Supporting Information

STRUCTURAL EFFECTS INFLUENCING THE *CIS-TRANS* ISOMERISATION IN METHOXY AND CYANO SUBSTITUTED STILBENE DERIVATIVES

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Cartesian coordinates for the calculated geometries of *Z*- and *E*-1-cyano-1,2-bis(2-methoxyphenyl)ethene (CBMPE) **1** at the B3LYP/6-31G* level.

	Z			*E*		
	x	***y***	***z***	***x***	***y***	***z***
C(1A)	-1.4975	-0.1284	-1.3609	1.5566	0.0935	-0.5021
C(2A)	-1.3336	-0.3546	-2.7580	2.9595	-0.1286	-0.5056
C(3A)	-2.4050	-0.1867	-3.6393	3.8514	0.9479	-0.5365
C(4A)	-3.6529	0.2051	-3.1521	3.3620	2.2547	-0.5715
C(5A)	-3.8395	0.4260	-1.7888	1.9886	2.4954	-0.5831
C(6A)	-2.7730	0.2574	-0.9099	1.1025	1.4218	-0.5500
O(9A)	-0.0851	-0.7298	-3.1619	3.3517	-1.4345	-0.4657
C(10A)	0.1397	-1.0008	-4.5369	4.7376	-1.7357	-0.5341
H(3A)	-2.2753	-0.3552	-4.7018	4.9215	0.7773	-0.5307
H(4A)	-4.4779	0.3337	-3.8476	4.0642	3.0837	-0.5950
H(5A)	-4.8113	0.7229	-1.4065	1.6081	3.5115	-0.6265
H(6A)	-2.9341	0.4176	0.1485	0.0350	1.6064	-0.5821
H(10A1)	1.1880	-1.2944	-4.6137	4.8051	-2.8247	-0.5234
H(10A2)	-0.4958	-1.8208	-4.8953	5.2790	-1.3302	0.3302
H(10A3)	-0.0338	-0.1105	-5.1547	5.1878	-1.3506	-1.4580
C(7)	-0.1020	0.0144	0.7958	-0.6174	-1.1845	-0.1080
C(8)	-0.3428	-0.3480	-0.4950	0.6663	-1.0687	-0.5374
H(8)	0.4737	-0.8755	-0.9771	1.1070	-1.9589	-0.9771
C(11)	-1.0277	0.7867	1.5738	-1.2785	-2.4358	-0.3647
N(12)	-1.7839	1.3836	2.2286	-1.8111	-3.4541	-0.5538
C(1B)	1.1421	-0.4317	1.4852	-1.3927	-0.1872	0.6866
C(2B)	1.9336	0.4702	2.2360	-2.6537	0.2681	0.2406
C(3B)	3.0925	0.0241	2.8793	-3.3981	1.1580	1.0234
C(4B)	3.4826	-1.3128	2.7692	-2.8895	1.6006	2.2464
C(5B)	2.7232	-2.2109	2.0239	-1.6460	1.1626	2.6978
C(6B)	1.5595	-1.7648	1.3956	-0.9108	0.2697	1.9175
O(9B)	1.5015	1.7603	2.2538	-3.0515	-0.2023	-0.9739
C(10B)	2.1579	2.6956	3.0953	-4.3672	0.0861	-1.4228
H(3B)	3.6999	0.7135	3.4542	-4.3661	1.5097	0.6856
H(4B)	4.3856	-1.6452	3.2743	-3.4770	2.2911	2.8456
H(5B)	3.0194	-3.2526	1.9444	-1.2548	1.5010	3.6525
H(6B)	0.9396	-2.4647	0.8425	0.0522	-0.0931	2.2642
H(10B1)	2.1509	2.3667	4.1421	-4.4828	-0.4524	-2.3646
H(10B2)	1.5916	3.6235	3.0028	-4.5062	1.1610	-1.5990
H(10B3)	3.1938	2.8675	2.7744	-5.1203	-0.2657	-0.7065
E (a.u.)	-861.9916574			-861.9890714		

Cartesian coordinates for the calculated geometries of *Z*- and *E*-1-cyano-2-(2-methoxyphenyl)-1-phenylethene (CPMPE) **2** at the B3LYP/6-31G* level.

	Z			*E*		
	x	***y***	***z***	***x***	***y***	***z***
C(1A)	0.9387	1.3063	-0.2316	1.0886	0.1003	-0.6510
C(2A)	2.3510	1.1789	-0.3741	2.4889	-0.1261	-0.5938
C(3A)	3.1607	2.3108	-0.4989	3.3854	0.9468	-0.6266
C(4A)	2.5862	3.5827	-0.4869	2.9019	2.2523	-0.7248
C(5A)	1.2063	3.7327	-0.3569	1.5304	2.4963	-0.7979
C(6A)	0.3989	2.6059	-0.2343	0.6400	1.4268	-0.7623
O(9A)	2.8398	-0.0946	-0.3714	2.8705	-1.4312	-0.4961
C(10A)	4.2343	-0.2965	-0.5475	4.2567	-1.7423	-0.5025
H(3A)	4.2347	2.2109	-0.6017	4.4540	0.7742	-0.5743
H(4A)	3.2266	4.4553	-0.5829	3.6071	3.0786	-0.7497
H(5A)	0.7571	4.7211	-0.3573	1.1562	3.5111	-0.8922
H(6A)	-0.6730	2.7346	-0.1516	-0.4253	1.6118	-0.8423
H(10A1)	4.3813	-1.3777	-0.5325	4.3161	-2.8308	-0.4570
H(10A2)	4.8109	0.1592	0.2671	4.7667	-1.3144	0.3698
H(10A3)	4.5809	0.1055	-1.5080	4.7441	-1.3875	-1.4194
C(7)	-1.1325	-0.1286	0.2704	-1.0967	-1.1774	-0.2876
C(8)	0.1514	0.0832	-0.1362	0.1942	-1.0581	-0.7007
H(8)	0.7002	-0.8093	-0.4158	0.6334	-1.9422	-1.1548
C(11)	-1.9490	0.9221	0.8058	-1.7674	-2.4042	-0.6235
N(12)	-2.6483	1.7364	1.2588	-2.3327	-3.3851	-0.8970
C(1B)	-1.7667	-1.4752	0.2333	-1.9051	-0.2059	0.5044
C(2B)	-2.7967	-1.8052	1.1310	-1.3618	0.4373	1.6285
C(3B)	-3.3736	-3.0736	1.1199	-2.1346	1.3181	2.3818
C(4B)	-2.9406	-4.0374	0.2081	-3.4637	1.5672	2.0302
C(5B)	-1.9304	-3.7162	-0.7011	-4.0175	0.9211	0.9241
C(6B)	-1.3547	-2.4480	-0.6947	-3.2472	0.0356	0.1710
H(2B)	-3.1422	-1.0637	1.8454	-0.3338	0.2369	1.9128
H(3B)	-4.1639	-3.3078	1.8280	-1.7007	1.8032	3.2520
H(4B)	-3.3937	-5.0248	0.1971	-4.0656	2.2523	2.6210
H(5B)	-1.5995	-4.4504	-1.4309	-5.0530	1.1009	0.6482
H(6B)	-0.5985	-2.2026	-1.4343	-3.6869	-0.4759	-0.6808
E (a.u.)	-747.4724845			-747.4680214		

Cartesian coordinates for the calculated geometries of *E*- and *Z*-1,2-bis-(2-methoxyphenyl)ethene (BMPE) **3** at the B3LYP/6-31G* level.

	E			*Z*		
	x	***y***	***z***	***x***	***y***	***z***
C(1A)	-1.8954	0.4041	-0.2276	-1.5433	0.2068	0.5131
C(2A)	-3.0791	-0.2912	0.1352	-2.9248	0.3031	0.2114
C(3A)	-4.3211	0.3500	0.1157	-3.8121	-0.7129	0.5813
C(4A)	-4.4095	1.6913	-0.2635	-3.3381	-1.8364	1.2622
C(5A)	-3.2627	2.3930	-0.6308	-1.9861	-1.9457	1.5824
C(6A)	-2.0287	1.7468	-0.6164	-1.1077	-0.9279	1.2128
O(9A)	-2.9114	-1.5985	0.5027	-3.3047	1.4345	-0.4574
C(10A)	-4.0534	-2.3579	0.8589	-4.6788	1.6202	-0.7504
H(3A)	-5.2213	-0.1842	0.3971	-4.8667	-0.6386	0.3421
H(4A)	-5.3809	2.1785	-0.2756	-4.0356	-2.6206	1.5448
H(5A)	-3.3283	3.4324	-0.9394	-1.6170	-2.8106	2.1260
H(6A)	-1.1414	2.2867	-0.9331	-0.0582	-0.9989	1.4787
H(10A1)	-3.6845	-3.3569	1.0993	-4.7488	2.5856	-1.2554
H(10A2)	-4.7701	-2.4259	0.0296	-5.2887	1.6427	0.1626
H(10A3)	-4.5593	-1.9383	1.7385	-5.0594	0.8354	-1.4175
C(7)	0.6076	0.2942	-0.2022	0.6514	1.3299	-0.1760
C(8)	-0.6076	-0.2942	-0.2022	-0.6514	1.3299	0.1760
H(7)	0.6747	1.3768	-0.1529	1.1260	2.3063	-0.2474
H(8)	-0.6747	-1.3768	-0.1529	-1.1260	2.3063	0.2474
C(1B)	1.8954	-0.4041	-0.2276	1.5433	0.2068	-0.5131
C(2B)	3.0791	0.2912	0.1352	2.9248	0.3031	-0.2114
C(3B)	4.3211	-0.3500	0.1157	3.8121	-0.7129	-0.5813
C(4B)	4.4095	-1.6913	-0.2635	3.3381	-1.8364	-1.2622
C(5B)	3.2627	-2.3930	-0.6308	1.9861	-1.9457	-1.5824
C(6B)	2.0287	-1.7468	-0.6164	1.1077	-0.9279	-1.2128
O(9B)	2.9114	1.5985	0.5027	3.3047	1.4345	0.4574
C(10B)	4.0534	2.3579	0.8589	4.6788	1.6202	0.7504
H(3B)	5.2213	0.1842	0.3971	4.8667	-0.6386	-0.3421
H(4B)	5.3809	-2.1785	-0.2756	4.0356	-2.6206	-1.5448
H(5B)	3.3283	-3.4324	-0.9394	1.6170	-2.8106	-2.1260
H(6B)	1.1414	-2.2867	-0.9331	0.0582	-0.9989	-1.4787
H(10B1)	3.6845	3.3569	1.0993	4.7488	2.5856	1.2554
H(10B2)	4.7701	2.4259	0.0296	5.2887	1.6427	-0.1626
H(10B3)	4.5593	1.9383	1.7385	5.0594	0.8354	1.4175
E (a.u.)	-769.7531249			-769.7460814		

Cartesian coordinates for the calculated geometries

of *E*- and *Z*-stilbene at the B3LYP/6-31G* level.

	E			*Z*		
	x	***y***	***z***	***x***	***y***	***z***
C(1A)	-1.9421	-0.1642	-0.0043	-1.6380	0.7182	0.1629
C(2A)	-2.8430	-1.2435	0.0655	-2.9212	0.8701	-0.3930
C(3A)	-4.2213	-1.0393	0.0725	-3.8843	-0.1302	-0.2707
C(4A)	-4.7367	0.2556	0.0077	-3.5917	-1.3003	0.4317
C(5A)	-3.8575	1.3408	-0.0654	-2.3302	-1.4560	1.0126
C(6A)	-2.4816	1.1358	-0.0729	-1.3653	-0.4600	0.8825
H(2A)	-2.4489	-2.2561	0.1167	-3.1587	1.7839	-0.9331
H(3A)	-4.8923	-1.8925	0.1283	-4.8652	0.0077	-0.7180
H(4A)	-5.8107	0.4203	0.0121	-4.3422	-2.0793	0.5355
H(5A)	-4.2485	2.3536	-0.1199	-2.0992	-2.3551	1.5781
H(6A)	-1.8201	1.9948	-0.1371	-0.3950	-0.5853	1.3513
C(7)	0.5037	0.4481	-0.0038	0.6738	1.8276	-0.0381
C(8)	-0.5037	-0.4481	-0.0038	-0.6738	1.8276	0.0381
H(7)	0.2605	1.5097	0.0042	1.1433	2.8115	-0.0228
H(8)	-0.2605	-1.5097	0.0042	-1.1433	2.8115	0.0228
C(1B)	1.9421	0.1642	-0.0043	1.6380	0.7182	-0.1629
C(2B)	2.8430	1.2435	0.0655	2.9212	0.8701	0.3930
C(3B)	4.2213	1.0393	0.0725	3.8843	-0.1302	0.2707
C(4B)	4.7367	-0.2556	0.0077	3.5917	-1.3003	-0.4317
C(5B)	3.8575	-1.3408	-0.0654	2.3302	-1.4560	-1.0126
C(6B)	2.4816	-1.1358	-0.0729	1.3653	-0.4600	-0.8825
H(2B)	2.4489	2.2561	0.1167	3.1587	1.7839	0.9331
H(3B)	4.8923	1.8925	0.1283	4.8652	0.0077	0.7180
H(4B)	5.8107	-0.4203	0.0121	4.3422	-2.0793	-0.5355
H(5B)	4.2485	-2.3536	-0.1199	2.0992	-2.3551	-1.5781
H(6B)	1.8201	-1.9948	-0.1371	0.3950	-0.5853	-1.3513
E (a.u.)		-540.7099729			-540.7019205	

Experimental (δ) and calculated (HF and DFT) ^{1}H chemical shifts (ppm), with reference to TMS, for *Z*-CBMPE **1** and *Z*-CPMPE **2** (see text for details).

		d			**J**	**HF**		**DFT**	
Z-CPMPE	H(6A)	8.14	dd	1H	7.8, 1.5	9.39	H(6A)	8.67	H(6A)
	H(8)	7.94	s	1H		8.74	H(8)	8.13	H(8)
	H(2B),H(6B)	7.68	m	2H		8.07	H(2B),H(6B)	7.62	H(2B),H(6B)
	H(4A)	7.33-7.44	m	4H		7.9	H(4A)	7.38	H(4A)
	H(3B),H(5B)	7.33-7.44	m			7.71	H(3B),H(5B)	7.34	H(3B),H(5B)
	H(4B)	7.33-7.44	m			7.62	H(4B)	7.3	H(4B)
	H(5A)	7.03	t	1H	7.8	7.34	H(5A)	7.05	H(5A)
	H(3A)	6.92	dd	1H	8.4, 0.9	6.87	H(3A)	6.47	H(3A)
	CH_3	3.87	s	3H		3.89	CH_3	3.81	CH_3
Z-CBMPE	H(6A)	8.18	dd	1H	7.8, 1.4	9.50	H(6A)	8.82	H(6A)
	H(8)	7.82	s	1H		8.33	H(8)	7.62	H(8)
	H(6B)	7.43	dd	1H	7.5, 1.7	7.87	H(4A)	7.37	H(4A)
	H(4A)	7.38	ddd	1H	8.3, 7.3, 1.5	7.79	H(6B)	7.33	H(4B)
	H(4B)	7.34	ddd	1H	8.2, 7.5, 1.7	7.79	H(4B)	7.25	H(6B)
	H(5A)	7.06	t	1H	7.3	7.33	H(5A)	7.09	H(5A)
	H(5B)	7.01	dt	1H	7.5, 1.1	7.20	H(5B)	6.97	H(5B)
	H(3B)	6.96	dd	1H	8.3, 0.8	6.93	H(3B)	6.54	H(3B)
	H(3A)	6.92	dd	1H	8.3, 0.7	6.84	H(3A)	6.45	H(3A)
	CH_3(B)	3.92	s	3H		3.90	CH_3(B)	3.88	CH_3(B)
	CH_3(A)	3.86	s	3H		3.83	CH_3(A)	3.82	CH_3(A)