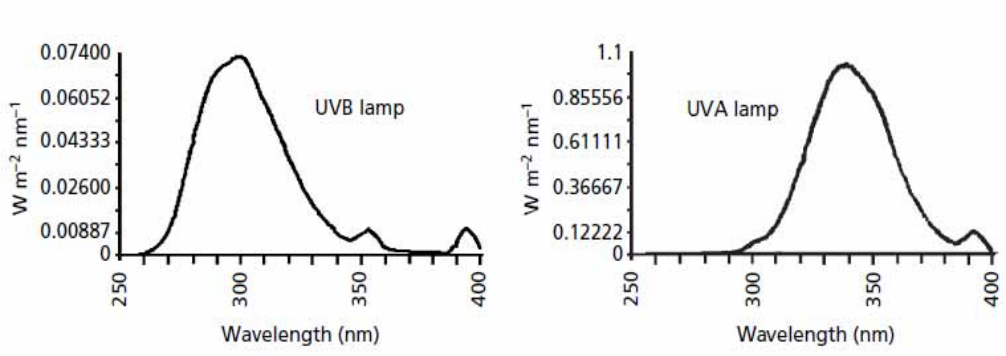
Electronic Supplementary Material (ESI) for Photochemical & Photobiological Sciences

Irradiance of the UVB and UVA lamps used in the photostability experiment.



Compound characterization

7-Hydroxy-4-methylcoumarin (H-7): 65%. Yellow solid. M.p. 186 - 187 ^{o}C. Retention factor (R_f) 0.23 (SiO_2, hexane/EtOAc, 70:30). Molar absorption coefficient (ε) 16,271 $M^{-1}cm^{-1}$. ATR-FTIR (neat, cm^{-1}); 3151 (OH str.) 3122 (=C-H str.), 3006 (=C-H str. of aromatic), 1673 (C=O str.), 1583 (C=C str.) and 1065 (C-O str.). ^{1}H NMR (d_6-DMSO, δ, ppm); 10.56 (br, s, 1H, -OH), 7.57 (d, J = 8.6 Hz, 1H, Ar-H), 6.78 (d, J = 8.8 Hz, 1H, Ar-H), 6.68 (s, 1H, Ar-H), 6.11 (s, 1H, =CH) and 2.31 (s, 3H, -CH_3); ^{13}C NMR (d_6-DMSO, δ, ppm); 161.5, 160.7, 155.2, 153.8, 126.9, 113.2, 112.4,110.6, 110.5 and 18.5. MS m/z: 177.033 [obtained M+1]$^+$, 176.169 [M cal].

7-Methoxy-4-methylcoumarin (M-7): 23%. Yellow solid. M.p. 159 - 160 ^{o}C. R_f 0.38 (SiO_2, hexane/EtOAc, 70:30). ε 15,496 $M^{-1}cm^{-1}$. ATR-FTIR (neat, cm^{-1}); 3061 (=C-H str.), 3019 (=C-H str. of aromatic), 2952 (-C-H str.), 1721 (C=O str.), 1605 (C=C str.), 1509 (C=C str.), 1217 (C-O str. of ether), 1065 (C-O str. of ester). ^{1}H NMR ($CDCl_3$, δ, ppm); 7.48 (d, J = 8.8 Hz, 1H, Ar-H), 6.84 (d, J = 8.8 Hz, 1H, Ar-H), 6.79 (s, 1H, Ar-H), 6.10 (s, 1H, =CH), 3.85 (s, 1H, OCH_3) and 2.38 (s, 3H, CH_3); ^{13}C NMR ($CDCl_3$, δ, ppm); 162.6, 161.3, 155.2, 152.6, 125.5, 113.5, 112.3, 111.9, 100.8, 55.7 and 18.7. MS m/z: 191.053 [obtained M+1]$^+$, 190.195 [M cal].

4-Methyl-7-octyloxycoumarin (O-7): 78%. Yellow wax. M.p. 40 - 41 ^{o}C. R_f 0.69 (SiO_2, hexane/EtOAc, 70:30). ε 16,243 $M^{-1}cm^{-1}$. ATR-FTIR (neat, cm^{-1}); 2921, 2853 (-C-H str.), 1720 (C=O str.), 1607 (C=C str.), 1505 (C=C str.), 1138 (C-O str. of ether), 1063 (C-O str. of ester). ^{1}H NMR ($CDCl_3$, δ, ppm); 7.45 (d, J = 8.8 Hz, 1H, Ar-H), 6.83 (d, J = 8.8 Hz, 1H, Ar-H), 6.77 (d, J = 2.4 Hz, 1H, Ar-H), 6.09 (s, 1H, =CH), 3.98 (t, J = 6.4 Hz, 2H, -$OCH_2C_7H_{15}$), 2.36 (s, 3H, -CH_3) and 1.85 - 0.81 (m, 15H, -C_7H_{15}); ^{13}C NMR ($CDCl_3$, δ, ppm); 162.2, 161.4, 155.2, 152.6, 125.4, 113.3, 112.6, 111.7, 101.3, 68.6, 31.8, 29.3, 29.2, 29.0, 25.9, 22.6, 18.7 and 14.1. MS m/z: 289.214 [obtained M+1]$^+$, 288.381 [M cal].

7,8-Dihydroxy-4-methylcoumarin (H-78): 72%. Yellow solid. M.p. 234 - 235 ^{o}C. R_f 0.11 (SiO_2, hexane/EtOAc, 70:30). ε 11,775 $M^{-1}cm^{-1}$. ATR-FTIR (neat, cm^{-1}); 3465 (OH str.), 3219 (=C-H str. of aromatic), 3106 (=C-H str. of aromatic), 2983 (-C-H str.), 1642 (C=O str.), 1578 (C=C str.) and 1057 (C-O str.). ^{1}H NMR (d_6-DMSO, δ, ppm); 10.07 (br, s, 1H, -OH), 9.28 (br, s, 1H, -OH), 7.01 (d, J = 8.6Hz, 1H, Ar-H), 6.77 (d, J = 8.4Hz, 1H, Ar-H), 6.04 (s, 1H, =CH) and 2.28 (s, 3H, -CH_3); ^{13}C NMR (d_6-DMSO, δ, ppm); 160.7, 154.4, 149.8, 143.7, 132.5, 115.9, 113.2, 112.5, 110.6 and 18.6. MS m/z: 193.068 [obtained M+1]$^+$, 192.168 [M cal].

5,7-Dihydroxy-4-methylcoumarin (H-57): 65%. Yellow solid. M.p. 285 - 286 ^{o}C. R_f 0.04 (SiO_2, hexane/EtOAc, 70:30). ε 13,324 $M^{-1}cm^{-1}$. ATR-FTIR (neat, cm^{-1}); 3419 (OH str.), 3126 (=C-H str.), 3029 (=C-H str. of aromatic), 2987 (-C-H str.), 1667 (C=O str.), 1556 (C=C str.), 1479 (C=C str.) and 1159 (C-O str.). ^{1}H NMR (d_6-Acetone, δ, ppm); 9.60 (br, s, 1H, -OH), 9.34 (br, s, 1H, -OH), 6.35 (s, 1H, Ar-H), 6.27 (s, 1H, Ar-H), 5.83 (s, 1H, =CH) and 2.55 (s, 3H, -CH_3); ^{13}C NMR (d_6-DMSO, δ, ppm); 161.5, 160.5, 158.4, 156.9, 155.4, 109.2, 102.5, 99.5, 94.9 and 23.9. MS m/z: 193.068 [obtained M+1]$^+$, 192.168 [M cal].

5,7-Dimethoxy-4-methylcoumarin (M-57): 68%. White solid. M.p. 173 - 174 ^{o}C. R_f 0.35 (SiO_2, hexane/EtOAc, 70:30). ε 15,810 $M^{-1}cm^{-1}$. ATR-FTIR (neat, cm^{-1}); 3003 (=C-H str. of aromatic), 2929 (-C-H str.), 1727 (C=O str.), 1605 (C=C str.), 1149, 1110 (C-O str. of ether) and 1065 (C-O str. of ester). ^{1}H NMR ($CDCl_3$, δ, ppm); 6.41 (s, 1H, Ar-H), 6.27 (s, 1H, Ar-H), 5.93 (s, 1H, =CH), 3.83 (s, 1H, -OCH_3), 2.51 (s, 3H, -OCH_3) and 1.73 (s, 1H, CH_3); ^{13}C NMR ($CDCl_3$, δ, ppm); 161.1, 162.7, 159.1, 156.9, 154.5, 111.3, 104.8, 95.4, 93.3, 55.7, 55.7 and 24.2. MS m/z: 221.089 [obtained M+1]$^+$, 220.221 [M cal].

6,7-Dimethoxy-4-methylcoumarin (M-67): 27%. White solid. M.p. 135 - 136 ^{o}C. R_f 0.14 (SiO_2, hexane/EtOAc, 70:30). ε 11,684 $M^{-1}cm^{-1}$. ATR-FTIR (neat, cm^{-1}); 3046 (=C-H str. of aromatic), 2985, 2931, 2837 (-C-H str.), 1711 (C=O str.), 1613 (C=C str.), 1512 (C=C str.), 1276, 1158 (C-O str. of ether) and 1067 (s, C-O str. of ester). ^{1}H NMR ($CDCl_3$, δ, ppm); 6.85 (s, 1H, Ar-H), 6.72 (s, 1H, Ar-H), 6.08 (s, 1H, =CH) and 2.39 (s, 3H, -CH_3); ^{13}C NMR ($CDCl_3$, δ, ppm); 161.4, 152.6, 152.5, 149.2, 146.0, 112.4, 112.1, 105.0, 99.9, 56.3, 56.3 and 18.9. MS m/z: 243.081 [obtained M+23]$^+$, 220.221 [M cal].

Text file of the optimized 3D structure of the dimer of EH-67 (Hyperchem 7)

HyperChem
Geometry optimization, SemiEmpirical, molecule = C:\Documents and Settings\customer\Desktop\hyperchem\dimer of EH-67-4.hin.
PM3
PolakRibiere optimizer
Convergence limit = 0.0100000 Iteration limit = 50
Accelerate convergence = YES
Optimization algorithm = Polak-Ribiere
Criterion of RMS gradient = 0.1000 kcal/(A mol) Maximum cycles = 2175
RHF Calculation:

Singlet state calculation
Number of electrons = 344
Number of Double Occupied Levels = 172
Charge on the System = 0
Total Orbitals = 328

Starting PM3 calculation with 328 orbitals

E=0.0000 Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=1 Diff=63855.80204]
E=0.0000 Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=2 Diff=372.50100]
E=0.0000 Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=3 Diff=54.49106]
E=0.0000 Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=4 Diff=11.56627]
E=0.0000 Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=5 Diff=1.03660]
E=0.0000 Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=6 Diff=0.24670]
E=0.0000 Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=7 Diff=0.10077]
E=0.0000 Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=8 Diff=0.01836]
E=0.0000 Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=9 Diff=0.00106]
E=-14323.7191 Grad=0.097 Conv=YES(0 cycles 1 points) [Iter=1 Diff=0.00000]

ENERGIES AND GRADIENT
Total Energy = -228976.8446502 (kcal/mol)
Total Energy = -364.890543252 (a.u.)
Binding Energy = -14323.7191122 (kcal/mol)
Isolated Atomic Energy = -214653.1255380 (kcal/mol)
Electronic Energy = -3596330.0775700 (kcal/mol)
Core-Core Interaction = 3367353.2329198 (kcal/mol)
Heat of Formation = -413.5091122 (kcal/mol)
Gradient = 0.0973491 (kcal/mol/Ang)

MOLECULAR POINT GROUP
C1

EIGENVALUES(eV)

Symmetry:	1 A	2 A	3 A	4 A	5 A
Eigenvalue:	-44.875061	-42.906612	-42.257526	-41.139751	-40.876259

Symmetry:	6 A	7 A	8 A	9 A	10 A
Eigenvalue:	-40.371109	-39.719563	-38.795212	-38.600304	-37.469254

Symmetry:	11 A	12 A	13 A	14 A	15 A
Eigenvalue:	-37.159336	-37.020721	-36.716259	-36.026741	-35.684929

Symmetry:	16 A	17 A	18 A	19 A	20 A

Eigenvalue:	-35.408714	-35.038952	-34.535320	-34.288685	-32.081879
Symmetry:	21 A	22 A	23 A	24 A	25 A
Eigenvalue:	-31.879143	-31.240995	-30.890764	-30.859276	-30.521347
Symmetry:	26 A	27 A	28 A	29 A	30 A
Eigenvalue:	-29.285208	-28.753849	-28.400866	-28.215801	-27.930532
Symmetry:	31 A	32 A	33 A	34 A	35 A
Eigenvalue:	-27.434753	-27.015152	-26.539385	-25.806587	-25.448765
Symmetry:	36 A	37 A	38 A	39 A	40 A
Eigenvalue:	-24.347672	-24.084171	-23.866587	-23.842350	-23.296528
Symmetry:	41 A	42 A	43 A	44 A	45 A
Eigenvalue:	-23.258936	-22.972261	-22.736303	-22.501358	-22.314377
Symmetry:	46 A	47 A	48 A	49 A	50 A
Eigenvalue:	-22.264120	-21.982531	-21.865177	-21.649086	-21.512369
Symmetry:	51 A	52 A	53 A	54 A	55 A
Eigenvalue:	-20.869610	-20.837622	-20.720392	-20.375446	-20.132452
Symmetry:	56 A	57 A	58 A	59 A	60 A
Eigenvalue:	-19.742813	-19.623632	-19.326096	-19.097673	-18.960621
Symmetry:	61 A	62 A	63 A	64 A	65 A
Eigenvalue:	-18.660545	-18.494577	-18.247934	-18.060591	-17.886328
Symmetry:	66 A	67 A	68 A	69 A	70 A
Eigenvalue:	-17.439085	-17.263132	-17.140793	-16.915689	-16.870651
Symmetry:	71 A	72 A	73 A	74 A	75 A
Eigenvalue:	-16.824800	-16.763443	-16.641529	-16.561588	-16.481707
Symmetry:	76 A	77 A	78 A	79 A	80 A
Eigenvalue:	-16.364256	-16.303303	-16.296141	-16.195910	-16.157837
Symmetry:	81 A	82 A	83 A	84 A	85 A
Eigenvalue:	-16.063566	-16.003561	-15.901015	-15.807764	-15.773310
Symmetry:	86 A	87 A	88 A	89 A	90 A
Eigenvalue:	-15.643689	-15.620778	-15.534667	-15.398162	-15.379847
Symmetry:	91 A	92 A	93 A	94 A	95 A
Eigenvalue:	-15.308391	-15.236953	-15.167840	-15.085799	-15.066725
Symmetry:	96 A	97 A	98 A	99 A	100 A
Eigenvalue:	-14.947688	-14.896455	-14.860745	-14.823191	-14.704031
Symmetry:	101 A	102 A	103 A	104 A	105 A
Eigenvalue:	-14.689554	-14.587900	-14.567878	-14.536782	-14.477372
Symmetry:	106 A	107 A	108 A	109 A	110 A
Eigenvalue:	-14.407774	-14.329296	-14.278560	-14.205961	-14.159431

Symmetry:	111 A	112 A	113 A	114 A	115 A
Eigenvalue:	-14.054877	-13.944592	-13.902613	-13.877948	-13.822707

Symmetry:	116 A	117 A	118 A	119 A	120 A
Eigenvalue:	-13.722523	-13.654029	-13.532920	-13.443342	-13.384642

Symmetry:	121 A	122 A	123 A	124 A	125 A
Eigenvalue:	-13.334540	-13.300450	-13.245397	-13.186399	-13.112423

Symmetry:	126 A	127 A	128 A	129 A	130 A
Eigenvalue:	-13.062754	-12.975987	-12.948813	-12.920347	-12.877932

Symmetry:	131 A	132 A	133 A	134 A	135 A
Eigenvalue:	-12.851955	-12.761524	-12.746979	-12.661724	-12.621163

Symmetry:	136 A	137 A	138 A	139 A	140 A
Eigenvalue:	-12.587151	-12.556046	-12.511679	-12.502710	-12.419311

Symmetry:	141 A	142 A	143 A	144 A	145 A
Eigenvalue:	-12.352450	-12.276207	-12.242054	-12.177514	-12.171997

Symmetry:	146 A	147 A	148 A	149 A	150 A
Eigenvalue:	-12.097619	-12.076070	-12.008366	-11.889535	-11.845014

Symmetry:	151 A	152 A	153 A	154 A	155 A
Eigenvalue:	-11.794250	-11.739104	-11.700638	-11.619184	-11.582847

Symmetry:	156 A	157 A	158 A	159 A	160 A
Eigenvalue:	-11.510509	-11.410488	-11.400829	-11.370610	-11.232810

Symmetry:	161 A	162 A	163 A	164 A	165 A
Eigenvalue:	-11.217950	-11.156642	-11.111074	-11.054314	-10.942421

Symmetry:	166 A	167 A	168 A	169 A	170 A
Eigenvalue:	-10.930963	-10.836268	-10.641062	-9.955121	-9.911338

Symmetry:	171 A	172 A	173 A	174 A	175 A
Eigenvalue:	-9.306362	-9.201542	-0.375232	-0.276869	-0.224417

Symmetry:	176 A	177 A	178 A	179 A	180 A
Eigenvalue:	-0.106161	0.595983	0.814166	1.259173	1.469181

Symmetry:	181 A	182 A	183 A	184 A	185 A
Eigenvalue:	1.758302	1.851446	1.928135	2.011019	2.068769

Symmetry:	186 A	187 A	188 A	189 A	190 A
Eigenvalue:	2.143586	2.190000	2.334582	2.368198	2.553112

Symmetry:	191 A	192 A	193 A	194 A	195 A
Eigenvalue:	2.665951	2.706729	2.811599	2.829330	2.892839

Symmetry:	196 A	197 A	198 A	199 A	200 A
Eigenvalue:	3.003141	3.088890	3.105106	3.172804	3.221043

Symmetry:	201 A	202 A	203 A	204 A	205 A
Eigenvalue:	3.250672	3.274386	3.299556	3.337359	3.355791

Symmetry:	206 A	207 A	208 A	209 A	210 A
Eigenvalue:	3.382210	3.399763	3.415379	3.443559	3.457056

Symmetry:	211 A	212 A	213 A	214 A	215 A
Eigenvalue:	3.465472	3.489036	3.503520	3.525632	3.554517

Symmetry:	216 A	217 A	218 A	219 A	220 A
Eigenvalue:	3.576111	3.589844	3.605505	3.608825	3.652972

Symmetry:	221 A	222 A	223 A	224 A	225 A
Eigenvalue:	3.682415	3.694726	3.713594	3.736015	3.743546

Symmetry:	226 A	227 A	228 A	229 A	230 A
Eigenvalue:	3.746600	3.772011	3.784936	3.801041	3.809765

Symmetry:	231 A	232 A	233 A	234 A	235 A
Eigenvalue:	3.820483	3.846165	3.862916	3.863981	3.878346

Symmetry:	236 A	237 A	238 A	239 A	240 A
Eigenvalue:	3.895996	3.915875	3.921990	3.954268	3.963914

Symmetry:	241 A	242 A	243 A	244 A	245 A
Eigenvalue:	3.974249	3.981852	3.996397	4.015051	4.045923

Symmetry:	246 A	247 A	248 A	249 A	250 A
Eigenvalue:	4.054005	4.071146	4.089569	4.096289	4.108818

Symmetry:	251 A	252 A	253 A	254 A	255 A
Eigenvalue:	4.120926	4.123839	4.139019	4.144416	4.156291

Symmetry:	256 A	257 A	258 A	259 A	260 A
Eigenvalue:	4.181939	4.188220	4.195916	4.205617	4.223155

Symmetry:	261 A	262 A	263 A	264 A	265 A
Eigenvalue:	4.231722	4.272217	4.286961	4.304687	4.327969

Symmetry:	266 A	267 A	268 A	269 A	270 A
Eigenvalue:	4.355357	4.369600	4.385199	4.389717	4.399780

Symmetry:	271 A	272 A	273 A	274 A	275 A
Eigenvalue:	4.413527	4.426725	4.458828	4.483694	4.497799

Symmetry:	276 A	277 A	278 A	279 A	280 A
Eigenvalue:	4.512997	4.522321	4.541050	4.558966	4.570983

Symmetry:	281 A	282 A	283 A	284 A	285 A
Eigenvalue:	4.585343	4.626620	4.633603	4.656351	4.676205

Symmetry:	286 A	287 A	288 A	289 A	290 A
Eigenvalue:	4.689061	4.722444	4.744257	4.756305	4.767586

Symmetry:	291 A	292 A	293 A	294 A	295 A
Eigenvalue:	4.795281	4.820664	4.831824	4.849032	4.883083

Symmetry:	296 A	297 A	298 A	299 A	300 A

Eigenvalue: 4.889971 4.895191 4.921332 4.963223 5.002479

Symmetry: 301 A 302 A 303 A 304 A 305 A
Eigenvalue: 5.013305 5.029659 5.033594 5.060184 5.065260

Symmetry: 306 A 307 A 308 A 309 A 310 A
Eigenvalue: 5.079001 5.090429 5.100073 5.138269 5.154849

Symmetry: 311 A 312 A 313 A 314 A 315 A
Eigenvalue: 5.193176 5.240541 5.256018 5.278534 5.289892

Symmetry: 316 A 317 A 318 A 319 A 320 A
Eigenvalue: 5.293774 5.344119 5.404444 5.510440 5.605680

Symmetry: 321 A 322 A 323 A 324 A 325 A
Eigenvalue: 5.658188 5.840594 5.905499 5.999612 6.210755

Symmetry: 326 A 327 A 328 A
Eigenvalue: 6.396995 6.662723 6.762603

ATOMIC ORBITAL ELECTRON POPULATIONS

AO:	1 S C	1 Px C	1 Py C	1 Pz C	2 S C
	1.182365	0.950926	0.982528	0.965189	1.171320
AO:	2 Px C	2 Py C	2 Pz C	3 S C	3 Px C
	1.005280	1.000305	0.953905	1.164971	1.005333
AO:	3 Py C	3 Pz C	4 S C	4 Px C	4 Py C
	0.985672	0.954397	1.162051	0.997814	0.993684
AO:	4 Pz C	5 S C	5 Px C	5 Py C	5 Pz C
	0.955444	1.167174	0.947974	0.946497	0.856789
AO:	6 S C	6 Px C	6 Py C	6 Pz C	7 S C
	1.177960	0.993744	1.010605	0.952462	1.165238
AO:	7 Px C	7 Py C	7 Pz C	8 S C	8 Px C
	0.903337	0.913347	0.934967	1.172105	0.922181
AO:	8 Py C	8 Pz C	9 S C	9 Px C	9 Py C
	0.959084	0.921638	1.176794	0.962963	0.981136
AO:	9 Pz C	10 S C	10 Px C	10 Py C	10 Pz C
	0.959560	1.172093	1.005811	1.018176	0.935039
AO:	11 S O	11 Px O	11 Py O	11 Pz O	12 S C
	1.824964	1.483537	1.531273	1.318982	1.187830
AO:	12 Px C	12 Py C	12 Pz C	13 S C	13 Px C
	0.801524	0.832422	0.821904	1.189597	0.929741
AO:	13 Py C	13 Pz C	14 S C	14 Px C	14 Py C
	0.930078	0.928764	1.192017	0.969797	0.958524
AO:	14 Pz C	15 S O	15 Px O	15 Py O	15 Pz O
	0.985487	1.840648	1.451409	1.729881	1.181762

AO:	17 S C	17 Px C	17 Py C	17 Pz C	18 S C
	1.144839	0.966669	1.021278	0.989173	1.187441
AO:	18 Px C	18 Py C	18 Pz C	19 S C	19 Px C
	0.928382	0.908181	0.950533	1.190819	0.932928
AO:	19 Py C	19 Pz C	20 S C	20 Px C	20 Py C
	0.964779	1.010020	1.190930	0.875331	0.793690
AO:	20 Pz C	21 S C	21 Px C	21 Py C	21 Pz C
	0.784942	1.171715	0.974868	0.985402	1.031628
AO:	22 S C	22 Px C	22 Py C	22 Pz C	23 S C
	1.160593	0.875399	0.896369	0.946583	1.175606
AO:	23 Px C	23 Py C	23 Pz C	24 S C	24 Px C
	1.007674	0.969585	1.048074	1.175783	0.979134
AO:	24 Py C	24 Pz C	25 S C	25 Px C	25 Py C
	0.932569	0.974110	1.165910	0.897835	0.946670
AO:	25 Pz C	26 S C	26 Px C	26 Py C	26 Pz C
	0.988137	1.167727	0.931742	0.883554	0.906060
AO:	27 S C	27 Px C	27 Py C	27 Pz C	34 S O
	1.146426	1.020382	1.014144	0.944438	1.834459
AO:	34 Px O	34 Py O	34 Pz O	38 S C	38 Px C
	1.579411	1.357556	1.409876	1.167428	0.890543
AO:	38 Py C	38 Pz C	39 S C	39 Px C	39 Py C
	0.957892	0.937466	1.168314	0.924076	0.978203
AO:	39 Pz C	40 S O	40 Px O	40 Py O	40 Pz O
	0.884040	1.843748	1.268316	1.173523	1.917031
AO:	42 S C	42 Px C	42 Py C	42 Pz C	43 S C
	1.186425	0.956881	1.023779	0.941274	1.187199
AO:	43 Px C	43 Py C	43 Pz C	45 S O	45 Px O
	1.027273	0.940490	0.952701	1.839236	1.334252
AO:	45 Py O	45 Pz O	46 S C	46 Px C	46 Py C
	1.227751	1.795378	1.165995	0.985196	0.838475
AO:	46 Pz C	47 S C	47 Px C	47 Py C	47 Pz C
	0.956752	1.167134	0.977121	1.025225	0.940398
AO:	48 S C	48 Px C	48 Py C	48 Pz C	49 S C
	1.166947	0.975225	0.993580	0.982919	1.162786
AO:	49 Px C	49 Py C	49 Pz C	50 S C	50 Px C
	0.972007	0.983626	0.994162	1.142748	0.989664
AO:	50 Py C	50 Pz C	56 S C	56 Px C	56 Py C

1.009764 0.986418 1.161568 1.007820 0.942993

AO: 56 Pz C 57 S C 57 Px C 57 Py C 57 Pz C
0.986887 1.142233 1.012043 0.964151 1.005669

AO: 61 S C 61 Px C 61 Py C 61 Pz C 62 S C
1.163801 0.952972 1.025271 0.971349 1.138081

AO: 62 Px C 62 Py C 62 Pz C 64 S C 64 Px C
1.000097 1.007492 0.963768 1.138119 0.993850

AO: 64 Py C 64 Pz C 73 S C 73 Px C 73 Py C
0.982308 0.995278 1.170106 1.012501 0.814505

AO: 73 Pz C 74 S C 74 Px C 74 Py C 74 Pz C
0.964915 1.189991 0.965955 0.979181 0.984052

AO: 75 S C 75 Px C 75 Py C 75 Pz C 76 S C
1.173121 0.958138 0.969736 1.030230 1.163284

AO: 76 Px C 76 Py C 76 Pz C 77 S C 77 Px C
0.957165 1.004742 0.980097 1.164182 0.961480

AO: 77 Py C 77 Pz C 79 S C 79 Px C 79 Py C
1.017017 0.977075 1.163961 0.949871 1.031071

AO: 79 Pz C 80 S C 80 Px C 80 Py C 80 Pz C
0.970225 1.152029 1.005343 1.022060 0.970860

AO: 83 S C 83 Px C 83 Py C 83 Pz C 90 S C
1.138464 0.954053 1.009061 1.008732 1.165421

AO: 90 Px C 90 Py C 90 Pz C 91 S C 91 Px C
0.998739 0.984229 0.957227 1.163875 1.007994

AO: 91 Py C 91 Pz C 92 S C 92 Px C 92 Py C
0.966840 0.966524 1.165049 0.959093 0.969048

AO: 92 Pz C 93 S C 93 Px C 93 Py C 93 Pz C
1.017671 1.159082 0.953538 0.968531 1.020844

AO: 94 S C 94 Px C 94 Py C 94 Pz C 95 S C
1.162358 0.941380 0.995931 1.003258 1.145824

AO: 95 Px C 95 Py C 95 Pz C 99 S C 99 Px C
0.985511 1.000058 1.007431 1.141064 1.000208

AO: 99 Py C 99 Pz C 141 S O 141 Px O 141 Py O
0.968216 1.010022 1.825502 1.410550 1.362049

AO: 141 Pz O 142 S O 142 Px O 142 Py O 142 Pz O
1.564364 1.862632 1.314504 1.265556 1.857339

AO: 144 S O 144 Px O 144 Py O 144 Pz O 31 S H
1.862412 1.273524 1.553839 1.608030 0.945354

AO:	63	S H	32	S H	65	S H	66	S H	67	S H
	0.961716		0.888793		0.962244		0.961692		0.947883	
AO:	68	S H	69	S H	70	S H	71	S H	72	S H
	0.948797		0.935082		0.922446		0.905758		0.876598	
AO:	44	S H	33	S H	16	S H	35	S H	36	S H
	0.874917		0.857068		0.858931		0.941658		0.943412	
AO:	78	S H	37	S H	28	S H	81	S H	82	S H
	0.934739		0.943053		0.888691		0.943399		0.953109	
AO:	51	S H	84	S H	85	S H	86	S H	87	S H
	0.959981		0.961961		0.961075		0.942786		0.929268	
AO:	88	S H	89	S H	52	S H	53	S H	54	S H
	0.936626		0.935995		0.958227		0.940777		0.945831	
AO:	55	S H	29	S H	30	S H	96	S H	97	S H
	0.932847		0.942182		0.942356		0.950331		0.957439	
AO:	98	S H	58	S H	100	S H	101	S H	102	S H
	0.910016		0.953651		0.950157		0.940709		0.946280	
AO:	103	S H	104	S H	105	S H	106	S H	107	S H
	0.933541		0.949103		0.938113		0.952549		0.937072	
AO:	108	S H	109	S H	110	S H	111	S H	112	S H
	0.947887		0.935115		0.908399		0.948932		0.962141	
AO:	113	S H	114	S H	115	S H	116	S H	117	S H
	0.949969		0.932539		0.957447		0.962369		0.962309	
AO:	118	S H	119	S H	120	S H	121	S H	122	S H
	0.950124		0.943319		0.946771		0.956318		0.940058	
AO:	123	S H	124	S H	125	S H	126	S H	127	S H
	0.946201		0.948615		0.940105		0.933530		0.940546	
AO:	128	S H	129	S H	130	S H	131	S H	132	S H
	0.935121		0.961680		0.962984		0.947271		0.948471	
AO:	133	S H	134	S H	135	S H	136	S H	137	S H
	0.934396		0.961425		0.945388		0.941242		0.949142	
AO:	138	S H	139	S H	140	S H	59	S H	60	S H
	0.945811		0.964180		0.949168		0.957576		0.948632	
AO:	143	S H	41	S H	145	S H				
	1.000233		0.959819		0.999621					

NET CHARGES AND COORDINATES

Atom	Z	Charge	Coordinates(Angstrom)			Mass
			x	y	z	
1	6	-0.081007	0.16689	4.79796	6.43005	12.01100
2	6	-0.130809	-0.22843	4.98304	4.96347	12.01100

3	6	-0.110373	0.55810	6.09738	4.29232	12.01100
4	6	-0.108993	0.23847	6.17394	2.80844	12.01100
5	6	0.081567	-0.19286	-2.44499	3.86389	12.01100
6	6	-0.134771	-1.21706	-3.32613	4.21029	12.01100
7	6	0.083111	-1.61857	-3.41058	5.54905	12.01100
8	6	0.024992	0.44112	-1.67149	4.86001	12.01100
9	6	-0.080454	0.01375	-1.76655	6.18715	12.01100
10	6	-0.131120	-1.02634	-2.62760	6.54941	12.01100
11	8	-0.158754	-2.61854	-4.34149	5.76328	15.99900
12	6	0.356320	-3.09352	-4.53397	7.03104	12.01100
13	6	0.021820	-1.45240	-2.74470	7.98100	12.01100
14	6	-0.105824	-2.65703	-3.71066	8.20562	12.01100
15	8	-0.203700	0.05674	-2.27003	2.51449	15.99900
17	6	-0.121959	-0.25599	-3.12380	8.83669	12.01100
18	6	0.025463	-2.34387	-1.55417	8.55464	12.01100
19	6	-0.098546	-3.55578	-2.52922	8.64772	12.01100
20	6	0.355107	-4.73719	-2.19845	7.77926	12.01100
21	6	-0.163612	-2.55806	-0.38781	7.64832	12.01100
22	6	0.121055	-3.70994	-0.26080	6.86647	12.01100
23	6	-0.200938	-3.89691	0.82231	5.99496	12.01100
24	6	-0.061596	-1.59430	0.62404	7.58616	12.01100
25	6	0.001448	-1.74556	1.70124	6.71837	12.01100
26	6	0.110917	-2.90390	1.79799	5.90393	12.01100
27	6	-0.125391	-1.91675	-1.06225	9.92810	12.01100
34	8	-0.181302	-2.96866	2.90512	5.09657	15.99900
38	6	0.046672	1.22479	-2.93407	2.03232	12.01100
39	6	0.045368	-3.91775	2.87907	4.03288	12.01100
40	8	-0.202618	1.57225	-0.92311	4.55604	15.99900
42	6	-0.108359	1.34397	-2.54998	0.55176	12.01100
43	6	-0.107663	-3.77175	4.21349	3.28802	12.01100
45	8	-0.196617	-0.65844	2.54574	6.57197	15.99900
46	6	0.053582	-0.81580	3.84810	7.13397	12.01100
47	6	-0.109878	-4.51418	4.13778	1.94900	12.01100
48	6	-0.118671	-3.63941	3.59309	0.82972	12.01100
49	6	-0.112582	-2.50515	4.55180	0.49831	12.01100
50	6	-0.128594	-1.56318	3.97893	-0.53431	12.01100
56	6	-0.099269	-4.29216	5.37443	4.13917	12.01100
57	6	-0.124095	-4.00125	6.70926	3.48917	12.01100
61	6	-0.113393	1.62109	4.33087	6.53553	12.01100
62	6	-0.109438	2.17659	4.45110	7.93582	12.01100
64	6	-0.109555	1.06240	7.23537	2.11663	12.01100
73	6	0.037974	1.38187	0.48351	4.47680	12.01100
74	6	-0.119180	0.92130	0.95880	3.09074	12.01100
75	6	-0.131226	1.44973	2.36911	2.81624	12.01100
76	6	-0.105289	2.96170	2.39647	2.67306	12.01100
77	6	-0.119755	3.42062	1.69510	1.40557	12.01100
79	6	-0.115129	-0.60272	0.95935	2.98200	12.01100
80	6	-0.150292	-1.04742	1.10312	1.54577	12.01100
83	6	-0.110310	4.92759	1.62008	1.32324	12.01100
90	6	-0.105615	0.35280	-3.33477	-0.30927	12.01100
91	6	-0.105233	0.27490	-2.76258	-1.71787	12.01100
92	6	-0.110861	-0.32963	-1.36654	-1.75132	12.01100
93	6	-0.101995	-1.83699	-1.37021	-1.55260	12.01100
94	6	-0.102927	2.77504	-2.78373	0.06626	12.01100
95	6	-0.138825	3.75798	-1.87866	0.77150	12.01100
99	6	-0.119510	-2.42505	0.01098	-1.73701	12.01100

141	8	-0.162465	-4.76097	-1.15633	6.88764	15.99900
142	8	-0.300031	-3.86607	-5.46551	7.01745	15.99900
144	8	-0.297805	-5.81291	-2.75061	7.74080	15.99900
31	1	0.054646	-0.52416	-3.16881	9.90533	1.00800
63	1	0.038284	3.22714	4.13515	7.97153	1.00800
32	1	0.111207	-3.93428	-2.65650	9.68781	1.00800
65	1	0.037756	0.81960	7.29353	1.04794	1.00800
66	1	0.038308	0.88829	8.22968	2.54883	1.00800
67	1	0.052117	-0.84540	6.37743	2.67000	1.00800
68	1	0.051203	0.34285	7.06888	4.78001	1.00800
69	1	0.064918	-1.31674	5.19437	4.88837	1.00800
70	1	0.077554	-0.06920	4.02575	4.41154	1.00800
71	1	0.094242	-2.68128	4.40382	3.06684	1.00800
72	1	0.123402	0.49824	-1.15121	6.95892	1.00800
44	1	0.125083	-0.70945	0.54638	8.23924	1.00800
33	1	0.142932	-4.81469	0.89119	5.39337	1.00800
16	1	0.141069	-1.70909	-3.93552	3.43982	1.00800
35	1	0.058342	-1.05738	-0.37685	9.83945	1.00800
36	1	0.056588	-2.73140	-0.51851	10.42211	1.00800
78	1	0.065261	0.71987	0.85513	5.28227	1.00800
37	1	0.056947	-1.61429	-1.89638	10.58146	1.00800
28	1	0.111309	-2.47503	-4.41511	9.05119	1.00800
81	1	0.056601	-0.82478	0.20108	0.95612	1.00800
82	1	0.046891	-2.13175	1.29578	1.47209	1.00800
51	1	0.040019	-0.79078	4.70612	-0.81454	1.00800
84	1	0.038039	5.38235	2.61861	1.28770	1.00800
85	1	0.038925	5.35443	1.09705	2.18967	1.00800
86	1	0.057214	3.41204	1.90708	3.56771	1.00800
87	1	0.070732	1.12957	3.06039	3.63145	1.00800
88	1	0.063374	0.95775	2.75154	1.89073	1.00800
89	1	0.064005	-1.01114	0.02279	3.41235	1.00800
52	1	0.041773	-2.09235	3.68643	-1.45086	1.00800
53	1	0.059223	-1.95171	4.78898	1.43898	1.00800
54	1	0.054169	-4.25685	3.41150	-0.07150	1.00800
55	1	0.067153	-4.86387	5.16097	1.67690	1.00800
29	1	0.057818	0.13943	-4.10431	8.54327	1.00800
30	1	0.057644	0.55606	-2.38994	8.73345	1.00800
96	1	0.049669	3.72469	-2.05028	1.86122	1.00800
97	1	0.042561	4.78536	-2.04917	0.43010	1.00800
98	1	0.089984	1.10096	-1.45365	0.42988	1.00800
58	1	0.046349	-4.41238	6.73869	2.46567	1.00800
100	1	0.049843	-2.31092	-2.07934	-2.26013	1.00800
101	1	0.059291	0.15492	-0.74723	-0.95988	1.00800
102	1	0.053720	-0.29902	-3.44666	-2.37199	1.00800
103	1	0.066459	-0.65021	-3.31753	0.16341	1.00800
104	1	0.050897	0.64834	-4.40212	-0.35098	1.00800
105	1	0.061887	2.12869	-2.59750	2.58877	1.00800
106	1	0.047451	-4.94316	2.73991	4.43134	1.00800
107	1	0.062928	-1.02358	1.78217	3.59930	1.00800
108	1	0.052113	-0.53179	1.95479	1.05773	1.00800
109	1	0.064885	2.41560	0.84308	4.67199	1.00800
110	1	0.091601	1.35624	0.27445	2.30787	1.00800
111	1	0.051068	3.32347	3.44293	2.68124	1.00800
112	1	0.037859	5.24862	1.07749	0.42423	1.00800
113	1	0.050031	3.01570	2.21765	0.51667	1.00800
114	1	0.067461	2.97741	0.66662	1.37195	1.00800

115	1	0.042553	-2.00368	0.73437	-1.02124	1.00800
116	1	0.037631	-3.51238	0.00240	-1.58837	1.00800
117	1	0.037691	-2.23485	0.40255	-2.74504	1.00800
118	1	0.049876	-0.08318	-0.88029	-2.71531	1.00800
119	1	0.056681	-2.08041	-1.75123	-0.53944	1.00800
120	1	0.053229	1.30814	-2.72578	-2.13329	1.00800
121	1	0.043682	-2.91932	6.89349	3.41320	1.00800
122	1	0.059942	-3.82350	5.33987	5.14363	1.00800
123	1	0.053799	3.52411	-0.81048	0.61465	1.00800
124	1	0.051385	3.05817	-3.84468	0.21575	1.00800
125	1	0.059895	2.79764	-2.61935	-1.03532	1.00800
126	1	0.066470	0.07684	5.78620	6.94786	1.00800
127	1	0.059454	2.23288	4.94426	5.83335	1.00800
128	1	0.064879	1.71890	3.28782	6.16827	1.00800
129	1	0.038320	1.62409	3.82620	8.65099	1.00800
130	1	0.037016	2.13200	5.48468	8.30456	1.00800
131	1	0.052729	-3.69242	2.02452	3.36276	1.00800
132	1	0.051529	-1.04636	3.07994	-0.15338	1.00800
133	1	0.065604	-3.22037	2.59758	1.11106	1.00800
134	1	0.038575	2.13797	7.02863	2.19823	1.00800
135	1	0.054612	0.41497	5.18530	2.33235	1.00800
136	1	0.058758	1.64739	5.91999	4.44793	1.00800
137	1	0.050858	-2.91872	5.51757	0.14591	1.00800
138	1	0.054189	-5.43005	3.52319	2.04933	1.00800
139	1	0.035820	-0.59121	3.77216	8.21546	1.00800
140	1	0.050832	-1.85422	4.21948	7.03163	1.00800
59	1	0.042424	-4.44216	7.53851	4.05464	1.00800
60	1	0.051368	-5.38133	5.25944	4.30820	1.00800
143	1	-0.000233	-6.60952	-6.16583	8.43210	1.00800
41	1	0.040181	1.12232	-4.02673	2.17077	1.00800
145	1	0.000379	-6.93962	-5.57161	8.59550	1.00800

ATOMIC GRADIENTS

Atom	Z	Gradients(kcal/mol/Angstrom)		
		x	y	z
1	6	-0.01340	0.03701	0.01401
2	6	0.02162	-0.00935	0.05230
3	6	0.01937	-0.00291	-0.01622
4	6	0.02892	0.03399	-0.05958
5	6	-0.01503	0.10499	0.07877
6	6	0.37703	0.27313	0.03675
7	6	-0.07931	0.01315	-0.06902
8	6	0.13874	-0.06469	-0.37679
9	6	-0.18004	-0.28006	0.16834
10	6	0.19953	0.35609	-0.09652
11	8	0.10935	0.07512	-0.04324
12	6	0.24162	0.19585	0.05030
13	6	-0.11368	-0.04459	-0.05255
14	6	-0.21491	0.02460	-0.39958
15	8	-0.00857	0.05345	0.20866
17	6	-0.03235	-0.02666	0.04599
18	6	-0.10424	0.04998	-0.03332
19	6	0.07081	0.11134	0.01043
20	6	-0.14762	-0.18918	-0.10798
21	6	-0.33455	-0.50622	0.00894
22	6	0.07764	-0.17143	0.07728

23	6	0.10585	0.21713	-0.07092
24	6	0.17530	0.62302	-0.40904
25	6	0.27656	-0.37070	0.55870
26	6	-0.09897	0.27782	-0.28573
27	6	-0.06071	-0.08284	-0.05409
34	8	-0.18609	-0.21203	0.05914
38	6	-0.00200	0.05099	0.05281
39	6	0.07866	-0.04370	0.10352
40	8	-0.22831	-0.00649	0.05646
42	6	-0.07178	-0.04023	-0.01264
43	6	-0.00390	0.05251	-0.05354
45	8	-0.20519	-0.02929	0.04132
46	6	-0.03514	-0.06393	-0.09083
47	6	-0.03226	0.05775	-0.04458
48	6	-0.08848	-0.00708	0.03008
49	6	-0.01608	0.06675	0.07470
50	6	-0.04389	-0.03017	0.00216
56	6	0.02514	0.03472	-0.01205
57	6	-0.00876	0.01422	0.02310
61	6	-0.02898	-0.01476	-0.00274
62	6	-0.03750	-0.03054	0.00260
64	6	0.05973	0.01210	-0.01381
73	6	0.05603	0.05688	0.00512
74	6	0.04484	0.04426	0.10202
75	6	0.01380	-0.06088	-0.02869
76	6	0.09017	-0.06146	-0.06236
77	6	0.07353	-0.04520	-0.05017
79	6	0.04168	0.05135	0.05017
80	6	0.00644	0.02383	-0.01824
83	6	0.01321	-0.00882	0.01319
90	6	0.00757	-0.03194	-0.00042
91	6	-0.00833	-0.02486	-0.02138
92	6	-0.07847	-0.03938	0.01384
93	6	-0.04302	-0.04902	0.04207
94	6	0.01836	-0.07953	0.03725
95	6	0.03606	0.01838	-0.02699
99	6	-0.00068	-0.08298	0.02470
141	8	0.10047	-0.04418	-0.01941
142	8	-0.13039	-0.19502	0.00139
144	8	0.13653	0.13742	0.04159
31	1	-0.03416	0.04207	-0.02089
63	1	0.00254	-0.04733	0.01665
32	1	-0.07291	-0.09090	-0.00020
65	1	0.03653	-0.03647	0.03182
66	1	0.06925	-0.02357	0.02888
67	1	0.02347	0.01898	0.01265
68	1	0.00596	0.00734	0.04102
69	1	-0.02309	-0.00931	0.00346
70	1	-0.00038	-0.05593	-0.00243
71	1	-0.03597	-0.01168	0.02214
72	1	0.10508	0.00875	0.14948
44	1	-0.02620	0.01145	-0.01365
33	1	-0.16689	-0.02668	0.05719
16	1	-0.01196	-0.00456	-0.11345
35	1	-0.06338	-0.00556	0.03747
36	1	-0.02355	-0.05020	-0.09622

78	1	0.04291	0.08863	-0.03300
37	1	-0.09074	-0.02929	-0.05801
28	1	0.07031	-0.15755	0.12549
81	1	-0.00537	-0.00155	0.00198
82	1	-0.05880	0.06986	0.00692
51	1	-0.00365	-0.00183	-0.00852
84	1	0.00251	-0.05150	-0.00943
85	1	0.00300	0.01830	-0.00834
86	1	0.01490	-0.00281	0.01866
87	1	0.00128	0.07846	0.01439
88	1	0.01120	0.01535	-0.06983
89	1	-0.02800	0.06329	0.01044
52	1	-0.01296	-0.01352	-0.03263
53	1	-0.00939	-0.00562	-0.00021
54	1	0.00739	-0.00417	0.05104
55	1	-0.01739	-0.04910	0.03706
29	1	0.00915	0.04039	-0.09541
30	1	0.13616	0.07427	-0.08058
96	1	-0.00708	0.01078	-0.00111
97	1	-0.01197	0.05679	-0.06128
98	1	-0.00467	0.03748	-0.04657
58	1	-0.00336	0.02209	-0.00069
100	1	-0.02473	-0.04779	0.09759
101	1	-0.01375	-0.06036	-0.02990
102	1	-0.05965	-0.07352	0.04229
103	1	-0.00342	0.00814	0.03788
104	1	-0.03946	-0.05549	0.04827
105	1	0.13360	0.16100	0.04986
106	1	-0.09855	0.05789	0.04198
107	1	-0.02726	0.07984	-0.00092
108	1	0.03423	0.04479	0.00263
109	1	0.06339	0.08177	0.04804
110	1	0.00605	-0.01753	-0.01220
111	1	0.03094	0.02892	-0.00058
112	1	0.00330	-0.00423	0.08569
113	1	0.02019	-0.05092	-0.00029
114	1	0.01364	-0.02030	0.04213
115	1	-0.02265	-0.08356	-0.02602
116	1	0.04713	-0.03025	0.04627
117	1	-0.04232	-0.09577	0.08062
118	1	-0.05514	-0.08766	0.03459
119	1	0.00971	-0.03601	0.03107
120	1	-0.07470	-0.08497	0.00546
121	1	0.06232	-0.00187	-0.00151
122	1	-0.01522	0.02291	0.01176
123	1	-0.06058	0.02545	-0.03339
124	1	0.02705	-0.00704	0.00076
125	1	0.00178	-0.02161	-0.08539
126	1	0.03669	0.08740	0.01181
127	1	0.03533	-0.00430	-0.00446
128	1	-0.01183	-0.09471	-0.02028
129	1	-0.04908	-0.04371	0.01471
130	1	0.02685	-0.04521	0.02108
131	1	-0.06331	-0.00001	0.03829
132	1	-0.00027	0.00281	-0.00912
133	1	-0.02650	0.01488	0.00017

134	1	0.02158	-0.03143	-0.01103
135	1	0.00399	0.00069	0.01751
136	1	0.04966	-0.06008	0.03056
137	1	-0.04168	0.02574	-0.04303
138	1	-0.02254	-0.04325	0.01129
139	1	-0.03690	0.00454	0.03719
140	1	0.00083	0.07019	-0.01086
59	1	0.02405	0.01869	0.00184
60	1	-0.04388	0.04502	0.01837
143	1	0.12265	0.13395	-0.06273
41	1	0.09214	0.00144	0.04713
145	1	0.14460	0.08265	-0.07471

Dipole (Debyes)	x	y	z	Total
Point-Chg.	4.145	4.404	1.330	6.193
sp Hybrid	-0.082	0.200	0.657	0.691
pd Hybrid	0.000	0.000	0.000	0.000
Sum	4.064	4.605	1.987	6.455