

SUPPLEMENTARY MATERIAL

A comparison of homopolymer and block copolymer structure in 6FDA-based polyimides

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Partial charges were extracted via *ab initio* calculations at the B3LYP/6-31G** level for representative three-fragment structures based on the 6FDA dianhydride and the mPDA and durene diamines. The terms 6FDA_end, mPDA_end and durene_end stand for terminating groups.

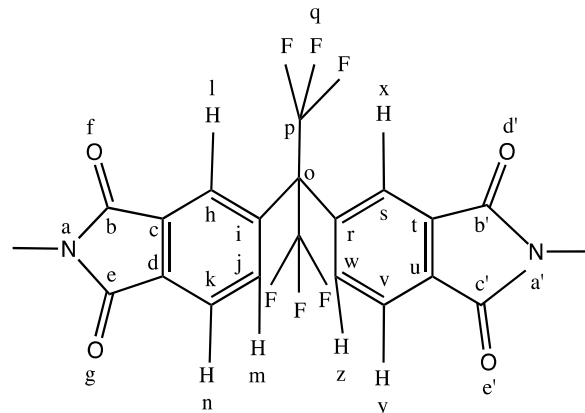
 6FDA	a	b	c	d	e	f	g	h	i	j	k
mPDA-6FDA-mPDA	-0.4475	0.6015	-0.0866	-0.0963	*	*	-0.4522	-0.1499	0.2291	-0.1488	-0.0964
durene-6FDA-durene	0.3200	0.3900	-0.1437	-0.1541	*	*	-0.4192	-0.0667	0.2690	-0.2098	-0.0112
mPDA-6FDA-durene	-0.3940	0.5944	-0.0344	-0.1361	*	*	-0.4308	-0.1911	0.2851	-0.1522	-0.0419
	l	m	n	o	p	q	r	s	t	u	v
mPDA-6FDA-mPDA	0.1331	0.1420	0.1395	-0.4088	0.3855	-0.1085	*	*	*	*	*
durene-6FDA-durene	0.1169	0.1462	0.1224	-0.5242	0.3704	-0.1014	*	*	*	*	*
mPDA-6FDA-durene	0.1413	0.1500	0.1401	-0.5686	0.4292	-0.0992	0.2851	-0.0195	-0.1574	-0.1361	-0.0419
	w	x	y	z	a'	b'	c'	d'	e'		
mPDA-6FDA-mPDA	*	*	*	*	*	*	*	*	*		
durene-6FDA-durene	*	*	*	*	*	*	*	*	*		
mPDA-6FDA-durene	-0.1522	0.1413	0.1401	0.1500	0.1820	0.4628	*	*	-0.4181		

Table S1. Partial charges for 6FDA fragment.

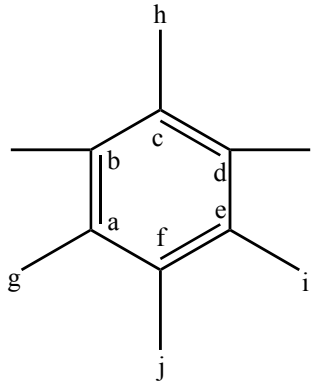
 <p style="text-align: center;">mPDA</p>	a	b	c	d	e	f	g	h	i	J
6FDA-mPDA-6FDA	-0.3793	0.4667	-0.4975	*	*	-0.0508	0.1893	0.2387	*	0.1098

Table S2. As table S1 for mPDA fragment.

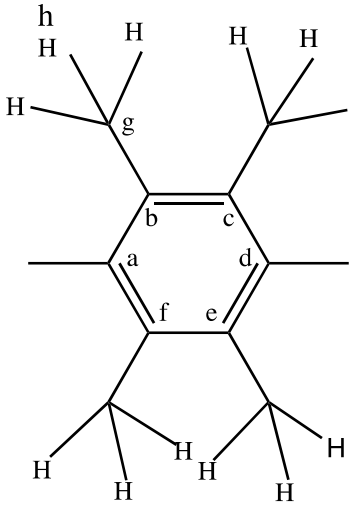
 <p style="text-align: center;">durene</p>	a	b	c	d	e	f	g	h
6FDA-durene-6FDA	-0.4137	0.1693	*	*	*	*	-0.2926	0.0876

Table S3. As table S1 for durene fragment.

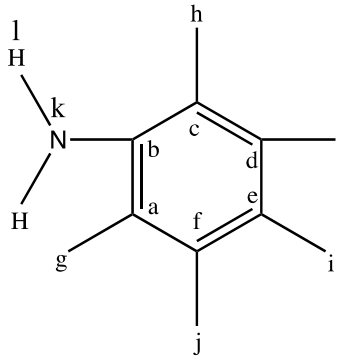
 <p style="text-align: center;">mPDA_end</p>	a	b	c	d	e	f	g	h	i	j
mPDA_end-6FDA-mPDA	-0.3289	0.4834	-0.4746	0.4020	-0.3559	-0.0176	0.1632	0.2099	0.1764	0.1230
	k	l								
	-0.7895	0.3250								

Table S4. As table S1 for mPDA_end fragment.

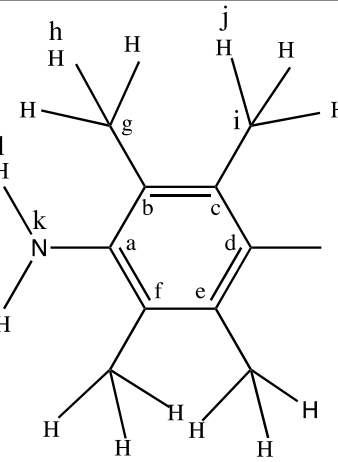
 <p style="text-align: center;">durene_end</p>	a	b	c	d	e	f	g	h
durene_end-6FDA-durene	0.3007	0.0132	0.1518	-0.6036	*	*	-0.3173	0.0966
	i	j	k	l				
	-0.3034	0.0981	-0.8647	0.3490				

Table S5. As table S1 for durene_end fragment.

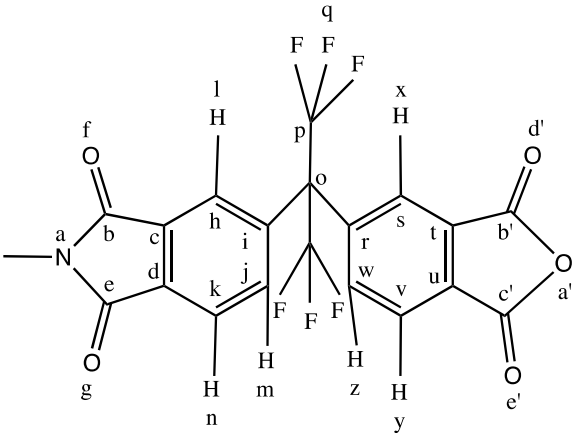
 6FDA_end	a	b	c	d	e	f	g	h	i	j	k
6FDA-mPDA-6FDA end	-0.4054	0.5418	-0.0342	-0.1307	0.5915	-0.4244	-0.4489	-0.1945	0.2658	-0.1543	-0.0877
6FDA-durene-6FDA end	-0.3932	0.5571	-0.0219	-0.1185	0.6068	-0.4141	-0.4379	-0.1822	0.2781	-0.1420	-0.0754
	l	m	n	o	p	q	r	s	t	u	v
6FDA-mPDA-6FDA end	0.1380	0.1448	0.1388	-0.5365	0.4526	-0.1212	0.3258	-0.1749	-0.0839	-0.1566	-0.0985
6FDA-durene-6FDA end	0.1503	0.1571	0.1511	-0.5243	0.4648	-0.1089	0.3381	-0.1626	-0.0717	-0.1443	-0.0863
	w	x	y	z	a'	b'	c'	d'	e'		
6FDA-mPDA-6FDA end	-0.1335	0.1293	0.1450	0.1308	-0.4282	0.6771	0.700	-0.4241	-0.4318		
6FDA-durene-6FDA end	-0.1212	0.1415	0.1573	0.1430	-0.4159	0.6864	0.7153	-0.4132	-0.4208		

Table S6. As table S1 for 6FDA_end fragment.