

SUPPLEMENTARY INFORMATION

Table . Isotropic hyperfine coupling constants of protons for the lutein triplet state as derived from DFT calculations

Position	a _{iso} (MHz)	
	Lut620	Lut621
1'	-6.0	-6.2
2'	2.6	2.4
4'	3.0	2.6
5'	-9.3	-9.5
6'	1.7	1.7
8'	-2.1	-2.1
9'	-7.3	7.3
1	-6.2	-6.2
2	2.5	2.3
4	2.7	2.9
5	-9.4	-9.1
6	1.4	1.6
8	-2.7	-2.5
9	-6.8	-7.0
Me-3	6.7	6.7
Me-7	9.0	8.8
Me-3'	7.0	6.8
Me-7'	8.8	8.6

Table . Mulliken Spin densities computed at the B3LYP/epr-II level for the triplet state of Lut620 and Lut621. Only densities larger than 0.02 (in absolute value) are reported.

atom	L620	L621
1	0.18	0.19
2	-0.08	-0.08
3	0.23	0.23
4	-0.09	-0.09
5	0.28	0.27
6	-0.06	-0.06
7	0.29	0.29
8	0.05	0.05
9	0.21	0.22
1'	0.19	0.19
2'	-0.09	-0.08
3'	0.24	0.23
4'	-0.09	-0.09
5'	0.28	0.28
6'	-0.05	-0.06
7'	0.29	0.29
8'	0.07	0.06
9'	0.20	0.20

Table . Isotropic hyperfine coupling constants of protons for the Lut620 triplet state as derived from DFT calculations by employing the PCM with $\epsilon = 2$ and $\epsilon = 3$.

Position	a_{iso} (MHz)	
	$\epsilon = 2$	$\epsilon = 3$
1'	-6.0	-6.0
2'	2.6	2.6
4'	3.0	3.0
5'	-9.3	-9.3
6'	1.7	1.7
8'	-2.1	-2.1
9'	-7.3	-7.3
1	-6.2	-6.2
2	2.5	2.5
4	2.7	2.7
5	-9.4	-9.4
6	1.4	1.4
8	-2.7	-2.7
9	-6.8	-6.8
Me-3	6.7	6.7
Me-7	9.0	9.0
Me-3'	7.0	7.0
Me-7'	8.8	8.8