

Supplementary Information

Microwave-assisted phenolation of acid-insoluble Klason lignin and its application to adhesion

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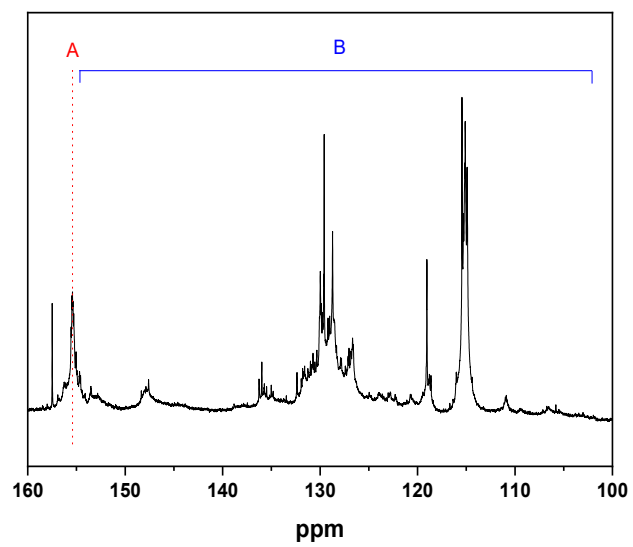


Fig. S1 ^{13}C NMR spectrum of the phenolated Klason lignin.

Table S1. ^{13}C NMR peak assignment for lignin unit after phenolation.

δ (ppm)	Assignment ^a
156.0 – 158.0	C1 in p-H (e and ne)
153.0 – 150.3	C2, C6 in S (e)
150.0 – 145.0	C1, C2 in G (e and ne); C2, C6 in S (ne)
136.3 – 131.0	C1 in S (e and ne); C4 in p-H, G and S (e and ne)
130.0 – 126.0	C3, C5 in p-H (e and ne)
119.0	C5 in G (e and ne)
116.0 – 114.0	C6 in G (e and ne), C2, C6 of p-H (e and ne)
111.7	C3 in G (e and ne)
104.0 – 103.0	C3, C5 in S (e and ne)

^a 'e' stand for etherified and 'ne' for non-etherified

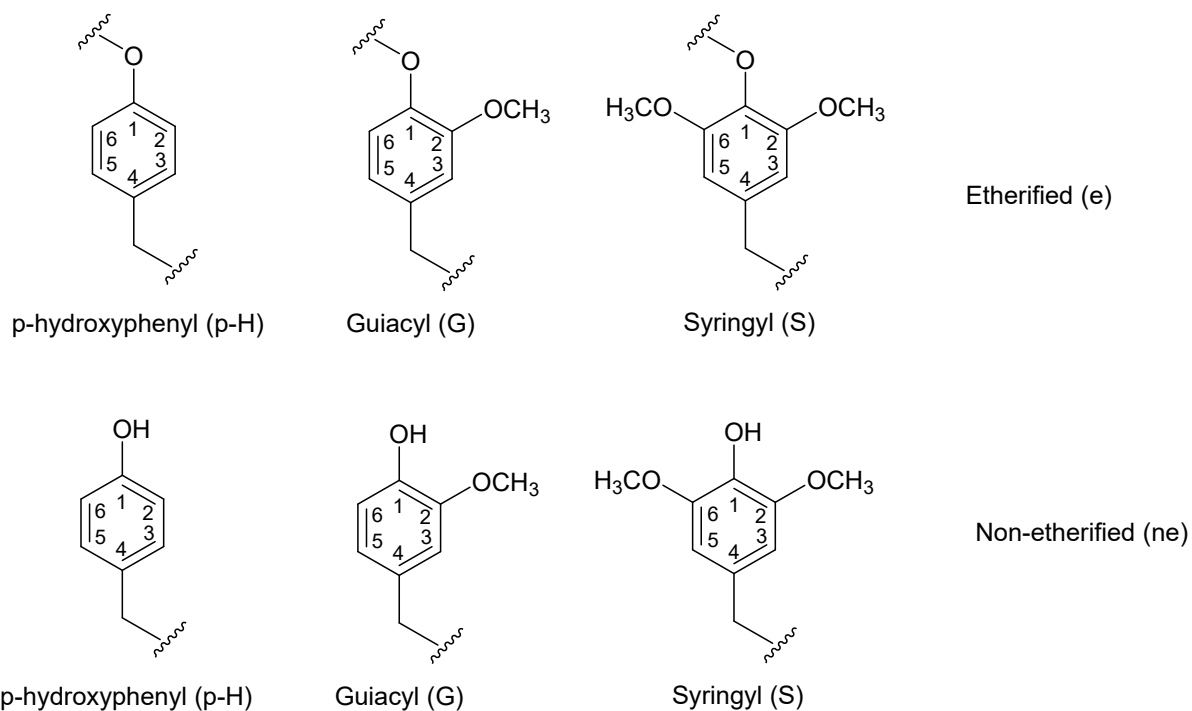
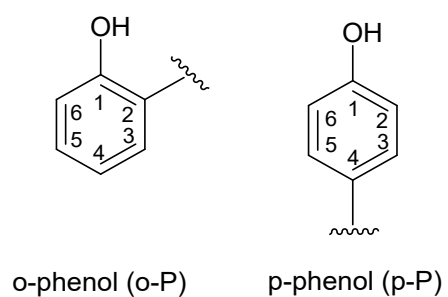


Table S2. ^{13}C NMR peak assignment for new phenyl group in lignin sample after phenolation.

δ (ppm)	Assignment
157.5	C1 of remained phenol
155	C1 of o-P and C1 of p-P
125 - 137	C2, C3, C5 of o-P; C3, C4, C5 of p-P
120	C4 of o-P
115	C6 of o-P and C2, C6 of p-P



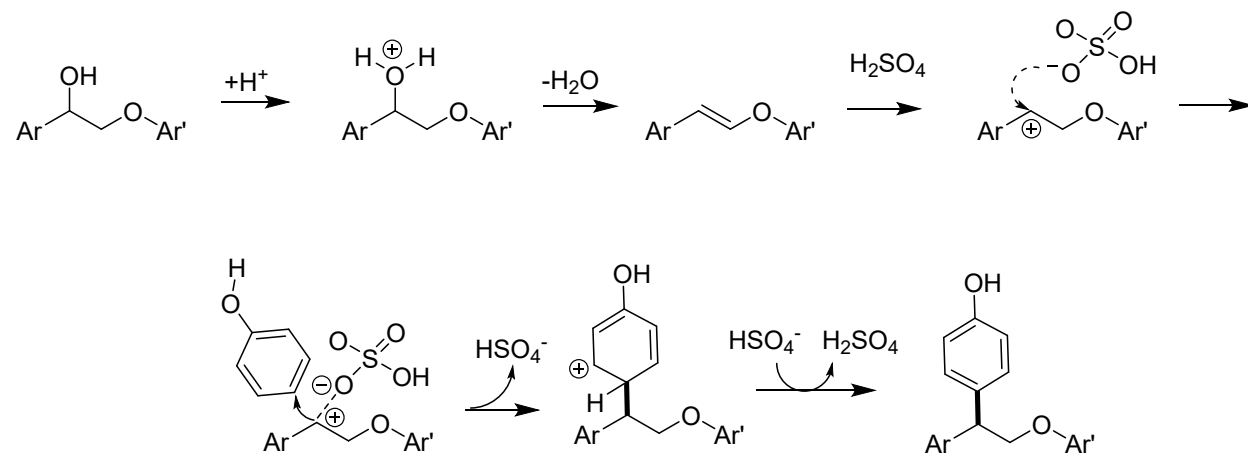
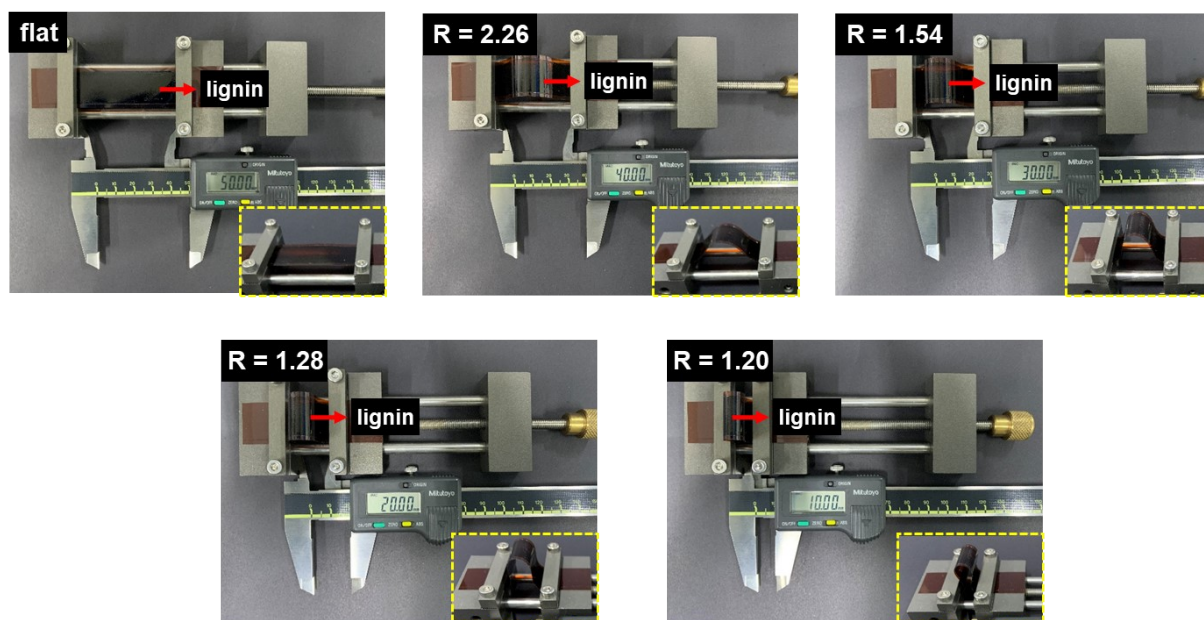


Fig. S2 Proposed reaction mechanism for the phenolation of lignin



$$R = \frac{L^2 + A^2}{2A} \text{ (cm)}$$

R : bending radius, L : half of device length, A : elevation distance

Fig. S3 Photographs showing the bending tests of the phenolated lignins on PEN and PI substrates as a function of the bending radius.

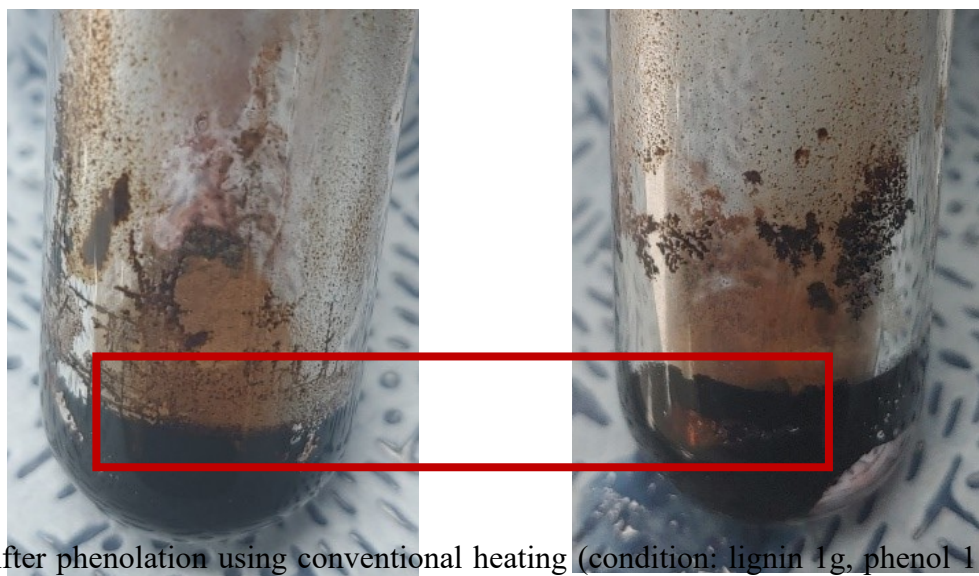


Fig. S4 After phenolation using conventional heating (condition: lignin 1g, phenol 1 g, 0.150 g H_2SO_4 as catalyst, 100°C for 4 hours (left) and 6 hours (right)), reaction mixture show two saperated phase, upper layer is original lignin, which have not dissolve into melted phenol (red box), and lower layer is the reacted mixture of lignin and phenol.

Reaction condition	Ar-H (mmol/g)
80°C, 10 min	0.86
80°C, 30 min	1.07
80°C, 60 min	1.36

Table S3: ^1H NMR and ^{31}P NMR analysis of phenolation lignin

Reaction at 80°C shown lignin solid particle after reaction, but there is still increasing in Ar-H due to the phenolation reaction.

Since guaiacyl and syringyl units contain methoxy functional group, the ratios of aromatic/methoxy (Ar/OMe) of phenolated lignin were calculated by ^{13}C -NMR, where the Ar/OMe increased with phenol to lignin feed ratios. Considering the similar Ar-H and Ar-OH concentration with increasing phenol to lignin feed ratios (Table 1), increasing Ar/OMe infers that lignin unit containing OMe might be substituted by phenol molecules.

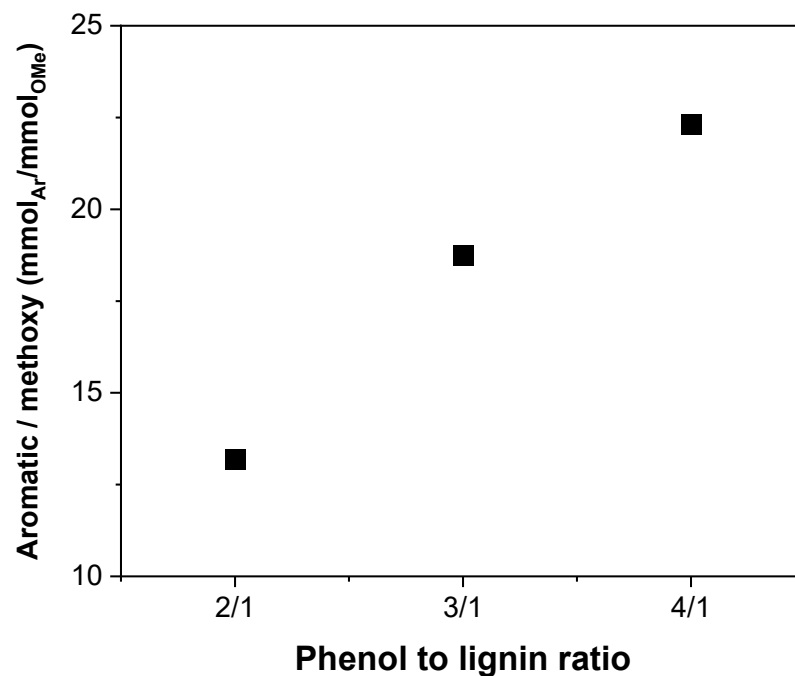


Fig. S5 Aromatic/methoxy of phenolated lignin along with phenol to lignin feed ratios. Reaction conditions: 100°C for 5 min

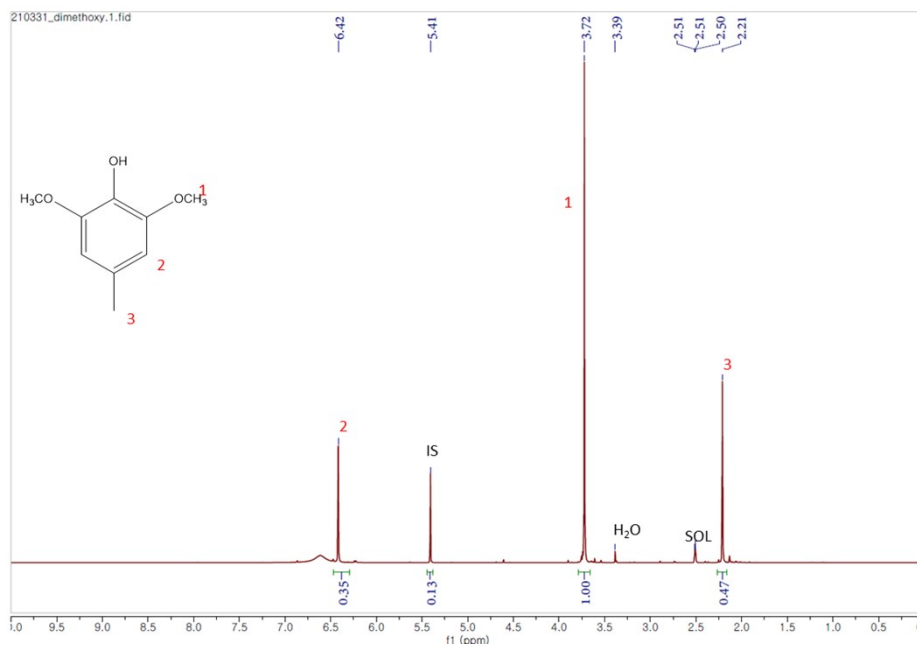


Fig. S6. The ¹H-NMR of 4-methyl-2,6-dimethoxyphenol under 15 wt.% H₂SO₄ at 100 °C for 5 min microwave irradiation.

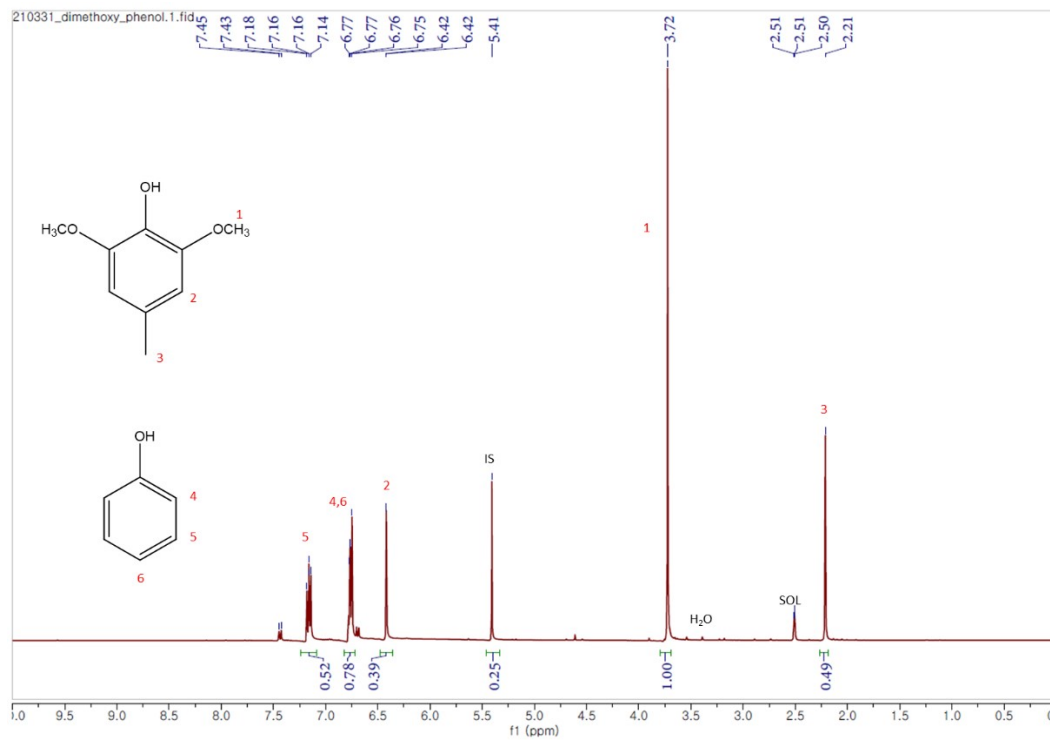


Fig. S7. The $^1\text{H-NMR}$ of product after reaction between 4-methyl-2,6-dimethoxyphenol and phenol (1/1, w/w) under 15 wt.% H_2SO_4 at 100 °C for 5 min microwave irradiation.

Table S4. M_w (g/mol) and polydispersity (\mathcal{D}) of the phenolated lignin as a function of reaction

Reaction time (min)	M_w (g/mol) ^a	Polydispersity (\mathcal{D})	T_g (°C)
5	1058	2.2	117
10	911	1.8	110
15	1013	1.8	115

time. Reaction conditions: 100°C, phenol:lignin = 2:1

Cartesian Coordinates Information

Result

1) Basis set : 6-31+G(d)

1-1) Normal Optimization (without electric field)

C	3.78837400	-2.00985800	0.70639400
C	3.33937600	-1.57148900	1.95451800
C	2.17440300	-0.80810000	2.05820700
C	1.43151500	-0.46253000	0.92182400
C	1.88447300	-0.91999100	-0.32614000
C	3.04441000	-1.68441500	-0.44506300
H	3.90684900	-1.82085100	2.84834700
H	1.84706200	-0.47920200	3.04115300
H	1.35035700	-0.69312700	-1.24470700
O	3.48264300	-2.04953300	-1.69895300
C	3.32225500	-3.44303000	-2.02699500
H	2.26066300	-3.71700300	-2.00574200
H	3.71276400	-3.56085900	-3.03950800
H	3.88671100	-4.07602400	-1.33554700
O	4.93256600	-2.73927300	0.53583700
H	5.35378100	-2.90425400	1.39585800
C	0.16401800	0.36291900	1.07218700
C	-1.06229800	-0.37557000	0.52308000
H	-0.96496700	-0.60314600	-0.54564500
H	-1.16273600	-1.32417100	1.06512400
O	-2.20486000	0.44833900	0.74554500
C	-3.44364600	-0.01716400	0.36567300
C	-3.67603100	-1.27077200	-0.20666800
C	-4.51937400	0.85539400	0.58979600
C	-4.98613700	-1.63813200	-0.54861900
H	-2.86587500	-1.96781500	-0.38985000
C	-5.81114400	0.46985200	0.24292900
H	-4.32725100	1.82723700	1.03617600
C	-6.07423700	-0.78637300	-0.33489800
H	-5.15093300	-2.61764600	-0.99231400
H	-6.63308300	1.15936000	0.42495900
C	-7.48335300	-1.19047800	-0.70716300
H	-7.91304300	-0.50740800	-1.45106600
H	-7.50829500	-2.20103800	-1.12791800
H	-8.14877500	-1.17403200	0.16534100
C	2.27087200	3.41815500	-0.81142200
C	1.33317300	2.69304100	-1.60755300
C	0.39234700	1.93161200	-0.99009900

C	0.27831200	1.83466000	0.48317100
C	1.27800000	2.63530900	1.22757300
C	2.22390500	3.39177600	0.61396000
H	1.38462700	2.76176700	-2.69001900
H	-0.33294200	1.39623200	-1.59573900
H	1.23464500	2.60685300	2.31301300
H	2.95037800	3.97688700	1.16736600
O	3.21799200	4.15503000	-1.34675000
H	3.20713800	4.13694500	-2.32379700
H	-0.01348900	0.51229600	2.14243700
H	-0.71560400	2.26360200	0.72848300

1-2) X-axis (Electric field : 0.0001 au)

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39744900
C	1.23213600	0.00000000	-0.68460600
O	-1.14035700	0.01331700	-0.75072300
C	1.20006500	-0.06357000	2.10663700
H	-0.94544200	0.03026600	1.93399800
C	2.43044900	-0.12818500	1.44072400
H	1.16601700	-0.07213400	3.19297800
C	2.42287500	-0.08116900	0.03720700
C	3.71212400	-0.27804800	2.24348500
H	3.34162500	-0.11268800	-0.54126100
O	1.28871200	-0.02317700	-2.06013300
C	0.87896500	1.18910000	-2.72352700
H	1.52820200	2.02062700	-2.42388500
H	0.99341800	0.99861200	-3.79219400
H	-0.16424900	1.42728100	-2.49867200
H	-1.92397900	0.01189500	-0.17555600
C	4.84836100	0.61091900	1.72983700
C	4.17772900	-1.79917000	2.38337700
H	3.51088100	0.04432700	3.27064100
H	5.16218200	0.35120000	0.71211500
H	4.50013100	1.65100000	1.72717800
O	5.95207500	0.46004300	2.62447900
C	7.10327100	1.17090300	2.38598100
C	7.27539600	2.07116500	1.33018700
C	8.15408900	0.95381200	3.29117700
C	8.49831400	2.74415600	1.19213100
H	6.48123300	2.26498700	0.61806100
C	9.35888300	1.63319700	3.13523100
H	8.00845400	0.25441400	4.10986300
C	9.55885100	2.54428200	2.08123500

H	8.61462600	3.44320900	0.36669200
H	10.16071300	1.45311100	3.84886100
C	10.87392400	3.27520400	1.92410100
H	11.70624000	2.57620300	1.76896300
H	10.84780700	3.95843600	1.06868300
H	11.11372500	3.86620800	2.81737000
C	4.41885400	-2.48177000	1.09103800
C	3.85695900	-3.67657000	0.77295300
C	2.99223900	-4.31139700	1.71690900
C	2.73591900	-3.74266400	2.99974100
O	2.39893400	-5.45432800	1.46123000
H	4.04705000	-4.15671600	-0.18241400
H	5.08380600	-2.00687300	0.37557200
C	3.29819900	-2.54727400	3.31237200
H	5.16193800	-1.70607600	2.88504400
H	3.10667200	-2.10339900	4.28566800
H	2.09000900	-4.27962500	3.68596000
H	2.59689000	-5.79725200	0.56762200

1-3) X-axis (Electric field : 0.001 au)

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40606700
C	1.26662900	0.00000000	-0.62998700
O	-1.07746100	0.26725800	-0.76470700
C	1.03781000	-0.60903100	2.09448200
H	-0.90436800	0.29802400	1.93190600
C	2.12243800	-1.13777100	1.37646000
H	0.93824300	-0.77074700	3.16398200
C	2.27517700	-0.72544700	0.03941600
C	2.82950700	-2.34459700	1.98431600
H	3.13712600	-1.01908200	-0.55732300
O	1.51721400	0.34824000	-1.92837000
C	0.74494700	1.41392900	-2.53482600
H	0.64136900	2.25426700	-1.84161800
H	1.32184200	1.71815200	-3.41072000
H	-0.24184500	1.06307600	-2.83535000
H	-1.90627200	0.29341400	-0.24943500
C	4.06889700	-2.75203000	1.19466000
C	1.79286100	-3.55211200	2.13276500
H	3.16601900	-2.10664100	3.00217200
H	3.81723200	-3.24916300	0.25154600
H	4.68039000	-1.86715400	0.98211800
O	4.85671100	-3.66228700	2.00573400
C	6.04120000	-4.10251800	1.54001500

C	6.59564900	-3.76581800	0.29290700
C	6.76455700	-4.96263400	2.39413400
C	7.84332300	-4.28522700	-0.07669000
H	6.05779400	-3.12725800	-0.39789900
C	8.00137400	-5.46558500	2.00546300
H	6.32118000	-5.23516500	3.34766700
C	8.57186900	-5.13873000	0.75977700
H	8.23799900	-4.02722900	-1.05904400
H	8.52400600	-6.14616200	2.67791800
C	9.89237100	-5.73907900	0.32237100
H	10.25184700	-5.26579500	-0.60068000
H	10.67327600	-5.61898600	1.08994500
H	9.80431400	-6.81731300	0.12301200
C	0.89678000	-3.73653500	0.94431000
C	-0.44488200	-3.90454900	1.03171600
C	-1.07833200	-3.87476000	2.32620700
C	-0.29414600	-3.68831900	3.52129700
O	-2.34715700	-4.00339300	2.51383800
H	-1.05999200	-4.04942600	0.14817800
H	1.35659300	-3.75760900	-0.04014600
C	1.04119500	-3.50901100	3.42626500
H	2.40862000	-4.47108800	2.19649400
H	1.61988800	-3.35216100	4.33365300
H	-0.82126400	-3.67480100	4.46980600
H	-2.90367700	-4.11258300	1.71024200

1-4) Y-axis (Electric field : 0.0001 au)

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39697600
C	1.23045000	0.00000000	-0.68678000
O	-1.14386200	0.03234700	-0.74967200
C	1.20148300	-0.09670900	2.10296800
H	-0.94439900	0.03514100	1.93526100
C	2.42993300	-0.17633200	1.43393700
H	1.17117000	-0.12227200	3.18929800
C	2.42138800	-0.10607900	0.03136800
C	3.71551700	-0.34140800	2.22975300
H	3.33998000	-0.14389400	-0.54750500
O	1.28020800	-0.01018400	-2.06316700
C	0.90931900	1.22127600	-2.70855400
H	1.58745800	2.02775900	-2.40348500
H	1.01138600	1.04107100	-3.78039000
H	-0.12471100	1.49228200	-2.47506500
H	-1.92302200	-0.00997300	-0.17057000

C	4.75661400	0.72712000	1.87715000
C	4.32689300	-1.80275900	2.15239500
H	3.47451800	-0.19951800	3.28880600
H	5.07888400	0.66815900	0.83056300
H	4.30985700	1.71580200	2.04123600
O	5.87701900	0.53984400	2.74083300
C	6.96641300	1.36780300	2.60870100
C	7.04217800	2.44019000	1.71530400
C	8.05389800	1.08576000	3.44997400
C	8.20929700	3.21770600	1.67165300
H	6.21716000	2.68397400	1.05519900
C	9.20139600	1.87085600	3.39016900
H	7.98453800	0.24927900	4.13982700
C	9.30613500	2.95447200	2.49781300
H	8.25411400	4.04717500	0.96890700
H	10.03528900	1.63445800	4.04804400
C	10.56460300	3.79147800	2.43754400
H	11.42957000	3.19217100	2.12522300
H	10.45783200	4.61777100	1.72662300
H	10.80925300	4.22022700	3.41771400
C	4.80173600	-2.23476500	0.81617400
C	4.51452100	-3.45352000	0.29033200
C	3.69349400	-4.35686500	1.03381900
C	3.18037700	-4.01490200	2.32104200
O	3.37321100	-5.54551900	0.58139300
H	4.89833300	-3.75581600	-0.67943600
H	5.44137800	-1.55909100	0.25601800
C	3.47451600	-2.79845200	2.84611700
H	5.24678200	-1.71284200	2.76923000
H	3.09244500	-2.53265300	3.82792200
H	2.56923700	-4.74215200	2.84451400
H	3.75046000	-5.73775600	-0.29996800

1-5) Y-axis (Electric field : 0.001 au)

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39882500
C	1.23622700	0.00000000	-0.67211700
O	-1.13474300	0.27824300	-0.74425900
C	1.11590300	-0.52311600	2.06722800
H	-0.93003400	0.17118300	1.93620200
C	2.26981000	-0.90753300	1.35946400
H	1.05879800	-0.69169600	3.13960900
C	2.34043200	-0.54551900	0.00174200
C	3.37175700	-1.69962900	2.06722200

H	3.23154600	-0.74188000	-0.58832800
O	1.36071200	0.22789700	-2.02620900
C	0.89834900	1.48213700	-2.51599100
H	1.43896600	2.30942200	-2.02766100
H	1.12130200	1.48549500	-3.58610000
H	-0.17873500	1.60420000	-2.36453500
H	-1.87395800	-0.25078500	-0.39707500
C	4.78895300	-1.28673700	1.59779400
C	3.16948800	-3.26901200	2.06191100
H	3.32546300	-1.42468600	3.12856900
H	5.08829400	-1.80755500	0.68202500
H	4.78680400	-0.21180300	1.38409400
O	5.78989900	-1.45531700	2.60906400
C	6.36461500	-2.73739300	2.74827200
C	7.07284000	-3.33524800	1.70264900
C	6.24444000	-3.38933700	3.97715700
C	7.62322400	-4.60845000	1.88488000
H	7.18152300	-2.83042900	0.74523700
C	6.81235700	-4.65777000	4.14678700
H	5.68921000	-2.92059600	4.78640400
C	7.49691600	-5.30202000	3.10235000
H	8.15111900	-5.08004000	1.05976200
H	6.69587400	-5.16795600	5.09955500
C	8.03997500	-6.69974600	3.26479300
H	7.30156800	-7.43950800	2.92994800
H	8.94239700	-6.85613100	2.66611000
H	8.27011800	-6.92655700	4.30968400
C	3.26200200	-4.00564300	0.76563300
C	2.62100500	-5.18087400	0.54068800
C	1.71921500	-5.69573200	1.53607800
C	1.41825800	-4.92776500	2.71576600
O	1.12372100	-6.83964600	1.44892400
H	2.79132600	-5.75179500	-0.36725000
H	3.96083700	-3.65255400	0.01279400
C	2.07707100	-3.76909900	2.94857400
H	4.07594600	-3.63435800	2.59798400
H	1.89062400	-3.23199000	3.87499100
H	0.69602800	-5.33881600	3.41347000
H	1.36579600	-7.39660800	0.67620800

1-6) Z-axis (Electric field : 0.0001 au)

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39718700

C	1.22492100	0.00000000	-0.69578700
O	-1.14908300	0.00547900	-0.74107200
C	1.20904000	-0.06371400	2.09732000
H	-0.94346600	0.01832600	1.93751700
C	2.43572600	-0.10493900	1.42035600
H	1.18872600	-0.08885600	3.18408200
C	2.41978900	-0.05042700	0.01811400
C	3.73742100	-0.19447700	2.20031300
H	3.33739400	-0.05726600	-0.56282300
O	1.26515200	-0.04034200	-2.06938900
C	0.88274500	1.17439700	-2.74574300
H	1.55798600	1.99097700	-2.46412800
H	0.98128900	0.96632500	-3.81237600
H	-0.15163700	1.44364700	-2.51351300
H	-1.92524400	-0.00116900	-0.15686900
C	4.58782900	1.06828200	2.01953000
C	4.57010400	-1.51377700	1.90027700
H	3.48997100	-0.26188600	3.26532500
H	4.84880200	1.23876600	0.96801300
H	4.00601400	1.93037400	2.36894600
O	5.77193000	0.91764600	2.80268400
C	6.71250900	1.92250300	2.78408200
C	6.57104400	3.12616600	2.08788600
C	7.87732800	1.68319000	3.52913800
C	7.60093000	4.07699400	2.14219900
H	5.68254400	3.34118600	1.50473000
C	8.88624500	2.64157500	3.56984800
H	7.97750400	0.74300200	4.06474700
C	8.77197500	3.86028900	2.87522800
H	7.47742000	5.00684500	1.59139700
H	9.78445200	2.43659500	4.14921300
C	9.88170200	4.88707000	2.91883100
H	10.81029700	4.49126200	2.48784400
H	9.61174700	5.78705000	2.35686100
H	10.10907200	5.18962500	3.94905200
C	5.21665700	-1.58927000	0.56825800
C	5.12867500	-2.68203600	-0.23464000
C	4.35596700	-3.80109200	0.20018800
C	3.70625500	-3.81570400	1.47169800
O	4.20880200	-4.87772000	-0.53568700
H	5.62986300	-2.71966100	-1.19751400
H	5.81944700	-0.74613200	0.24401700
C	3.80585900	-2.72723500	2.27600800
H	5.41191700	-1.43406800	2.61906700
H	3.31025900	-2.72634100	3.24309000

H	3.14432600	-4.69940700	1.75403400
H	4.66382200	-4.81618300	-1.39878200

1-7) Z-axis (Electric field : 0.001 au)

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39821900
C	1.18091700	0.00000000	-0.76474100
O	-1.19257000	0.03888700	-0.67413300
C	1.23918000	-0.20088800	2.05277300
H	-0.93656800	0.04672400	1.94655800
C	2.43570200	-0.30184800	1.30694100
H	1.26492000	-0.30516600	3.13850100
C	2.37954300	-0.13953400	-0.07508500
C	3.78974800	-0.63393700	1.94056800
H	3.26844800	-0.14419300	-0.68932400
O	1.27154700	0.01812800	-2.10357800
C	0.30369000	0.66604400	-2.97867500
H	0.06312600	1.66243100	-2.60022700
H	0.81397200	0.74143300	-3.93772800
H	-0.59475400	0.05826700	-3.07576400
H	-1.94243600	0.00822300	-0.06054300
C	4.37221900	0.60096600	2.63489900
C	4.81897800	-1.33061200	0.95537600
H	3.61472100	-1.37677300	2.73211800
H	4.78744700	1.31660100	1.91916400
H	3.58303500	1.10072200	3.20848600
O	5.40792100	0.17281400	3.55683400
C	6.08156100	1.10654300	4.27316500
C	5.87882300	2.49302900	4.17753600
C	7.05020300	0.62047300	5.17184400
C	6.64859900	3.36250900	4.95837000
H	5.15974200	2.90528900	3.47926300
C	7.80378900	1.50529500	5.94166700
H	7.22184800	-0.45174400	5.22019700
C	7.62430000	2.89673300	5.84980600
H	6.49858000	4.43334600	4.83499400
H	8.57589500	1.10453600	6.59924700
C	8.51318500	3.85775400	6.61106900
H	8.84877600	3.42690900	7.56560600
H	9.41386600	4.11085800	6.03505000
H	7.99532000	4.80151300	6.82275500
C	5.49119600	-0.49036700	-0.09189300
C	5.71364100	-0.90737900	-1.36398400

C	5.21007800	-2.18731100	-1.78737300
C	4.50323000	-3.03496500	-0.86030000
O	5.33403800	-2.65307800	-2.98454200
H	6.23502100	-0.27919200	-2.08044800
H	5.87419100	0.48427900	0.19621300
C	4.29284000	-2.62058200	0.40973300
H	5.65761300	-1.62217800	1.62039500
H	3.73430100	-3.25937500	1.08979200
H	4.12511000	-3.98042600	-1.23528700
H	5.77906700	-2.06827500	-3.63904400

2) Basis set : 6-31+G(3df,2p)

2-1) Normal Optimization (without electric field)

C	3.77849900	-1.99478400	0.70719900
C	3.34060600	-1.53392600	1.94359300
C	2.18187600	-0.77425700	2.04299100
C	1.43217200	-0.45387900	0.91280700
C	1.87379200	-0.93085900	-0.32351400
C	3.02772600	-1.69309700	-0.43912900
H	3.91534800	-1.76520200	2.83200500
H	1.86330600	-0.42881500	3.01770700
H	1.33338300	-0.72426600	-1.23772500
O	3.45285300	-2.08082300	-1.68439600
C	3.28735500	-3.47300000	-1.99064600
H	2.22924000	-3.74159300	-1.97323300
H	3.68189400	-3.61459000	-2.99325100
H	3.83844100	-4.09806100	-1.28875300
O	4.91804700	-2.72175400	0.54825500
H	5.34072900	-2.86522200	1.40242200
C	0.16731800	0.36761400	1.05855500
C	-1.05701800	-0.37175300	0.51993000
H	-0.96762900	-0.59341300	-0.54623000
H	-1.14381700	-1.32133800	1.05383500
O	-2.19879900	0.43972900	0.75782900
C	-3.43136200	-0.01942600	0.37546800
C	-3.66256400	-1.26286700	-0.20297100
C	-4.50410200	0.84568100	0.60284000
C	-4.96538600	-1.62662900	-0.54789800
H	-2.85508900	-1.95474800	-0.38893300
C	-5.78807100	0.46387900	0.25326000
H	-4.31460600	1.81052600	1.05393600
C	-6.04846500	-0.78186100	-0.33094400

H	-5.12882200	-2.59863800	-0.99682900
H	-6.60689400	1.14872800	0.43806900
C	-7.45206500	-1.18212500	-0.70660200
H	-7.87982900	-0.49277700	-1.43749600
H	-7.47580000	-2.18210500	-1.13759900
H	-8.11306700	-1.17641000	0.16243600
C	2.26352200	3.41179800	-0.81769400
C	1.34538100	2.67355700	-1.61405400
C	0.40821600	1.91538500	-1.00602500
C	0.27868900	1.83154800	0.45941600
C	1.25540100	2.64489000	1.20592100
C	2.19739700	3.39835000	0.60139800
H	1.41216400	2.73309300	-2.69179500
H	-0.30106200	1.36812600	-1.61188500
H	1.19644600	2.62551100	2.28634600
H	2.90806400	3.99281800	1.15642200
O	3.20463700	4.14546100	-1.34880600
H	3.20485900	4.11619100	-2.31804900
H	-0.00606000	0.52431000	2.12349600
H	-0.71859300	2.25153400	0.68864800

2-2) X-axis (Electric field : 0.0001 au)

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39041700
C	1.22698500	0.00000000	-0.68226000
O	-1.13525600	0.00935600	-0.74686200
C	1.19327300	-0.06055100	2.09668500
H	-0.94292800	0.02825200	1.92214500
C	2.41752700	-0.12160200	1.43479700
H	1.16001300	-0.06801700	3.17822900
C	2.41106400	-0.07741000	0.03859100
C	3.69461500	-0.26481500	2.23686400
H	3.32703200	-0.10638800	-0.53578600
O	1.28330800	-0.02325400	-2.05178700
C	0.88818600	1.18609300	-2.71739200
H	1.55064000	2.00655100	-2.43409600
H	0.98398200	0.99213600	-3.78228500
H	-0.14299100	1.44601400	-2.48421800
H	-1.91287800	0.00947100	-0.17689300
C	4.83542800	0.60133600	1.70978600
C	4.14527400	-1.78320700	2.40424800
H	3.49505200	0.07539900	3.25335700
H	5.14979700	0.31589600	0.70376100
H	4.49220700	1.63798200	1.67575600

O	5.93014400	0.47076700	2.61032700
C	7.08164200	1.16293500	2.35987200
C	7.26189600	2.03237100	1.28864900
C	8.12568300	0.96299100	3.26702600
C	8.48310200	2.69093400	1.13766100
H	6.47408700	2.21142900	0.57288000
C	9.32827300	1.62752600	3.09811900
H	7.97589600	0.28649300	4.09782100
C	9.53473900	2.50782000	2.02897600
H	8.60564900	3.36543500	0.29910000
H	10.12432700	1.45970900	3.81379700
C	10.84739900	3.23010400	1.86274700
H	11.68283600	2.52955300	1.80082900
H	10.85192100	3.83688600	0.95807500
H	11.04709500	3.89186100	2.70850400
C	4.37979300	-2.48853300	1.13126200
C	3.81633400	-3.68005500	0.84192700
C	2.95576900	-4.29142600	1.79643800
C	2.70235200	-3.69437900	3.06050300
O	2.36726500	-5.43298700	1.56527500
H	4.00017400	-4.17975400	-0.09943000
H	5.04035000	-2.03043500	0.40773200
C	3.26720100	-2.50289500	3.34533800
H	5.12722700	-1.68802100	2.90114300
H	3.07974500	-2.03710400	4.30405100
H	2.05754700	-4.21141900	3.75577000
H	2.56720000	-5.79399300	0.68763700

2-3) X-axis (Electric field : 0.001 au)

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39878600
C	1.26131500	0.00000000	-0.62904200
O	-1.07406900	0.25291900	-0.76223900
C	1.03625700	-0.59530400	2.08654900
H	-0.90292700	0.29413900	1.91971000
C	2.11875700	-1.11727000	1.37501800
H	0.93757400	-0.75155800	3.15185500
C	2.26860400	-0.71270700	0.04272300
C	2.83566900	-2.30859100	1.98912200
H	3.12959900	-1.00152300	-0.54884600
O	1.50953900	0.35208200	-1.91925200
C	0.73871300	1.41337100	-2.52269400
H	0.60061200	2.23528000	-1.82143000
H	1.32566400	1.74773500	-3.37472500
H	-0.23031900	1.05642500	-2.85534900

H	-1.89581900	0.28723500	-0.25107300
C	4.07857000	-2.70489600	1.20941500
C	1.81217600	-3.52295900	2.14125200
H	3.16289200	-2.06195900	3.00241900
H	3.83637200	-3.20442100	0.27012700
H	4.67530800	-1.81618600	0.99413600
O	4.87409300	-3.60054900	2.02219800
C	6.06633800	-4.01179400	1.57415700
C	6.62278100	-3.66974400	0.33592400
C	6.80161100	-4.84584700	2.43402800
C	7.88037100	-4.15575300	-0.01693800
H	6.07777700	-3.04932800	-0.35837700
C	8.04789400	-5.31599600	2.06120400
H	6.36002300	-5.12221400	3.38198800
C	8.61894400	-4.98165400	0.82620600
H	8.27767800	-3.89116200	-0.99109300
H	8.58045100	-5.97413100	2.74019500
C	9.95457100	-5.54743400	0.40592800
H	10.34137900	-5.02556200	-0.47209100
H	10.69986800	-5.46391600	1.20436500
H	9.88183100	-6.60869100	0.14702500
C	0.92634600	-3.72113400	0.95620500
C	-0.40593000	-3.89480800	1.04012000
C	-1.04263200	-3.86322000	2.32698200
C	-0.26555000	-3.66497900	3.51819100
O	-2.30390000	-3.99915900	2.50454300
H	-1.01609000	-4.04674000	0.15955600
H	1.38844100	-3.74256100	-0.02212200
C	1.06076600	-3.48179000	3.42685000
H	2.43457100	-4.43160000	2.21101200
H	1.63463100	-3.31791200	4.33052400
H	-0.79330800	-3.65008200	4.46123200
H	-2.84989700	-4.11593300	1.70412100

2-4) Y-axis (Electric field : 0.0001 au)

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.38988100
C	1.22544500	0.00000000	-0.68418400
O	-1.13859700	0.02982600	-0.74605500
C	1.19456700	-0.09646500	2.09314600
H	-0.94178000	0.03520700	1.92340000
C	2.41681800	-0.17522700	1.42822600
H	1.16457800	-0.12154700	3.17461100
C	2.40934600	-0.10606100	0.03288700

C	3.69750100	-0.33958800	2.22284500
H	3.32484200	-0.14247100	-0.54240900
O	1.27498100	-0.00763700	-2.05468400
C	0.92048200	1.22227800	-2.69994200
H	1.61279300	2.01570200	-2.41001300
H	1.00324500	1.04112100	-3.76831700
H	-0.10019900	1.51568100	-2.45694600
H	-1.91189300	-0.01044600	-0.17222000
C	4.74167700	0.71839500	1.86904100
C	4.30040300	-1.80084500	2.15269100
H	3.45575600	-0.19320600	3.27609900
H	5.07215000	0.64460100	0.83058400
H	4.29479700	1.70573700	2.01053500
O	5.84826100	0.54463400	2.74489100
C	6.94140800	1.35470300	2.60612000
C	7.03281200	2.40527200	1.69887100
C	8.01735900	1.08125400	3.45440000
C	8.20155300	3.16701000	1.64749900
H	6.21720000	2.64315400	1.03291900
C	9.16616700	1.85027700	3.38678900
H	7.93748600	0.26203700	4.15628400
C	9.28546800	2.91074600	2.47996500
H	8.25797500	3.97970000	0.93351800
H	9.99028900	1.61963000	4.05102300
C	10.54868500	3.73009600	2.41012200
H	11.39898700	3.12233700	2.09310400
H	10.44710700	4.55319000	1.70363300
H	10.80418700	4.15218600	3.38406400
C	4.76821300	-2.24052600	0.82444900
C	4.47351900	-3.45276300	0.31010900
C	3.65444300	-4.34534100	1.05755000
C	3.15040800	-3.99382100	2.33955600
O	3.33146700	-5.52718000	0.61212800
H	4.84917900	-3.76258400	-0.65546400
H	5.40469900	-1.57221900	0.26074800
C	3.45184300	-2.78390700	2.85353200
H	5.21895100	-1.70996000	2.76422800
H	3.07733800	-2.50980800	3.83102800
H	2.54052100	-4.71190800	2.86770100
H	3.70297000	-5.72258200	-0.26258600

2-5) Y-axis (Electric field : 0.001 au)

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39290800

C	1.22962600	0.00000000	-0.66760400
O	-1.12515500	0.29068700	-0.73697300
C	1.11744700	-0.49928700	2.06068800
H	-0.92389900	0.17515800	1.93022900
C	2.27500400	-0.86351800	1.36280600
H	1.06293800	-0.65938200	3.12975400
C	2.33870500	-0.51348100	0.00859100
C	3.38401500	-1.63135000	2.07522600
H	3.23634300	-0.69032000	-0.56974300
O	1.30129100	0.32060300	-2.00306300
C	1.21355400	-0.81752900	-2.89480600
H	0.26103300	-1.32918900	-2.76451900
H	1.28870800	-0.42512800	-3.90553100
H	2.02931900	-1.51461200	-2.70891100
H	-1.88416900	-0.14835600	-0.33531600
C	4.79153600	-1.20640700	1.60429400
C	3.20369300	-3.19900500	2.07954800
H	3.33364600	-1.35069600	3.12989100
H	5.07985200	-1.70735600	0.67934900
H	4.77917100	-0.13300900	1.40490600
O	5.79610000	-1.38870300	2.60031000
C	6.37941700	-2.66294100	2.71374500
C	7.03256500	-3.26398800	1.64388500
C	6.32279800	-3.30546800	3.94421300
C	7.59076800	-4.52864500	1.80547300
H	7.09415700	-2.76882600	0.68296300
C	6.89764200	-4.56516000	4.09210900
H	5.80966600	-2.83514500	4.77348400
C	7.52735300	-5.21183900	3.02485100
H	8.07668800	-5.00190500	0.96190500
H	6.83121700	-5.06710600	5.04876700
C	8.07715100	-6.60273600	3.16835100
H	7.31649400	-7.34131900	2.90579600
H	8.92570500	-6.77117500	2.50755100
H	8.38366200	-6.81134700	4.19162800
C	3.30897700	-3.93942400	0.79476900
C	2.68736000	-5.11649500	0.57785000
C	1.80058800	-5.64113000	1.57336200
C	1.49321300	-4.87537800	2.74592200
O	1.23372300	-6.79060700	1.48878300
H	2.86115500	-5.68825100	-0.32359900
H	3.99771100	-3.57868100	0.04290600
C	2.13070500	-3.71274600	2.97016100
H	4.11392800	-3.54770300	2.61340800
H	1.93811300	-3.17451400	3.88927100

H	0.78253900	-5.29243900	3.44500000
H	1.48145600	-7.33652500	0.71937600

2-6) Z-axis (Electric field : 0.0001 au)

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39008100
C	1.21985300	0.00000000	-0.69329600
O	-1.14391700	0.00355300	-0.73735500
C	1.20221400	-0.06326100	2.08733300
H	-0.94085500	0.01745000	1.92563200
C	2.42285800	-0.10316700	1.41466100
H	1.18219600	-0.08834300	3.16921000
C	2.40782400	-0.05013300	0.01959800
C	3.71942600	-0.18953400	2.19446100
H	3.32174100	-0.05482300	-0.55862200
O	1.26000300	-0.03780900	-2.06095900
C	0.89227100	1.17504100	-2.73727700
H	1.58334300	1.97799700	-2.47407000
H	0.96732300	0.96470900	-3.80040400
H	-0.12768500	1.46800500	-2.49264000
H	-1.91421200	-0.00156900	-0.15850800
C	4.56800200	1.06881000	2.01521400
C	4.55062400	-1.50589400	1.89934100
H	3.46984200	-0.25582600	3.25401100
H	4.83694700	1.23119600	0.96897900
H	3.98124800	1.92892500	2.34724900
O	5.73925700	0.92884700	2.80988100
C	6.67948100	1.92421000	2.78660800
C	6.54725800	3.11492000	2.08000500
C	7.83421700	1.69318100	3.53787800
C	7.57403300	4.05894800	2.12957200
H	5.66661200	3.32422000	1.49182400
C	8.83995100	2.64414600	3.57330100
H	7.92872500	0.76336300	4.08287800
C	8.73379500	3.84900500	2.86796200
H	7.45698500	4.97921000	1.57073600
H	9.72978700	2.44452500	4.15834200
C	9.84336200	4.86837600	2.90443700
H	10.75858500	4.47459300	2.45713600
H	9.56943800	5.77006700	2.35851900
H	10.08649500	5.15651800	3.92912100
C	5.19104300	-1.58672300	0.57276000
C	5.10332600	-2.67792100	-0.21759400
C	4.34008500	-3.79323200	0.22401100

C	3.69775500	-3.80066500	1.49306200
O	4.19760600	-4.86673700	-0.50332900
H	5.59774900	-2.72112900	-1.17866900
H	5.78492200	-0.74531900	0.24281300
C	3.79641500	-2.71364100	2.28500300
H	5.39148400	-1.41969900	2.61256000
H	3.30718000	-2.70651100	3.25028500
H	3.14269300	-4.68079000	1.78256700
H	4.64777300	-4.80776700	-1.36062100

2-7) Z-axis (Electric field : 0.001 au)

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39107200
C	1.17485200	0.00000000	-0.76389300
O	-1.18925400	0.02329800	-0.66957700
C	1.23630700	-0.16731700	2.04504700
H	-0.93406900	0.03943600	1.93464700
C	2.42855400	-0.25584300	1.30314200
H	1.26303800	-0.25634300	3.12687600
C	2.36883600	-0.11822600	-0.07319800
C	3.78668500	-0.54424000	1.94016800
H	3.25264300	-0.12001200	-0.68631200
O	1.26929100	0.01527600	-2.09451900
C	0.28471600	0.60594500	-2.98359500
H	-0.01497900	1.58495000	-2.61740600
H	0.79837200	0.70619800	-3.93318900
H	-0.57541800	-0.04529600	-3.09225900
H	-1.93281300	0.00466100	-0.06034400
C	4.29435400	0.68160600	2.69601000
C	4.86256700	-1.14348900	0.94890900
H	3.63919200	-1.32524800	2.69281900
H	4.70342800	1.43708900	2.02529500
H	3.46842600	1.12670400	3.25292200
O	5.31050200	0.26254800	3.63869200
C	5.86152300	1.17236800	4.46287700
C	5.58306900	2.54308200	4.44296700
C	6.77943800	0.68478800	5.40457500
C	6.22116800	3.39201400	5.34284300
H	4.90241000	2.95869400	3.71601700
C	7.40201300	1.54931100	6.29152500
H	7.01119100	-0.37220300	5.39895300
C	7.13900700	2.92306300	6.28119700
H	6.01048700	4.45334500	5.28260800
H	8.13306500	1.14871600	6.98704400

C	7.88388200	3.87185600	7.18872400
H	7.28971700	4.76077800	7.40918100
H	8.14988800	3.39350400	8.13620700
H	8.81396500	4.21700500	6.72847800
C	5.48116700	-0.23884300	-0.06722000
C	5.74112100	-0.60937100	-1.33753200
C	5.33525300	-1.90690000	-1.79299200
C	4.68433500	-2.81783100	-0.89417600
O	5.50139900	-2.32957600	-2.99230400
H	6.21987600	0.06693700	-2.03316600
H	5.78626600	0.75084300	0.24511200
C	4.43772300	-2.45021100	0.37451400
H	5.71195400	-1.39300300	1.61087900
H	3.92423100	-3.13872000	1.03387800
H	4.38006400	-3.77602700	-1.29053200
H	5.90695900	-1.70527000	-3.62394900