

## Electronic Supplementary Information (ESI)

*New Journal of Chemistry*

### Theoretical study on homolytic C(sp<sup>2</sup>)-O cleavage in ethers and phenols

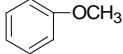
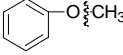
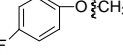
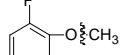
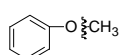
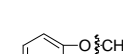

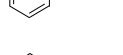
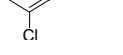
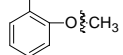
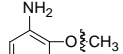
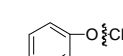
Lanlan Ding, Wenrui Zheng\*, Yingxing Wang

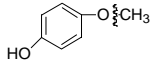
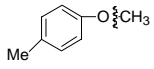
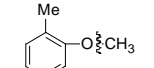
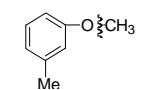
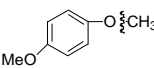
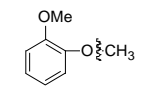
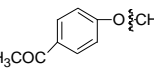
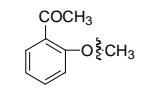
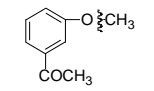
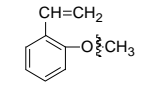
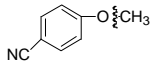
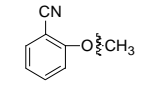
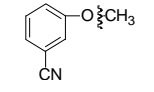
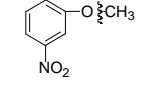
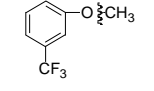
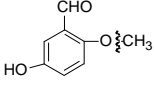
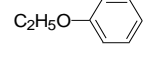
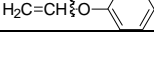
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Table S1. The 72 calculated C-O BDEs using 26 kinds of DFTs (kJ/mol)

No.	compounds	Exp	B3P86	BMK	M05	BH&HLYP	B3LYP	M06-L
1	H <sub>3</sub> C-OCH <sub>3</sub>	349.8±4.2	333.9	340.9	330.4	301.3	315.6	323.8
2	H <sub>3</sub> C-OC <sub>2</sub> H <sub>5</sub>	348.1±4.2	352.5	358.4	349.1	318.7	333.7	344.3
3	C <sub>2</sub> H <sub>5</sub> -OCH <sub>3</sub>	353.1±5.4	335.4	345.8	330.2	306.3	317.2	323.3
4	C <sub>2</sub> H <sub>3</sub> -OC <sub>2</sub> H <sub>3</sub>	326.8±10.5	314.1	320.3	292.9	288.7	295.8	296.4
5	C <sub>2</sub> H <sub>5</sub> -OC <sub>2</sub> H <sub>3</sub>	272.8±10.5	249.9	259.0	231.2	228.0	233.4	236.6
6	C <sub>2</sub> H <sub>5</sub> -OC <sub>2</sub> H <sub>5</sub>	355.6±6.3	353.5	362.4	348.8	323.3	334.9	343.4
7	nC <sub>3</sub> H <sub>7</sub> -OCH <sub>3</sub>	356.5±6.3	328.7	339.7	323.6	279.0	309.9	318.2
8	H <sub>3</sub> C-OiC <sub>3</sub> H <sub>7</sub>	350.2±6.3	331.2	338.8	327.6	299.5	311.9	325.2
9	iC <sub>3</sub> H <sub>7</sub> -OCH <sub>3</sub>	358.6±4.2	327.9	342.1	320.3	300.9	309.1	316.3
10	C <sub>2</sub> H <sub>5</sub> -OC <sub>3</sub> H <sub>7</sub>	358.4±8.4	332.0	342.7	327.0	304.6	313.8	320.3
11	C <sub>3</sub> H <sub>7</sub> -OC <sub>2</sub> H <sub>5</sub>	355.2±8.4	353.3	362.5	348.9	323.2	334.5	344.0
12	C <sub>3</sub> H <sub>7</sub> -OC <sub>2</sub> H <sub>3</sub>	274.1±10.5	249.7	258.8	231.3	228.0	233.0	237.0
13	C <sub>4</sub> H <sub>9</sub> -OCH <sub>3</sub>	343.9±6.3	332.4	343.0	327.8	303.4	296.8	323.1
14	H <sub>3</sub> C-OC <sub>4</sub> H <sub>9</sub>	353.1±6.3	331.9	339.4	328.6	301.1	313.5	323.0
15	C <sub>2</sub> H <sub>5</sub> O-C <sub>3</sub> H <sub>7</sub>	356.9±6.3	353.3	362.5	348.9	323.2	334.5	344.0
16	C <sub>2</sub> H <sub>3</sub> -OC <sub>4</sub> H <sub>9</sub>	419.2±8.4	405.0	411.7	398.3	374.5	385.5	388.0

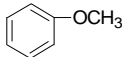
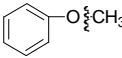
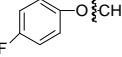
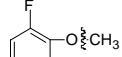
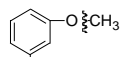
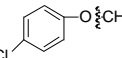
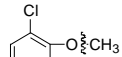
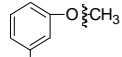
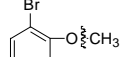
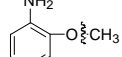
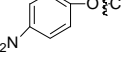
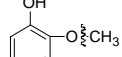
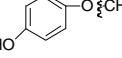
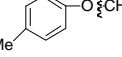
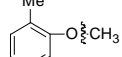
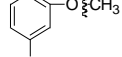
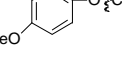
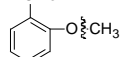
\* Corresponding author. Tel.: +86 21 67791216; fax: +86 21 67791220.  
E-mail address: wrzheng@sues.edu.cn (W.R. Zheng).

17	$C_4H_9-OC_2H_5$	$273.2 \pm 10.5$	253.3	262.3	235.0	231.8	219.7	241.1
18	$tC_4H_9-OC_2H_5$	$347.3 \pm 6.3$	332.7	350.8	322.6	305.9	312.1	326.3
19	$C_2H_5-OtC_4H_9$	$349.6 \pm 6.3$	325.5	336.2	319.3	296.1	305.0	321.5
20	$sC_4H_9-OnC_4H_9$	$348.2 \pm 8.4$	337.4	347.3	370.0	360.3	319.0	326.1
21	$sC_4H_9-OsC_4H_9$	$359.4 \pm 8.4$	315.3	336.2	363.1	340.4	297.8	317.9
22	$tC_4H_9-OtC_4H_9$	$324.7 \pm 8.4$	283.9	305.7	317.8	298.6	261.1	287.1
23	$nC_4H_9-OtC_4H_9$	$351.9 \pm 8.4$	326.3	366.8	371.5	344.7	305.4	323.5
24	$nC_4H_9O-tC_4H_9$	$348.1 \pm 8.4$	315.9	335.2	338.3	338.9	296.0	307.2
25	$iC_4H_9-OtC_4H_9$	$353.1 \pm 8.4$	226.3	377.6	317.9	344.3	304.9	325.5
26	$nC_5H_{11}-OtC_4H_9$	$349.4 \pm 8.4$	322.8	333.5	367.3	340.1	301.5	321.5
27		$416.7 \pm 5.9$	407.5	416.1	462.9	436.3	386.2	392.8
28		$268.6 \pm 7.1$	361.3	269.3	282.9	272.0	240.2	254.2
29		261.1	253.3	261.4	275.7	265.3	233.2	244.8
30		257.7	254.2	262.4	276.2	266.8	234.0	254.4
31		269.4	265.5	274.4	289.6	278.3	244.6	257.5
32		261.1	256.6	265.9	279.3	296.6	236.1	247.3
33		256.5	255.3	264.6	277.0	268.8	234.9	246.1
34		266.5	265.7	265.7	288.6	277.8	244.7	257.6
35		258.6	254.6	254.6	277.0	268.3	234.1	244.6
36		234.7	213.2	213.2	232.6	229.4	194.0	205.2
37		255.2	257.9	257.9	280.4	271.5	237.1	249.4
38		243.1	236.2	236.2	256.7	252.5	217.7	222.6

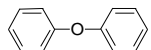
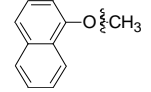
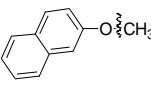
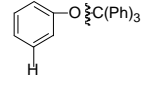
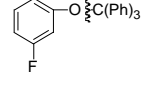
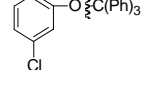
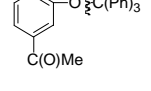
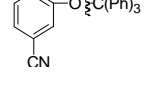
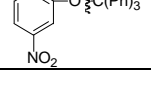
39		266.9	257.1	257.1	279.1	269.4	236.2	248.9
40		257.7	252.5	252.5	272.7	263.2	231.6	244.2
41		254.8	257.9	257.9	278.8	269.8	237.2	250.0
42		263.6	258.6	258.6	280.0	268.5	237.6	251.1
43		260.2	251.4	251.4	274.2	263.5	230.2	244.5
44		248.1	229.0	229.0	249.6	245.9	209.5	216.0
45		268.2	269.3	269.3	292.9	281.2	248.1	260.9
46		259.4	254.4	254.4	264.9	246.5	224.3	239.2
47		266.5	269.3	269.3	291.6	279.6	248.2	262.3
48		255.2	245.0	245.0	263.1	255.6	224.2	236.3
49		266.9	269.2	269.2	291.5	286.3	249.9	259.0
50		265.3	269.4	269.4	293.6	283.3	248.2	260.7
51		270.3	273.4	273.4	296.8	284.9	252.3	265.9
52		263.6	274.2	274.2	297.3	286.2	253.3	266.4
53		282.4	270.3	270.3	293.1	281.7	249.5	261.7
54		260.7	266.8	266.8	292.4	283.0	246.4	254.0
55		416.7±5.4	419.1	419.1	477.1	447.6	397.0	407.8
56		331.0±10.5	322.2	322.2	349.1	343.8	300.1	306.8

57		320.5 ±20.9	316.3	316.3	340.7	339.9	297.1	298.5
58		304.6 ±8.4	273.7	273.7	305.7	285.7	253.9	260.9
59		303.7 ±8.4	292.6	292.6	326.7	305.2	271.6	282.4
60		298.3 ±8.4	263.9	263.9	296.5	274.2	241.8	259.9
61		298.7 ±8.4	275.9	275.9	290.9	289.6	255.8	263.0
62		300.8 ±8.4	264.8	264.8	295.8	277.2	243.7	258.5
63		332.2 ±8.4	321.8	321.8	347.8	345.9	298.9	306.6
64		208.4 ±8.4	192.6	192.6	196.6	195.8	171.3	183.6
65		240.6	233.7	233.7	299.1	242.6	213.2	226.0
66		255.2	253.0	253.0	272.2	263.0	231.9	244.7
67		155	122.7	122.7	116.7	120.0	97.1	122.8
68		145	126.7	126.7	122.8	125.6	101.4	125.6
69		166	127.5	127.5	122.7	126.1	102.1	126.6
70		163	136.0	136.0	131.3	131.9	109.7	138.1
71		166	141.0	141.0	137.9	137.9	114.6	143.5
72		167	142.0	142.0	138.2	139.7	115.9	143.5

No.	compounds	Exp	TPSS1KCIS	B97-1	B97-2	B98	wB97	wB97X
1	H <sub>3</sub> C-OCH <sub>3</sub>	349.8±4.2	317.5	334.1	332.8	329.9	342.5	339.3
2	H <sub>3</sub> C-OC <sub>2</sub> H <sub>5</sub>	348.1±4.2	335.4	338.9	338.2	334.8	360.7	345.9
3	C <sub>2</sub> H <sub>5</sub> -OCH <sub>3</sub>	353.1±5.4	318.7	334.5	331.8	330.5	346.9	342.7
4	C <sub>2</sub> H <sub>3</sub> -OC <sub>2</sub> H <sub>3</sub>	326.8±10.5	297.0	311.8	309.8	307.5	315.6	315.0
5	C <sub>2</sub> H <sub>5</sub> -OC <sub>2</sub> H <sub>3</sub>	272.8±10.5	234.5	250.4	247.2	245.8	257.0	255.7
6	C <sub>2</sub> H <sub>5</sub> -OC <sub>2</sub> H <sub>5</sub>	355.6±6.3	336.3	339.0	336.7	335.0	364.9	349.2
7	nC <sub>3</sub> H <sub>7</sub> -OCH <sub>3</sub>	356.5±6.3	311.8	328.1	324.8	323.9	341.9	337.3
8	H <sub>3</sub> C-OiC <sub>3</sub> H <sub>7</sub>	350.2±6.3	313.7	330.9	328.8	326.6	342.7	338.9
9	iC <sub>3</sub> H <sub>7</sub> -OCH <sub>3</sub>	358.6±4.2	310.4	326.5	321.4	322.4	344.7	339.0
10	C <sub>2</sub> H <sub>5</sub> -OC <sub>3</sub> H <sub>7</sub>	358.4±8.4	315.3	331.1	328.4	327.2	344.4	340.1
11	C <sub>3</sub> H <sub>7</sub> -OC <sub>2</sub> H <sub>5</sub>	355.2±8.4	335.8	328.8	336.5	334.8	365.4	349.5
12	C <sub>3</sub> H <sub>7</sub> -OC <sub>2</sub> H <sub>3</sub>	274.1±10.5	234.1	250.2	247.1	254.6	257.6	256.1
13	C <sub>4</sub> H <sub>9</sub> -OCH <sub>3</sub>	343.9±6.3	314.8	331.4	328.2	327.2	346.2	341.5
14	H <sub>3</sub> C-OC <sub>4</sub> H <sub>9</sub>	353.1±6.3	315.3	331.9	330.6	327.8	342.0	338.6
15	C <sub>2</sub> H <sub>5</sub> O-C <sub>3</sub> H <sub>7</sub>	356.9±6.3	335.8	338.8	336.5	334.8	365.4	349.5
16	C <sub>2</sub> H <sub>3</sub> -OC <sub>4</sub> H <sub>9</sub>	419.2±8.4	386.9	401.2	400.3	397.7	411.3	408.1
17	C <sub>4</sub> H <sub>9</sub> -OC <sub>2</sub> H <sub>3</sub>	273.2±10.5	237.1	253.4	250.4	248.8	261.6	260.0
18	tC <sub>4</sub> H <sub>9</sub> -OC <sub>2</sub> H <sub>5</sub>	347.3±6.3	313.2	317.1	309.8	312.7	355.8	336.7
19	C <sub>2</sub> H <sub>5</sub> -OtC <sub>4</sub> H <sub>9</sub>	349.6±6.3	306.2	323.3	319.2	318.8	342.4	336.8
20	sC <sub>4</sub> H <sub>9</sub> -OnC <sub>4</sub> H <sub>9</sub>	348.2±8.4	370.8	335.9	333.8	332.0	350.8	346.4
21	sC <sub>4</sub> H <sub>9</sub> -OsC <sub>4</sub> H <sub>9</sub>	359.4±8.4	347.3	318.0	309.9	313.1	344.1	336.8
22	tC <sub>4</sub> H <sub>9</sub> -OtC <sub>4</sub> H <sub>9</sub>	324.7±8.4	304.4	271.6	270.7	276.2	315.5	290.0
23	nC <sub>4</sub> H <sub>9</sub> -OtC <sub>4</sub> H <sub>9</sub>	351.9±8.4	354.9	323.7	319.8	319.2	344.4	338.6
24	nC <sub>4</sub> H <sub>9</sub> O-tC <sub>4</sub> H <sub>9</sub>	348.1±8.4	344.2	313.7	306.4	309.5	339.8	316.5
25	iC <sub>4</sub> H <sub>9</sub> -OtC <sub>4</sub> H <sub>9</sub>	353.1±8.4	354.9	324.1	319.5	319.4	345.8	339.7
26	nC <sub>5</sub> H <sub>11</sub> -OtC <sub>4</sub> H <sub>9</sub>	349.4±8.4	350.6	320.3	315.8	315.6	342.1	336.1

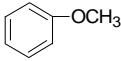
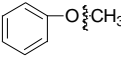
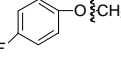
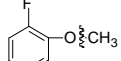
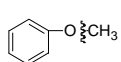
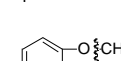
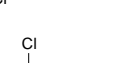
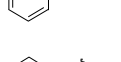
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28		268.6±7.1	284.3	259.1	257.5	254.5	267.2	266.6
29		261.1	275.6	241.2	249.6	246.8	260.2	259.4
30		257.7	276.5	252.0	250.3	247.6	261.0	260.1
31		269.4	289.1	263.3	261.8	258.8	273.2	272.2
32		261.1	279.2	254.7	252.8	250.3	264.3	263.6
33		256.5	277.6	253.4	251.3	249.1	263.0	262.2
34		266.5	289.2	263.5	261.9	259.0	272.4	271.6
35		258.6	276.7	252.5	250.6	248.2	262.6	261.9
36		234.7	229.8	212.3	210.1	208.1	224.9	222.7
37		255.2	280.1	256.1	254.4	251.6	267.0	265.7
38		243.1	256.0	235.0	232.8	230.9	246.1	245.0
39		266.9	279.4	255.0	253.5	231.1	265.1	264.0
40		257.7	274.7	250.4	248.8	245.9	258.9	258.2
41		254.8	281.1	256.0	254.0	251.4	264.4	263.5
42		263.6	281.2	256.5	255.2	251.9	265.1	264.4
43		260.2	272.3	248.7	247.3	244.3	258.0	257.4
44		248.1	246.5	227.7	226.3	223.7	239.0	238.5

45		268.2	293.6	266.8	265.5	262.3	274.0	273.5
46		259.4	266.5	243.5	242.2	238.8	249.9	249.5
47		266.5	293.5	267.0	265.3	262.4	273.8	273.3
48		255.2	265.6	243.1	241.2	238.5	253.4	252.6
49		266.9	293.4	269.1	266.2	263.2	263.8	276.3
50		265.3	293.3	266.9	265.4	262.5	276.4	275.6
51		270.3	298.0	271.1	269.5	266.6	278.3	277.8
52		263.6	299.0	271.9	270.1	267.4	278.9	278.4
53		282.4	295.0	268.0	266.2	263.5	275.5	274.9
54		260.7	290.0	264.5	262.1	260.2	275.1	274.0
55		416.7±5.4	461.4	298.2	398.2	376.9	430.5	414.1
56		331.0±10.5	353.0	316.8	315.0	312.7	325.5	324.8
57		320.5±20.9	344.1	313.1	310.1	308.8	322.0	320.4
58		304.6±8.4	297.3	271.1	265.4	267.5	292.9	287.9
59		303.7±8.4	318.4	276.5	270.9	272.7	312.4	295.7
60		298.3±8.4	285.4	261.5	253.9	257.4	289.1	282.9
61		298.7±8.4	299.5	273.1	267.5	269.6	296.4	291.2
62		300.8±8.4	285.9	262.4	255.2	258.5	289.2	283.5
63		332.2±8.4	350.0	315.5	313.2	311.6	329.8	328.1

64		208.4±8.4	204.8	188.4	184.3	184.3	204.0	202.2
65		240.6	263.0	231.9	229.7	227.3	239.0	238.6
66		255.2	274.7	250.7	249.1	246.2	258.2	258.1
67		155	120.4	118.3	106.8	113.6	157.7	152.0
68		145	125.1	122.3	110.9	117.8	138.9	156.6
69		166	125.9	123.2	111.6	118.6	162.5	156.8
70		163	135.5	130.6	119.3	125.9	168.9	162.9
71		166	141.1	135.5	124.4	130.8	174.4	168.3
72		167	142.2	136.5	125.2	132.0	174.8	168.8

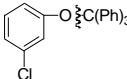
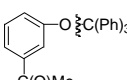
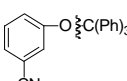
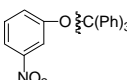
No.	compounds	Exp	wB97X-D	PBE1PBE	MPW1P86	MPW1B95	MPWCIS1K
1	H <sub>3</sub> C-OCH <sub>3</sub>	349.8±4.2	337.4	328.7	331.1	341.0	319.5
2	H <sub>3</sub> C-OC <sub>2</sub> H <sub>5</sub>	348.1±4.2	344.0	346.3	349.5	359.3	337.7
3	C <sub>2</sub> H <sub>5</sub> -OCH <sub>3</sub>	353.1±5.4	341.2	330.3	333.7	342.9	322.3
4	C <sub>2</sub> H <sub>3</sub> -OC <sub>2</sub> H <sub>3</sub>	326.8±10.5	314.6	310.5	313.2	324.2	305.2
5	C <sub>2</sub> H <sub>5</sub> -OC <sub>2</sub> H <sub>3</sub>	272.8±10.5	255.3	247.1	249.9	262.5	241.9
6	C <sub>2</sub> H <sub>5</sub> -OC <sub>2</sub> H <sub>5</sub>	355.6±6.3	348.1	348.3	351.7	360.7	340.1
7	nC <sub>3</sub> H <sub>7</sub> -OCH <sub>3</sub>	356.5±6.3	337.1	323.6	327.1	336.5	315.2
8	H <sub>3</sub> C-OiC <sub>3</sub> H <sub>7</sub>	350.2±6.3	338.1	355.5	329.2	339.2	317.2
9	iC <sub>3</sub> H <sub>7</sub> -OCH <sub>3</sub>	358.6±4.2	338.2	323.4	327.5	336.3	314.8
10	C <sub>2</sub> H <sub>5</sub> -OC <sub>3</sub> H <sub>7</sub>	358.4±8.4	339.8	327.2	330.6	339.6	319.8



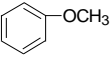
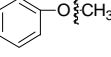
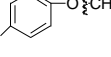
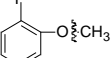
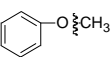
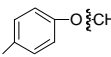
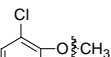
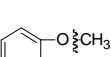
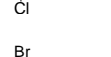
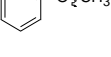
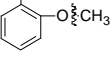
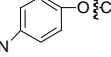
11	$C_3H_7-OC_2H_5$	$355.2 \pm 8.4$	349.0	348.2	351.5	360.6	340.1
12	$C_3H_7-OC_2H_3$	$274.1 \pm 10.5$	256.4	247.0	249.8	262.5	242.0
13	$C_4H_9-OCH_3$	$343.9 \pm 6.3$	341.0	327.7	331.0	340.6	319.6
14	$H_3C-OC_4H_9$	$353.1 \pm 6.3$	337.2	336.2	329.6	339.4	318.5
15	$C_2H_5O-C_3H_7$	$356.9 \pm 6.3$	349.0	348.2	351.5	360.6	340.1
16	$C_2H_3-OC_4H_9$	$419.2 \pm 8.4$	407.4	399.4	402.6	409.4	392.2
17	$C_4H_9-OC_2H_3$	$273.2 \pm 10.5$	260.1	250.8	253.5	266.2	246.0
18	$tC_4H_9-OC_2H_5$	$347.3 \pm 6.3$	336.9	328.3	333.3	342.3	318.6
19	$C_2H_5-OtC_4H_9$	$349.6 \pm 6.3$	362.6	321.0	324.9	334.6	312.7
20	$sC_4H_9-OnC_4H_9$	$348.2 \pm 8.4$	345.9	333.0	336.2	345.1	378.2
21	$sC_4H_9-OC_4H_9$	$359.4 \pm 8.4$	341.1	315.3	319.9	344.4	354.8
22	$tC_4H_9-OtC_4H_9$	$324.7 \pm 8.4$	335.1	280.3	335.1	298.1	275.0
23	$nC_4H_9-OtC_4H_9$	$351.9 \pm 8.4$	365.1	322.2	375.8	335.6	364.2
24	$nC_4H_9O-tC_4H_9$	$348.1 \pm 8.4$	332.8	312.0	315.8	325.9	314.6
25	$iC_4H_9-OtC_4H_9$	$353.1 \pm 8.4$	367.3	322.2	457.7	336.4	363.7
26	$nC_5H_{11}-OtC_4H_9$	$349.4 \pm 8.4$	363.6	318.7	346.2	332.5	359.7
27		$416.7 \pm 5.9$	413.2	401.1	405.8	413.2	465.9
28		$268.6 \pm 7.1$	280.5	259.4	261.3	274.1	293.8
29		261.1	273.0	251.7	253.7	266.1	285.6
30		257.7	273.6	252.5	254.5	267.4	286.7
31		269.4	285.7	263.8	265.7	278.9	299.6
32		261.1	277.3	255.1	257.0	269.6	289.7
33		256.5	275.9	253.9	256.0	268.5	288.3
34		266.5	285.2	263.9	265.8	278.8	299.3

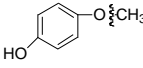
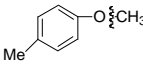
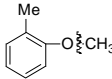
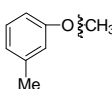
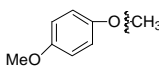
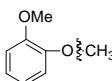
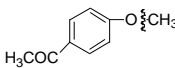
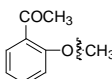
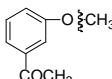
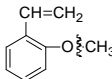
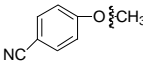
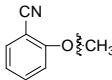
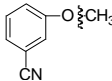
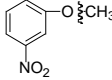
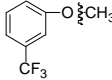
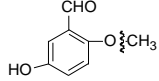
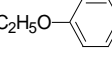
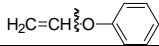
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36		234.7	234.8	213.2	215.2	225.9	244.0
37		255.2	278.8	256.6	258.5	271.3	292.0
38		243.1	257.5	235.0	237.5	249.2	268.6
39		266.9	277.4	255.6	257.5	270.5	290.3
40		257.7	272.0	250.9	252.7	265.4	284.2
41		254.8	277.6	256.5	258.3	271.1	290.4
42		263.6	278.2	256.9	258.8	271.3	291.0
43		260.2	271.1	250.3	251.8	264.3	284.4
44		248.1	251.7	229.1	230.9	241.9	263.4
45		268.2	288.6	267.5	269.9	281.6	303.0
46		259.4	265.2	244.0	245.5	285.5	275.5
47		266.5	287.6	267.1	269.0	281.6	301.9
48		255.2	266.7	243.9	245.8	259.0	276.6
49		266.9	289.3	267.2	270.5	279.4	306.7
50		265.3	289.6	267.9	269.8	282.7	304.4

51		270.3	292.1	271.2	273.2	285.9	307.1
52		263.6	292.7	271.9	273.9	286.6	307.9
53		282.4	289.1	268.2	270.1	283.0	303.4
54		260.7	287.9	264.9	267.7	278.9	301.3
55		416.7±5.4	463.2	413.4	417.4	425.1	469.3
56		331.0±10.5	326.1	320.6	322.5	332.4	356.5
57		320.5±20.9	321.4	313.1	316.4	327.2	357.7
58		304.6±8.4	287.7	270.8	274.2	281.7	304.1
59		303.7±8.4	345.8	289.6	293.1	300.4	225.0
60		298.3±8.4	288.5	261.8	265.6	274.7	292.7
61		298.7±8.4	294.3	273.3	276.8	283.7	307.4
62		300.8±8.4	288.6	262.8	266.6	274.6	294.8
63		332.2±8.4	332.2	320.7	323.1	332.6	366.7
64		208.4±8.4	203.0	192.7	194.2	205.2	216.7
65		240.6	253.2	232.5	234.5	274.6	262.9
66		255.2	272.7	251.6	253.4	266.1	284.09
67		155	164.7	126.3	129.7	140.6	137.3
68		145	169.3	130.4	133.7	144.9	142.5

69		166	170.0	131.1	134.4	145.3	143.0
70		163	175.5	139.1	142.3	154.4	150.5
71		166	180.7	144.2	147.3	160.5	156.7
72		167	181.5	145.0	148.2	138.1	157.7

No.	compounds	Exp	B97-D	MPW1K	MPWB1K	MPWLYP1M	MPW1KCIS
1	H <sub>3</sub> C-OCH <sub>3</sub>	349.8±4.2	319.7	315.5	337.7	317.5	326.4.
2	H <sub>3</sub> C-OC <sub>2</sub> H <sub>5</sub>	348.1±4.2	338.7	333.3	355.7	335.6	345.1
3	C <sub>2</sub> H <sub>5</sub> -OCH <sub>3</sub>	353.1±5.4	320.5	319.4	341.0	318.0	326.3
4	C <sub>2</sub> H <sub>3</sub> -OC <sub>2</sub> H <sub>3</sub>	326.8±10.5	290.1	301.1	323.9	295.2	306.7
5	C <sub>2</sub> H <sub>5</sub> -OC <sub>2</sub> H <sub>3</sub>	272.8±10.5	230.2	238.4	262.7	233.1	242.5
6	C <sub>2</sub> H <sub>5</sub> -OC <sub>2</sub> H <sub>5</sub>	355.6±6.3	339.4	336.8	358.6	335.6	344.7
7	nC <sub>3</sub> H <sub>7</sub> -OCH <sub>3</sub>	356.5±6.3	317.5	312.5	334.6	310.6	319.3
8	H <sub>3</sub> C-OiC <sub>3</sub> H <sub>7</sub>	350.2±6.3	319.9	313.7	336.7	312.6	308.5
9	iC <sub>3</sub> H <sub>7</sub> -OCH <sub>3</sub>	358.6±4.2	316.1	313.2	335.4	309.2	302.9
10	C <sub>2</sub> H <sub>5</sub> -OC <sub>3</sub> H <sub>7</sub>	358.4±8.4	317.8	317.3	338.5	313.1	322.2
11	C <sub>3</sub> H <sub>7</sub> -OC <sub>2</sub> H <sub>5</sub>	355.2±8.4	340.5	336.9	358.7	334.8	344.2
12	C <sub>3</sub> H <sub>7</sub> -OC <sub>2</sub> H <sub>3</sub>	274.1±10.5	231.4	238.5	262.8	232.4	242.2
13	C <sub>4</sub> H <sub>9</sub> -OCH <sub>3</sub>	343.9±6.3	319.9	316.8	339.0	313.8	323.1
14	H <sub>3</sub> C-OC <sub>4</sub> H <sub>9</sub>	353.1±6.3	317.6	314.9	337.0	313.9	323.5
15	C <sub>2</sub> H <sub>5</sub> O-C <sub>3</sub> H <sub>7</sub>	356.9±6.3	340.5	336.9	358.7	334.8	344.2
16	C <sub>2</sub> H <sub>3</sub> -OC <sub>4</sub> H <sub>9</sub>	419.2±8.4	384.8	388.9	407.7	384.5	395.7
17	C <sub>4</sub> H <sub>9</sub> -OC <sub>2</sub> H <sub>3</sub>	273.2±10.5	234.5	242.4	266.7	235.6	245.9

18	$tC_4H_9-OC_2H_5$	$347.3 \pm 6.3$	326.6	318.3	342.3	311.1	318.7
19	$C_2H_5-OtC_4H_9$	$349.6 \pm 6.3$	316.3	310.1	333.6	304.3	315.0
20	$sC_4H_9-OnC_4H_9$	$348.2 \pm 8.4$	322.2	323.5	344.4	368.2	378.2
21	$sC_4H_9-OsC_4H_9$	$359.4 \pm 8.4$	317.5	305.4	331.3	343.7	354.8
22	$tC_4H_9-OtC_4H_9$	$324.7 \pm 8.4$	289.1	270.0	300.4	301.0	275.0
23	$nC_4H_9-OtC_4H_9$	$351.9 \pm 8.4$	318.4	311.5	335.0	352.5	364.2
24	$nC_4H_9O-tC_4H_9$	$348.1 \pm 8.4$	308.1	303.7	328.2	340.1	314.6
25	$iC_4H_9-OtC_4H_9$	$353.1 \pm 8.4$	312.2	311.4	335.7	352.2	363.7
26	$nC_5H_{11}-OtC_4H_9$	$349.4 \pm 8.4$	317.0	307.8	331.9	348.2	359.7
27		$416.7 \pm 5.9$	390.5	391.2	412.1	446.8	456.9
28		$268.6 \pm 7.1$	239.7	250.8	275.1	274.9	293.8
29		261.1	231.4	244.1	267.5	266.1	285.6
30		257.7	231.7	245.0	269.0	266.9	286.7
31		269.4	243.0	255.8	280.4	279.3	299.6
32		261.1	233.9	247.8	278.1	268.7	289.7
33		256.5	232.2	246.8	270.6	267.2	288.3
34		266.5	243.3	255.5	280.1	279.3	299.3
35		258.6	231.5	246.5	270.3	266.0	287.9
36		234.7	191.3	210.6	230.1	218.3	244.0
37		255.2	234.7	249.6	273.4	269.6	292.0
38		243.1	213.6	230.2	252.3	246.6	268.6

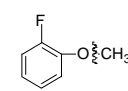
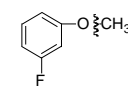
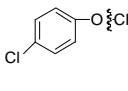
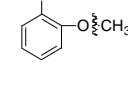
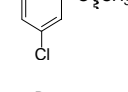
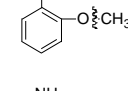
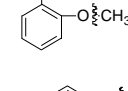
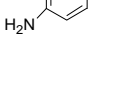
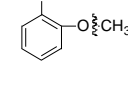
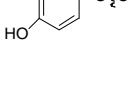
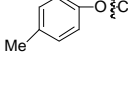
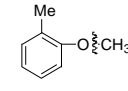
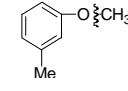
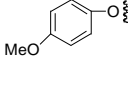
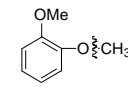
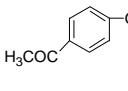
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40		257.7	230.6	242.9	266.7	264.6	284.2
41		254.8	236.8	248.4	272.5	271.2	290.4
42		263.6	237.0	243.3	272.5	271.6	291.0
43		260.2	228.0	225.8	266.4	261.6	284.4
44		248.1	206.7	200.8	246.1	235.4	263.4
45		268.2	247.7	258.8	282.7	283.8	303.0
46		259.4	226.9	234.8	258.8	257.1	275.5
47		266.5	248.5	257.5	282.1	284.9	301.9
48		255.2	222.4	230.0	261.0	254.9	276.6
49		266.9	248.7	261.0	287.8	280.2	306.7
50		265.3	246.4	260.2	284.6	282.9	304.4
51		270.3	251.9	261.9	286.6	289.0	307.1
52		263.6	252.7	262.8	287.3	290.2	307.9
53		282.4	249.3	259.0	283.7	286.2	303.4
54		260.7	244.8	258.0	281.3	280.7	301.3
55		416.7 ± 5.4	406.6	401.8	423.5	459.6	469.3
56		331.0 ± 10.5	296.1	313.0	334.4	342.6	356.6

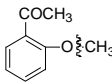
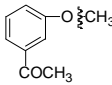
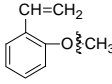
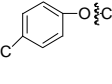
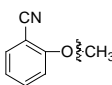
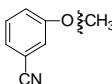
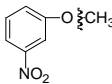
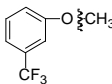
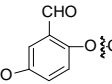
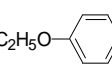
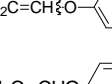
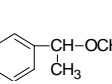
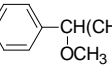
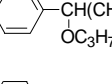
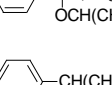
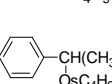


57		320.5 ±20.9	294.4	305.0	328.3	341.9	357.7
58		304.6 ±8.4	259.1	260.8	281.8	292.1	304.1
59		303.7 ±8.4	283.4	278.9	300.2	312.6	225.0
60		298.3 ±8.4	260.1	252.1	285.6	288.6	292.7
61		298.7 ±8.4	265.4	264.4	284.6	292.2	307.4
62		300.8 ±8.4	259.1	253.7	275.9	278.3	294.8
63		332.2 ±8.4	300.1	314.6	336.0	339.4	366.7
64		208.4 ±8.4	169.1	185.1	208.0	192.6	316.7
65		240.6	211.8	224.5	249.6	234.2	262.9
66		255.2	230.6	243.1	267.5	264.4	284.9
67		155	118.7	121.2	147.2	103.3	137.3
68		145	122.5	125.7	151.7	107.9	142.5
69		166	124.0	126.2	150.2	108.6	143.0
70		163	134.8	132.6	160.3	118.8	150.3
71		166	138.9	138.0	166.5	123.8	156.7
72		167	132.7	139.0	166.6	125.5	157.7

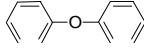
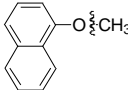
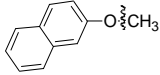
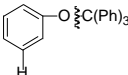
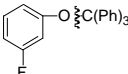
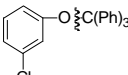
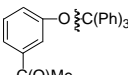
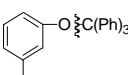
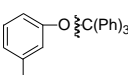
No.	compounds	Exp	CAM-B3LYP	B3LYP-D3	B97-D3	M06-2X	(wB97 opt)
1	H <sub>3</sub> C-OCH <sub>3</sub>	349.8 ±4.2	328.5	323.3	322.8	352.5	343.0
2	H <sub>3</sub> C-OC <sub>2</sub> H <sub>5</sub>	348.1 ±4.2	335.2	342.1	341.8	370.1	348.7

3	<chem>C2H5-OCH3</chem>	353.1±5.4	332.4	327.1	322.1	358.3	347.7
4	<chem>C2H3-OC2H3</chem>	326.8±10.5	309.1	305.6	295.6	330.7	315.6
5	<chem>C2H5-OC2H3</chem>	272.8±10.5	247.7	243.8	233.6	274.7	239.6
6	<chem>C2H5-OC2H5</chem>	355.6±6.3	338.6	345.7	340.8	375.7	353.6
7	<chem>nC3H7-OCH3</chem>	356.5±6.3	325.5	322.1	317.7	353.0	342.8
8	<chem>H3C-OiC3H7</chem>	350.2±6.3	326.3	322.9	321.1	337.2	343.1
9	<chem>iC3H7-OCH3</chem>	358.6±4.2	327.0	323.1	315.2	341.2	345.9
10	<chem>C2H5-OC3H7</chem>	358.4±8.4	329.5	324.7	318.4	356.3	345.7
11	<chem>C3H7-OC2H5</chem>	355.2±8.4	338.5	345.9	341.2	376.0	353.5
12	<chem>C3H7-OC2H3</chem>	274.1±10.5	247.7	244.1	234.0	274.9	256.5
13	<chem>C4H9-OCH3</chem>	343.9±6.3	329.9	325.5	320.0	356.3	346.9
14	<chem>H3C-OC4H9</chem>	353.1±6.3	327.3	322.3	320.0	352.3	342.0
15	<chem>c2H5O-c3H7</chem>	356.9±6.3	338.5	345.9	241.2	376.0	353.5
16	<chem>C2H3-OC4H9</chem>	419.2±8.4	399.9	394.8	388.9	420.0	409.2
17	<chem>C4H9-OC2H3</chem>	273.2±10.5	251.7	247.7	237.0	278.1	258.2
18	<chem>tC4H9-OC2H5</chem>	347.3±6.3	321.8	332.3	322.7	368.7	340.2
19	<chem>C2H5-OtC4H9</chem>	349.6±6.3	323.1	321.8	314.9	353.1	337.6
20	<chem>sC4H9-OnC4H9</chem>	348.2±8.4	335.8	329.9	322.5	418.9	351.7
21	<chem>sC4H9-OCsC4H9</chem>	359.4±8.4	319.3	322.7	313.7	414.6	346.1
22	<chem>tC4H9-OtC4H9</chem>	324.7±8.4	285.6	291.5	280.4	381.5	317.5
23	<chem>nC4H9-OtC4H9</chem>	351.9±8.4	324.4	323.3	315.9	410.3	347.5
24	<chem>nC4H9O-tC4H9</chem>	348.1±8.4	317.8	315.6	304.0	41.0	344.2
25	<chem>iC4H9-OtC4H9</chem>	353.1±8.4	324.3	325.0	318.1	412.6	346.1
26	<chem>nC5H11-OtC4H9</chem>	349.4±8.4	341.2	346.5	338.6	407.6	336.2
27	<chem>c1ccc(OCH3)cc1</chem>	416.7±5.9	403.0	400.7	393.9	493.9	418.7
28	<chem>c1ccc(OCC)cc1</chem>	268.6±7.1	255.2	251.6	244.1	336.5	265.5
29	<chem>Fc1ccc(OCC)cc1</chem>	261.1	248.5	244.6	235.8	326.7	258.0



30		257.7	249.4	245.5	236.1	327.9	259.6
31		269.4	260.4	256.1	247.4	342.6	271.0
32		261.1	252.1	247.5	238.1	331.8	262.6
33		256.5	251.0	246.9	236.9	330.4	261.5
34		266.5	260.2	256.2	247.7	342.6	270.9
35		258.6	248.6	256.3	258.4	330.0	232.9
36		234.7	210.6	205.9	195.2	280.5	233.3
37		255.2	253.5	248.6	239.1	335.4	265.0
38		243.1	234.2	229.7	217.8	309.0	244.5
39		266.9	252.1	247.9	239.0	333.4	263.1
40		257.7	246.8	243.0	235.0	326.3	257.6
41		254.8	252.2	249.2	241.0	330.0	256.4
42		263.6	252.8	249.1	241.3	333.9	263.4
43		260.2	246.1	241.5	232.4	324.6	243.2
44		248.1	226.8	221.9	210.5	300.7	238.6
45		268.2	262.8	259.6	252.1	283.6	272.4

46		259.4	238.2	236.6	230.6	256.3	264.0
47		266.5	262.6	259.8	252.9	283.9	272.4
48		255.2	240.7	236.4	226.8	320.5	252.0
49		266.9	268.3	265.3	257.8	260.1	278.1
50		265.3	264.3	260.3	251.1	255.5	274.5
51		270.3	267.1	263.9	256.3	258.6	276.8
52		263.6	267.9	264.8	257.0	259.5	277.4
53		282.4	264.3	261.2	253.4	346.4	274.1
54		260.7	262.8	260.3	249.5	344.1	274.0
55		416.7±5.4	402.5	415.1	409.3	416.6	419.8
56		331.0±10.5	316.1	313.8	302.2	402.7	341.5
57		320.5±20.9	313.1	312.5	300.0	390.9	305.4
58		304.6±8.4	274.7	269.6	259.5	358.2	293.4
59		303.7±8.4	281.0	292.2	283.7	290.0	300.2
60		298.3±8.4	264.7	268.5	258.9	298.8	289.7
61		298.7±8.4	277.0	275.8	265.3	363.7	296.6
62		300.8±8.4	266.7	268.2	256.9	355.2	290.2
63		332.2±8.4	317.8	320.2	306.5	407.4	329.0

64		208.4±8.4	190.5	186.0	172.1	270.2	201.8
65		240.6	228.1	225.4	216.2	305.6	237.1
66		255.2	245.2	243.6	234.9	327.1	256.7
67		155	157.1	162.6	148.4	223.0	159.8
68		145	133.6	147.7	128.1	162.7	161.2
69		166	134.2	149.4	129.9	165.6	161.6
70		163	141.0	155.6	138.4	170.3	166.8
71		166	146.3	160.3	142.6	146.7	172.1
72		167	147.4	161.7	143.6	147.2	154.1

Note: The values of (wb97 opt) are calculated at wb97/6-311++G(2df,2p)//wb97/6-31+G(d) level.