144730019	1	-
0.1921	C(173)	-3.257212735	1	-12.130821191	1	2.937290615	1	-
0.0056	C(174)	-3.068272622	1	-12.309476575	1	1.541960402	1	
0.0096	C(175)	-4.081325845	1	-12.947141861	1	3.656492304	1	-
0.0426	C(176)	-3.720629428	1	-13.355965249	1	0.864253298	1	-
0.0000	C(177)	-4.768708916	1	-14.000076181	1	2.981571968	1	
0.0900	C(178)	-4.583505601	1	-14.215814901	1	1.622911355	1	
0.1518	C(179)	-2.210491332	1	-11.441684424	1	0.815189124	1	-
0.0020	C(180)	-2.013179552	1	-11.635650235	1	-0.525596976	1	
0.1520	C(181)	-2.673609215	1	-12.689789292	1	-1.207549256	1	-
0.1169	C(182)	-3.506034069	1	-13.525407100	1	-0.529064118	1	-
0.0968	C(183)	-1.097436282	1	-10.760993742	1	-1.240469663	1	
0.4374	O(184)	2.573514727	1	-2.796775432	1	-2.763362121	1	-
0.3918	O(185)	-2.601759257	1	-1.574893317	1	-5.235855116	1	-
0.4008	O(186)	-4.633273865	1	-2.583878978	1	-3.856993537	1	-
0.1809	H(187)	-9.079049639	1	-12.666079981	1	7.387128716	1	
0.0947	C(188)	-6.776297316	1	-6.737671479	1	6.461958610	1	

0.3666	O(189)	-2.805281377	1	-9.274042227	1	7.723505313	1	-
0.1210	C(190)	-4.814933903	1	-9.637925543	1	8.979457061	1	
0.1850	C(191)	-6.179818136	1	-9.373918224	1	9.159839832	1	-
0.0905	C(192)	-6.814184586	1	-8.436590847	1	8.365089173	1	-
0.1193	C(193)	-6.118315205	1	-7.759307849	1	7.369427535	1	-
0.1362	C(194)	-4.760332196	1	-7.995496885	1	7.182072211	1	-
0.0155	C(195)	-4.111154491	1	-8.940987260	1	7.971343659	1	-
0.1286	C(196)	-7.271342534	1	-13.791902047	1	7.050484076	1	-
0.1869	C(197)	-6.022644421	1	-13.819500018	1	6.455681347	1	-
0.0125	C(198)	-5.573009488	1	-12.745636038	1	5.687837015	1	-
0.1421	C(199)	-6.392900403	1	-11.628287638	1	5.499075357	1	-
0.1060	C(200)	-7.655490054	1	-11.612238252	1	6.128523484	1	
0.1953	C(201)	-8.093947793	1	-12.691321785	1	6.906586321	1	-
0.1384	C(202)	-5.977963275	1	-10.464514175	1	4.651652287	1	-
0.1588	C(203)	-6.703304393	1	-10.484874666	1	3.303468695	1	-
0.1090	H(204)	-4.883061463	1	-10.461046871	1	4.475958563	1	
0.1588	C(205)	-5.441301610	1	-9.610307726	1	1.318829416	1	-
0.1467	C(206)	-5.018431958	1	-8.571477568	1	0.506738687	1	-
0.0484	C(207)	-5.374559479	1	-7.255477500	1	0.800414294	1	-
0.1545	C(208)	-6.181234549	1	-7.003036265	1	1.911646385	1	-
0.1686	C(209)	-6.609350177	1	-8.045687098	1	2.715016795	1	-
0.0519	C(210)	-6.238880704	1	-9.359158301	1	2.431283372	1	-
0.1296	C(211)	-4.941294261	1	-6.151890621	1	-0.057918233	1	-
0.1747	C(212)	-3.760915553	1	-6.149330117	1	-0.667974637	1	-
0.2118	C(213)	-4.197532868	1	-4.266541264	1	-2.265300763	1	-
0.0166	C(214)	-3.287382556	1	-5.116463938	1	-1.587537742	1	
0.1831	C(215)	-1.943309280	1	-4.990827305	1	-1.819993528	1	-
0.1110	C(216)	-3.739252020	1	-3.353281995	1	-3.183600072	1	
0.1103	C(217)	-2.340965720	1	-3.242476617	1	-3.489239587	1	-

0.0256	C(218)	-1.450435974	1	-4.053295006	1	-2.762875604	1	
0.1489	C(219)	-0.056686845	1	-3.924941611	1	-2.979799700	1	-
0.1117	C(220)	-1.800706082	1	-2.369753703	1	-4.487630135	1	
0.0892	C(221)	-0.431020801	1	-2.251559082	1	-4.689068305	1	-
0.1023	C(222)	0.442056371	1	-3.037989118	1	-3.892218802	1	-
0.1909	C(223)	1.966469160	1	-2.980364672	1	-3.999036166	1	
0.0550	C(224)	0.052209672	1	-1.296277391	1	-5.744856741	1	-
0.2075	O(225)	3.685699670	1	-1.594916853	1	-5.153764747	1	-
0.0664	C(226)	1.515133393	1	-1.187940967	1	-5.769493516	1	-
0.0535	C(227)	2.347011306	1	-1.920330314	1	-4.980427809	1	-
0.1061	C(228)	2.371553708	1	-0.315980227	1	-6.544194917	1	-
0.0950	C(229)	3.696948147	1	-0.600447907	1	-6.107930234	1	
0.1473	C(230)	4.815229837	1	0.056992777	1	-6.588225115	1	-
0.1003	C(231)	4.611370564	1	1.031309266	1	-7.558955981	1	-
0.0188	C(232)	3.315762043	1	1.313080597	1	-8.039602395	1	-
0.1480	C(233)	2.175374804	1	0.641150085	1	-7.534234618	1	
0.2080	C(234)	-6.622076406	1	-5.326273451	1	7.085144619	1	-
0.0398	C(235)	5.820574234	1	1.772321593	1	-8.068208813	1	
0.2053	C(236)	-8.207891690	1	-3.630941649	1	6.140119403	1	-
0.0390	C(237)	-6.984548220	1	-4.281701398	1	6.078415282	1	-
0.0420	C(238)	-6.097620098	1	-3.971977724	1	5.034939973	1	-
0.1081	C(239)	-6.459375884	1	-3.017150655	1	4.058909968	1	
0.1945	C(240)	-7.701660185	1	-2.377371366	1	4.134412533	1	-
0.0325	C(241)	-8.565255944	1	-2.686713793	1	5.177391270	1	
0.1613	C(242)	-9.870069169	1	-2.023112443	1	5.268750032	1	-
0.2605	C(243)	-10.662271603	1	-1.829738075	1	4.233217485	1	-
0.3588	O(244)	0.909668407	1	0.891484550	1	-7.913341700	1	-
0.3944	O(245)	-4.927945070	1	-4.647046594	1	4.883283743	1	-
0.3390	O(246)	-5.518837579	1	-14.882250256	1	3.709397370	1	-

0.4583	O(247)	-8.120046626	1	-7.098101506	1	6.285803188	1	-
0.0318	C(248)	-1.824856008	1	-8.377758376	1	8.246552065	1	-
0.3565	O(249)	-4.244114899	1	-10.536131328	1	9.803255605	1	-
0.3865	O(250)	-8.539175971	1	-10.595674286	1	5.986174365	1	-
0.3854	O(251)	3.070200647	1	2.270181516	1	-8.971931034	1	-
0.3788	O(252)	-5.645547223	1	-2.661185095	1	3.042146623	1	-
0.1180	C(253)	-6.924474395	1	-14.729789342	1	3.650685618	1	-
0.2113	H(254)	0.609923613	1	-10.325227805	1	0.081034537	1	
0.1660	H(255)	2.634625934	1	-7.429119667	1	-3.735754990	1	
0.1719	H(256)	2.447380923	1	-8.518907963	1	-1.502077525	1	
0.3105	H(257)	-2.072003912	1	-9.517979800	1	-4.939454774	1	
0.3086	H(258)	-5.354916111	1	-15.974845242	1	1.472464134	1	
0.1160	H(259)	-3.618746271	1	-11.915154171	1	5.494221973	1	
0.1257	H(260)	-3.638094701	1	-13.684025613	1	5.580260885	1	
0.1770	H(261)	-2.716085782	1	-11.312530702	1	3.429857982	1	
0.1805	H(262)	-1.720569028	1	-10.616192341	1	1.346860387	1	
0.1830	H(263)	-2.505051027	1	-12.831977734	1	-2.281664910	1	
0.1847	H(264)	-4.013297296	1	-14.336289276	1	-1.065737687	1	
0.2974	H(265)	2.299143422	1	-1.980452514	1	-2.341857008	1	
0.3200	H(266)	-3.331030875	1	-2.061315901	1	-5.620108286	1	
0.3173	H(267)	-4.815291095	1	-1.778643298	1	-3.364542584	1	
0.1299	H(268)	-6.254592701	1	-6.764852327	1	5.463812489	1	
0.1860	H(269)	-7.881110934	1	-8.244318371	1	8.535176707	1	
0.1762	H(270)	-4.202784172	1	-7.438375830	1	6.418588536	1	
0.1605	H(271)	-7.609234233	1	-14.643055274	1	7.652055608	1	
0.1697	H(272)	-5.386148817	1	-14.702554566	1	6.587857902	1	
0.1210	H(273)	-7.802863782	1	-10.413868803	1	3.439229576	1	
0.1173	H(274)	-6.520844929	1	-11.461283265	1	2.805051722	1	
0.1728	H(275)	-5.142274657	1	-10.637062138	1	1.072999170	1	

0.1600	H(276)	-6.488082741	1	-5.978242799	1	2.148886751	1	
0.1590	H(277)	-7.262101665	1	-7.834698184	1	3.569577684	1	
0.1685	H(278)	-4.416799972	1	-8.801283207	1	-0.380421107	1	
0.1672	H(279)	-3.044943673	1	-6.969764639	1	-0.508360281	1	
0.1996	H(280)	-5.275629794	1	-4.357301960	1	-2.073240824	1	
0.1802	H(281)	-1.220499508	1	-5.623154541	1	-1.288508959	1	
0.1850	H(282)	0.616868445	1	-4.560246283	1	-2.388501392	1	
0.1649	H(283)	2.346999466	1	-3.973681261	1	-4.368393998	1	
0.1365	H(284)	-0.369123587	1	-0.282052062	1	-5.561971543	1	
0.1363	H(285)	-0.311733804	1	-1.627958540	1	-6.743042342	1	
0.2015	H(286)	5.819198195	1	-0.182875733	1	-6.218736234	1	
0.1347	H(287)	-5.574195636	1	-5.190962847	1	7.427509350	1	
0.1344	H(288)	-7.248588219	1	-5.234070068	1	7.998019395	1	
0.3639	O(289)	11.001219695	1	3.183073537	1	0.200731332	1	-
0.1775	H(290)	-8.902788864	1	-3.859076335	1	6.957749752	1	
0.1962	H(291)	-7.980758538	1	-1.625943062	1	3.384307894	1	
0.1604	H(292)	-10.149963027	1	-1.694150157	1	6.278682664	1	
0.1503	H(293)	-11.628832518	1	-1.331831723	1	4.334618209	1	
0.1536	H(294)	-10.424561529	1	-2.153638831	1	3.217570979	1	
0.3123	H(295)	0.855181471	1	1.393147514	1	-8.725273532	1	
0.3043	H(296)	-4.232994304	1	-4.236411689	1	5.399327599	1	
0.2912	H(297)	-8.590952648	1	-6.413329518	1	5.815445160	1	
0.1082	H(298)	-1.899482511	1	-8.332678454	1	9.360242916	1	
0.1179	H(299)	-1.987208091	1	-7.344169464	1	7.856680192	1	
0.3097	H(300)	-3.420957680	1	-10.881649244	1	9.465197066	1	
0.3081	H(301)	-8.113880202	1	-9.739108441	1	5.985267998	1	
0.2994	H(302)	3.628451736	1	2.148277876	1	-9.739233489	1	
0.3191	H(303)	-4.963475129	1	-3.307254235	1	2.860301961	1	
0.0940	H(304)	-7.335307221	1	-15.043987783	1	2.669408632	1	

0.1240	H(305)	-7.261890238	1	-13.692887098	1	3.857507348	1	
0.1365	H(306)	-7.289814731	1	-15.404545604	1	4.452916910	1	
0.0993	H(307)	-6.170069686	1	-9.509485941	1	5.188368682	1	
0.1649	H(308)	-5.667833187	1	-5.335124291	1	-0.166445627	1	
0.1978	C(309)	8.672508778	1	4.871977068	1	0.595047574	1	-
0.0062	C(310)	12.142769451	1	4.383453738	1	1.868510112	1	
0.0534	C(311)	12.247615504	1	5.431847864	1	2.821413957	1	-
0.1204	C(312)	10.983718114	1	4.166652102	1	1.117595510	1	
0.1427	C(313)	11.167892997	1	6.267395548	1	3.047453721	1	-
0.0858	C(314)	9.905995009	1	5.035988787	1	1.363865966	1	-
0.1319	C(315)	10.012423586	1	6.054622153	1	2.319805928	1	-
0.2153	O(316)	13.317375892	1	3.667215073	1	1.806480202	1	-
0.2322	C(317)	13.592530376	1	5.320192599	1	3.357868754	1	-
0.0424	C(318)	14.169771172	1	4.265994389	1	2.721441107	1	-
0.4548	O(319)	5.142291936	1	5.287029786	1	3.218150117	1	-
0.3928	O(320)	2.933283508	1	7.342494737	1	3.069804264	1	-
0.1665	C(321)	4.136499227	1	10.647517053	1	-1.764846266	1	-
0.1224	C(322)	4.217742772	1	10.476811033	1	-0.450966232	1	-
0.2064	C(323)	5.054684854	1	8.140571833	1	-0.377687657	1	-
0.0215	C(324)	5.110474709	1	6.869453481	1	0.197462336	1	
0.0051	C(325)	4.279736035	1	9.153326819	1	0.168323475	1	
0.1490	C(326)	4.378994603	1	6.586898214	1	1.344841231	1	-
0.0047	C(327)	3.535203380	1	8.880542507	1	1.326036402	1	
0.0926	C(328)	3.592104875	1	7.604196375	1	1.916743081	1	
0.1710	C(329)	5.912215980	1	5.826098445	1	-0.509431268	1	-
0.0601	C(330)	6.241971567	1	4.587995221	1	0.326366506	1	-
0.2144	C(331)	5.030716952	1	4.141490973	1	1.134606051	1	-
0.1286	C(332)	4.413642442	1	5.232212494	1	2.024508701	1	
0.1477	C(333)	7.474189645	1	4.790039403	1	1.157616572	1	-

0.4528	O(334)	1.972439560	1	-1.535071320	1	4.407812653	1	-
0.4112	O(335)	-3.338487095	1	-1.078120145	1	2.042753882	1	-
0.4004	O(336)	-4.098564336	1	1.402781553	1	1.453002461	1	-
0.1879	H(337)	3.797448095	1	15.512505743	1	-4.124127117	1	
0.0622	C(338)	-5.304338938	1	7.995686957	1	-6.437884262	1	-
0.2312	O(339)	-6.228811567	1	10.224089303	1	-6.020116444	1	-
0.0995	C(340)	-4.143906880	1	11.285610324	1	-6.634475832	1	
0.2536	C(341)	-3.077063185	1	12.121743166	1	-6.280209641	1	-
0.0870	C(342)	-2.978886778	1	12.608305131	1	-4.989199812	1	-
0.0834	C(343)	-3.956440625	1	12.311713996	1	-4.044041886	1	-
0.1180	C(344)	-5.065969900	1	11.549261881	1	-4.397422067	1	-
0.0721	C(345)	-5.148408618	1	11.013382587	1	-5.678563010	1	
0.1796	H(346)	-2.300295485	1	12.377163758	1	-7.011406400	1	
0.1238	C(347)	4.708565929	1	13.536755323	1	-4.116050520	1	-
0.1871	C(348)	4.795504423	1	12.285544476	1	-3.509349033	1	-
0.0282	C(349)	4.036419437	1	11.965341467	1	-2.385809964	1	
0.1035	C(350)	3.174392972	1	12.935540448	1	-1.890105160	1	-
0.0613	C(351)	3.104223801	1	14.204297586	1	-2.534708589	1	
0.1531	C(352)	3.862305816	1	14.529932690	1	-3.647114916	1	-
0.2230	C(353)	2.222290151	1	13.005701112	1	-0.795182142	1	-
0.0615	C(354)	1.678280063	1	14.250229242	1	-0.847997947	1	-
0.2162	H(355)	2.001916840	1	12.205969816	1	-0.092275724	1	
0.1476	C(356)	-0.730723595	1	7.021565242	1	1.019621666	1	-
0.1475	C(357)	-1.027416330	1	5.671769200	1	1.124495837	1	-
0.0312	C(358)	-1.086937520	1	5.068567319	1	2.379822160	1	-
0.1489	C(359)	-0.847086866	1	5.824546925	1	3.525258748	1	-
0.1756	C(360)	-0.554685460	1	7.175632209	1	3.410710119	1	-
0.1700	C(361)	-0.494958702	1	7.775867599	1	2.160595100	1	-
0.2032	C(362)	-2.583667570	1	3.155865023	1	1.866055755	1	-

0.0165	C(363)	-1.407207148	1	3.637537891	1	2.491207055	1	
0.1749	C(364)	-0.591799459	1	2.786189629	1	3.177061446	1	-
0.1112	C(365)	-2.907923387	1	1.824018063	1	1.946661416	1	
0.1007	C(366)	-2.053576573	1	0.892443980	1	2.630450095	1	-
0.0223	C(367)	-0.901045828	1	1.401432967	1	3.258095092	1	
0.1554	C(368)	-0.048067201	1	0.522642422	1	3.967619925	1	-
0.1077	C(369)	-2.302947115	1	-0.514992217	1	2.712492321	1	
0.0825	C(370)	-1.450961474	1	-1.367012804	1	3.404288259	1	-
0.0960	C(371)	-0.312869774	1	-0.816432905	1	4.046817833	1	-
0.1833	C(372)	0.662473992	1	-1.645989887	1	4.876679720	1	
0.0528	C(373)	-1.767207950	1	-2.834715983	1	3.424724011	1	-
0.1749	N(374)	0.818691668	1	-4.033260476	1	5.791522383	1	-
0.0626	C(375)	-0.863507244	1	-3.601416412	1	4.291388093	1	-
0.1600	C(376)	0.217205923	1	-3.067494154	1	4.939547823	1	-
0.1325	C(377)	-0.923654386	1	-4.996728170	1	4.641316919	1	-
0.0224	C(378)	0.166154003	1	-5.254879722	1	5.520722542	1	
0.2095	C(379)	0.399062655	1	-6.514113332	1	6.068949531	1	-
0.0115	C(380)	-0.456058200	1	-7.545165077	1	5.730645459	1	-
0.0745	C(381)	-1.539833118	1	-7.318706596	1	4.843067500	1	-
0.1739	C(382)	-1.789173569	1	-6.044160443	1	4.298969501	1	
0.0604	C(383)	-6.059570638	1	8.908839576	1	-5.749176397	1	
0.1548	C(384)	-0.212140037	1	-8.898911183	1	6.328212136	1	-
0.1993	C(385)	-0.451213629	1	-8.909433780	1	7.834867819	1	-
0.0136	C(386)	-6.258030263	1	6.852796484	1	-4.798498977	1	-
0.0563	C(387)	-6.707268183	1	8.191139093	1	-4.657425896	1	-
0.0858	C(388)	-7.579817646	1	8.535749334	1	-3.633816322	1	
0.0740	C(389)	-7.988794988	1	7.501101533	1	-2.756323759	1	
0.2567	C(390)	-7.524150050	1	6.183204974	1	-2.889351857	1	-
0.2075	C(391)	-6.651983675	1	5.842311975	1	-3.924608861	1	

0.3700	O(392)	-2.795168118	1	-5.742635878	1	3.463275419	1	-
0.3615	O(393)	-7.931648461	1	9.824580652	1	-3.461352629	1	-
0.3388	O(394)	2.676219480	1	9.818828524	1	1.831877759	1	-
0.2061	O(395)	-5.410593012	1	6.735433774	1	-5.881007432	1	-
0.3527	O(396)	-4.254299920	1	10.689601692	1	-7.838457959	1	-
0.2261	O(397)	2.189029754	1	15.008900892	1	-1.891093833	1	-
0.3916	O(398)	-2.333966476	1	-8.333150320	1	4.408000257	1	-
0.3601	O(399)	-8.867585214	1	7.864442760	1	-1.794636869	1	-
0.1190	C(400)	3.134798867	1	10.555658381	1	2.948002852	1	-
0.3198	H(401)	10.130531593	1	2.820911887	1	0.026861785	1	
0.1567	H(402)	8.813114931	1	4.833791331	1	-0.494444374	1	
0.1722	H(403)	11.235032665	1	7.074897613	1	3.782382450	1	
0.1749	H(404)	9.146605235	1	6.708657376	1	2.480927673	1	
0.2062	H(405)	14.028276914	1	5.967291579	1	4.112575457	1	
0.2297	H(406)	15.155507361	1	3.799389292	1	2.781459993	1	
0.3192	H(407)	1.994970151	1	7.529879051	1	2.986004346	1	
0.1747	H(408)	4.239745378	1	11.330235670	1	0.240521909	1	
0.1589	H(409)	4.146830683	1	9.802882526	1	-2.466746176	1	
0.1773	H(410)	5.655481515	1	8.352957131	1	-1.271329438	1	
0.1253	H(411)	6.849837339	1	6.277957424	1	-0.900603827	1	
0.1082	H(412)	5.318530304	1	5.509507470	1	-1.396560936	1	
0.1224	H(413)	6.470328582	1	3.756959614	1	-0.393696571	1	
0.1420	H(414)	5.295375768	1	3.252016706	1	1.747289786	1	
0.1208	H(415)	4.234293033	1	3.816955827	1	0.429171284	1	
0.1095	H(416)	3.348029586	1	4.923138506	1	2.225207294	1	
0.1839	H(417)	7.350607991	1	4.833416602	1	2.246715716	1	
0.2939	H(418)	2.053114037	1	-1.788455092	1	3.488885063	1	
0.3319	H(419)	-4.180583608	1	-0.695829159	1	2.299219836	1	
0.3172	H(420)	-4.035344745	1	1.194464024	1	0.517414847	1	

0.2516	H(421)	-4.673256262	1	8.053551955	1	-7.328913253	1
0.1725	H(422)	-2.115558709	1	13.223851737	1	-4.710503264	1
0.1996	H(423)	-5.874353902	1	11.364707103	1	-3.677869691	1
0.1701	H(424)	5.331813526	1	13.745624242	1	-4.993707108	1
0.1727	H(425)	5.487710589	1	11.542564700	1	-3.922695884	1
0.1668	H(426)	-0.272529565	1	8.845461135	1	2.071868711	1
0.2289	H(427)	0.936225011	1	14.772910987	1	-0.240593286	1
0.1689	H(428)	-0.689033968	1	7.493834887	1	0.031325383	1
0.1691	H(429)	-0.903884424	1	5.356906342	1	4.514779487	1
0.1608	H(430)	-0.391049422	1	7.772347663	1	4.315025212	1
0.1917	H(431)	-3.241191165	1	3.865155018	1	1.346201611	1
0.1761	H(432)	0.320102804	1	3.153485796	1	3.663356526	1
0.1821	H(433)	0.838712547	1	0.945544585	1	4.458844420	1
0.1591	H(434)	0.695994188	1	-1.218864460	1	5.918725946	1
0.1367	H(435)	-1.711207196	1	-3.243754662	1	2.390810247	1
0.1154	H(436)	-2.811448822	1	-2.981891288	1	3.778144545	1
0.2687	H(437)	1.802516554	1	-3.999130090	1	5.980097571	1
0.1778	H(438)	1.245445544	1	-6.680597095	1	6.743548861	1
0.1183	H(439)	0.844098397	1	-9.186857280	1	6.128725550	1
0.1244	H(440)	-0.817861951	1	-9.691892910	1	5.845364540	1
0.1193	H(441)	0.297298922	1	-8.269690470	1	8.351627714	1
0.1203	H(442)	-0.299979943	1	-9.943133512	1	8.213655300	1
0.1992	H(443)	-7.839207695	1	5.406474040	1	-2.179536281	1
0.3295	H(444)	-3.368635299	1	-6.481567950	1	3.255470739	1
0.3072	H(445)	-8.881482394	1	9.929999336	1	-3.508375596	1
0.2991	H(446)	-3.667469761	1	11.074178313	1	-8.486066435	1
0.3031	H(447)	-2.779661593	1	-8.756698088	1	5.143197577	1
0.3021	H(448)	-9.079164983	1	7.143840237	1	-1.205840757	1
0.1304	H(449)	2.286352123	1	11.232274232	1	3.180043802	1

0.1033	H(450)	4.040324782	1	11.152910174	1	2.714529151	1
0.1125	H(451)	3.356336166	1	9.913318737	1	3.824866451	1
0.1683	H(452)	-1.205246764	1	5.078112301	1	0.220578658	1
0.1678	H(453)	0.652876449	1	-0.379671312	1	0.267347433	1
0.2888	H(454)	4.758353841	1	5.890204354	1	3.846734979	1