Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

On the radical scavenging activity of isoflavones: Thermodynamics of O–H bond cleavage

(*Electronic Supplementary Information*)

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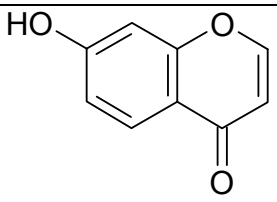
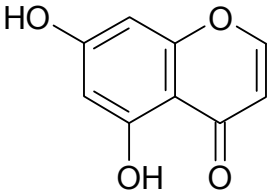
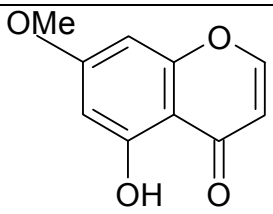
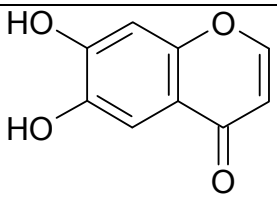
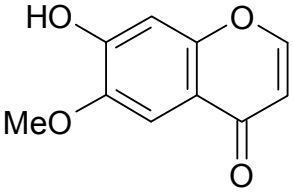
Model molecule	Parent molecules	Structure of model molecule
I	daidzein formononetin	
II	genistein biochanin A orobol	
III	prunetin santal	
IV	6-hydroxydaidzein	
V	glycitein	

Fig. 1S Model molecules without B ring.

Table 1S Published gas-phase reaction enthalpies in kJ mol^{-1}.

Molecule	BDE	IP	PDE	PA	ETE
daidzein[a]		733			
4'-OH	**340**		**924**	1419	**239**
7-OH	359		943	**1375**	306
formononetin[a]	703				
7-OH	358		976	1377	303
genistein[a]		724			
4'-OH	**339**		**945**	1411	**252**
5-OH	378		983	**1350**	308
7-OH	368		972	1373	316
biochanin A[a]	705				
5-OH	383		1001	**1369**	336
7-OH	**367**		**985**	1375	**315**
prunetin[b]		708			
4'-OH	**340**		**954**	**1411**	**251**
5-OH	469		1083	1450	340
glycitein[b]		704			
4'-OH	338		956	1425	**234**
7-OH	**336**		**954**	**1373**	285

a. J. Zhang, F. Du, B. Peng, R. Lu, H. Gao and Z. Zhou, *J. Mol. Struct. THEOCHEM*, 2010, **955**, 1–6.
b. K. Senthil kumar and R. Kumaresan, *Comp. Theor. Chem.*, 2012, **985**, 14–22.

Table 2S Gas-phase B3LYP/6-311+G** reaction enthalpies in kJ mol^{-1} of model molecules of isoflavones without B ring.

Model molecule	BDE	IP	PDE	PA	ETE
I		827			
7-OH	360		855	1378	304
II		792			
5-OH	415		945	1452	285
7-OH	371		894	1376	316
III		773			
5-OH	412		961	1457	277
IV		787			
6-OH	321		855	1365	278
7-OH	327		862	1345	305
V		767			
7-OH	358		912	1398	282

Table 3S Parameters of 5-OH hydrogen bonds in isoflavones and corresponding model molecules. Bond lengths in Ångströms, angle in deg.

Molecule	Bond lengths		Angle
	O–H	H···O	O–H···O
genistein	0.99296	1.68869	148.5
biochanin A	0.99315	1.68752	148.6
orobol	0.99347	1.68424	148.7
model **II**	*0.99273*	*1.70462*	*148.5*
santal	0.99296	1.68869	148.5
prunetin	0.99276	1.69000	148.5
model **III**	*0.99251*	*1.70588*	*148.6*

Table 4S Published reaction enthalpies in kJ mol^{-1} in benzene and water.[a]

Molecule	BDE	IP	PDE	PA	ETE
prunetin (benzene)		601			
4'-OH	**343**		**187**	**477**	**310**
5-OH	438		283	505	380
glycitein (benzene)		599			
4'-OH	341		187	485	**301**
7-OH	341		187	**440**	346
prunetin (water)		436			
4'-OH	**353**		**65**	**204**	**297**
5-OH	387		150	206	380
glycitein (water)		436			
4'-OH	**349**		**64**	207	**293**
7-OH	355		68	**169**	334

a. K. Senthil kumar and R. Kumaresan, *Comp. Theor. Chem.*, 2012, **985**, 14–22.