

Toward an Understanding of the Ambiguous Electron Paramagnetic Resonance Spectra of the Iminoxy Radical from o-Fluorobenzaldehyde Oxime: Density Functional Theory and *ab Initio* Studies

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Isotropic hyperfine couplings calculated using EPR-II and EPR-III basis sets; experimental values are the ones determined from the dominant EPR spectrum of unknown isomer/conformer

		E^{anti}			E^{syn}			Z^{anti}			Z^{syn}		
		A_N	A_{CH3}	A_F	A_N	A_{CH3}	A_F	A_N	A_{CH3}	A_F	A_N	A_{CH3}	A_F
VACUUM ε = 1.00	BP/EPR-II	28.90	-1.52	-0.37	31.96	-1.52	22.33	31.78	-1.52	0.42	28.69	-1.52	8.16
	BP/EPR-III	29.05	-1.48	-0.40	31.99	-1.49	22.04	29.95	-0.96	0.31	28.85	-1.49	7.81
	B3LYP/EPR-II	30.78	-2.18	-0.69	34.04	-2.17	21.62	32.01	-2.08	-0.35	30.54	-2.06	6.58
	B3LYP/EPR-III	29.05	-1.48	-0.40	31.99	-1.49	22.04	29.95	-0.96	0.31	28.85	-1.49	7.81
	TPSS/EPR-II	28.11	-1.43	-0.51	31.24	-1.42	20.23	29.18	-1.52	0.14	27.98	-1.52	7.14
	TPSS/EPR-III	29.93	-1.34	-0.60	33.02	-1.36	21.28	30.89	-1.46	-0.08	29.77	-1.49	7.14
	B2PLYP/EPR-II	28.95	0.56	4.67	31.93	0.87	30.06	30.11	0.93	5.77	29.84	0.23	9.82
	B2PLYP/EPR-III	28.68	0.72	4.71	31.42	1.04	29.75	29.68	1.07	5.77	29.56	0.34	9.55
	OO-SCS-RI-MP2/EPR-II	32.97	-1.21	-0.27	36.68	-1.26	21.93	34.11	-0.99	-0.01	32.84	-0.92	7.08
	OO-SCS-RI-MP2/EPR-III	32.52	-0.96	-0.22	35.89	-1.00	21.05	33.49	-0.81	0.05	32.34	-0.49	6.65
	QCISD/EPR-II	30.37	-3.08	1.05	34.38	-3.34	20.60	31.94	-2.91	0.50	29.86	-2.27	9.61
PhCH₃ ε = 2.40	BP/EPR-II	29.09	-1.48	-0.34	31.78	-1.49	22.67	29.93	-1.55	0.54	29.02	-1.55	8.22
	BP/EPR-III	29.29	-1.44	-0.37	31.89	-1.46	22.33	30.03	-1.51	0.45	29.19	-1.51	7.85
	B3LYP/EPR-II	31.13	-2.15	-0.65	33.99	-2.14	22.02	32.08	-2.10	-0.17	31.03	-2.08	6.62
	B3LYP/EPR-III	31.20	-2.08	-0.65	33.93	-2.08	21.77	32.04	-2.03	-0.22	31.07	-2.01	6.41
	TPSS/EPR-II	28.31	-1.39	-0.48	31.07	-1.39	20.57	29.20	-1.56	0.28	28.31	-1.54	7.21
	TPSS/EPR-III	30.20	-1.31	-0.57	32.94	-1.32	21.62	30.98	-1.50	0.08	30.14	-1.50	7.18
	B2PLYP/EPR-II	29.46	0.40	4.15	31.89	0.77	29.91	30.50	0.63	4.87	30.39	0.12	9.60
	B2PLYP/EPR-III	29.24	0.56	4.20	31.47	1.80	29.59	30.16	0.75	4.87	30.12	0.23	9.32
	OO-SCS-RI-MP2/EPR-II	32.91	-1.21	-0.27	36.65	-1.25	21.88	33.85	-0.99	0.14	32.69	-0.92	7.01
	OO-SCS-RI-MP2/EPR-III	32.46	-0.95	-0.21	35.87	-0.99	21.01	33.28	-0.81	0.18	32.20	-0.48	6.59
	QCISD/EPR-II	30.49	-2.95	1.17	34.10	-3.27	20.66	31.63	-2.73	1.06	30.07	-2.20	9.42
	EXP*	31.95	1.50	6.60	31.95	1.50	6.60	31.95	1.50	6.60	31.95	1.50	6.60
CH₂Cl₂ ε = 9.08	BP/EPR-II	29.24	-1.44	-0.31	31.60	-1.46	23.07	30.01	-1.58	0.66	29.37	-1.56	8.39
	BP/EPR-III	29.49	-1.40	-0.34	31.80	-1.42	22.68	30.17	-1.53	0.58	29.56	-1.52	7.99
	B3LYP/EPR-II	31.46	-2.12	-0.60	33.97	-2.11	22.47	32.24	-2.12	-0.01	31.55	-2.09	6.74
	B3LYP/EPR-III	31.60	-2.05	-0.61	34.01	-2.05	22.19	32.27	-2.05	-0.05	31.62	-2.02	6.50
	TPSS/EPR-II	28.49	-2.04	-0.45	30.90	-1.36	20.95	29.28	-1.59	0.41	28.66	-1.56	7.38
	TPSS/EPR-III	30.44	-2.21	-0.52	32.88	-1.28	22.00	31.12	-1.52	0.26	30.52	-1.50	7.31
	B2PLYP/EPR-II	29.96	0.25	3.69	31.94	0.64	29.80	30.98	0.34	4.11	30.98	-0.01	9.50
	B2PLYP/EPR-III	29.79	0.42	3.77	31.59	0.79	29.46	30.69	0.47	4.14	30.73	0.10	9.23
	OO-SCS-RI-MP2/EPR-II	32.85	-1.20	-0.23	36.63	-1.25	21.89	33.63	-0.99	0.28	32.57	-0.92	7.03
	OO-SCS-RI-MP2/EPR-III	32.42	-0.95	-0.20	35.86	-0.98	21.02	33.08	-0.81	0.31	32.08	-0.75	6.61
	QCISD/EPR-II	30.52	-2.82	1.31	33.79	-3.19	20.85	31.40	-2.55	1.64	30.30	-2.13	9.37
	EXP	32.25	1.50	7.50	32.25	1.50	7.50	32.25	1.50	7.50	32.25	1.50	7.50
CH₃CN ε = 36.6	BP/EPR-II	29.29	-2.12	-0.30	31.54	-1.44	23.24	30.04	-1.59	0.71	29.37	-1.56	8.39
	BP/EPR-III	29.57	-1.39	-0.33	31.77	-1.41	22.83	30.23	-1.55	0.63	29.71	-1.52	8.06
	B3LYP/EPR-II	31.58	-2.10	-0.58	33.96	-2.10	22.67	32.32	-2.12	0.06	31.76	-2.09	6.81
	B3LYP/EPR-III	31.76	-2.03	-0.59	34.04	-2.03	22.37	32.38	-2.05	0.01	31.84	-2.03	6.56
	TPSS/EPR-II	28.56	-1.35	-0.44	30.85	-1.34	21.12	29.32	-1.59	0.47	28.80	-1.57	7.46
	TPSS/EPR-III	30.53	-1.25	-0.51	32.87	-1.26	22.17	31.19	-1.52	0.33	30.68	-1.51	7.38
	B2PLYP/EPR-II	30.14	0.20	3.55	31.97	0.58	29.77	31.18	0.23	3.84	31.22	-0.06	9.50
	B2PLYP/EPR-III	30.00	0.36	3.63	31.67	1.65	29.40	30.92	0.35	3.88	30.98	0.05	9.22
	OO-SCS-RI-MP2/EPR-II	32.91	-1.22	-0.16	36.63	-1.24	21.91	33.54	-0.99	0.34	32.53	-0.91	7.06
	OO-SCS-RI-MP2/EPR-III	32.40	-0.94	-0.19	35.86	-0.98	21.02	33.00	-0.81	0.36	32.04	-0.75	6.64
	QCISD/EPR-II	30.51	-2.78	1.35	33.67	-3.15	20.95	31.32	-1.01	1.88	30.40	-2.11	9.38
	EXP	32.35	1.50	9.25	32.35	1.50	9.25	32.35	1.50	9.25	32.35	1.50	9.25
DMF ε = 38.3	BP/EPR-II	29.29	-1.42	-0.30	31.54	-1.44	23.25	30.04	-1.59	0.71	29.50	-1.56	8.49
	BP/EPR-III	29.57	-1.39	-0.33	31.77	-1.41	22.84	30.23	-1.54	0.63	29.72	-1.52	8.06
	B3LYP/EPR-II	31.59	-2.10	-0.58	33.96	-2.10	22.67	32.32	-2.12	0.06	31.76	-2.08	6.81
	B3LYP/EPR-III	31.76	-2.03	-0.59	34.04	-2.03	22.38	32.38	-2.05	0.01	31.84	-2.03	6.57
	TPSS/EPR-II	28.56	-1.34	-0.44	30.85	-1.34	21.13	29.32	-1.59	0.47	28.80	-1.57	7.46

DMSO $\epsilon = 42.7$	TPSS/EPR-III	30.53	-1.25	-0.51	32.86	-1.25	22.20	31.19	-1.51	0.33	30.69	-1.51	7.39
	B2PLYP/EPR-II	30.15	0.20	3.53	31.97	0.58	29.77	31.19	0.23	3.83	31.22	-0.06	9.50
	B2PLYP/EPR-III	30.00	0.36	3.61	31.67	0.73	29.40	30.93	0.35	3.88	30.98	0.05	9.22
	OO-SCS-RI-MP2/EPR-II	32.91	-1.22	-0.16	36.63	-1.24	21.92	33.54	-0.99	0.34	32.52	-0.91	7.06
	OO-SCS-RI-MP2/EPR-III	32.41	-0.94	-0.19	35.86	-0.98	21.04	33.00	-0.81	0.37	32.04	-0.68	6.64
	QCISD/EPR-II	30.50	-2.78	1.37	33.67	-3.15	20.95	31.32	-2.47	1.89	30.40	-2.11	9.38
	EXP	32.35	1.50	10.00	32.35	1.50	10.00	32.35	1.50	10.00	32.35	1.50	10.00
	BP/EPR-II	29.29	-1.42	-0.30	31.53	-1.44	23.26	30.04	-1.59	0.71	29.51	-1.56	8.50
	BP/EPR-III	29.58	-1.38	-0.33	31.77	-1.40	22.86	30.23	-1.54	0.63	29.73	-1.52	8.07
	B3LYP/EPR-II	31.59	-2.10	-0.58	33.97	-2.10	22.69	32.32	-2.12	0.07	31.78	-2.09	6.82
	B3LYP/EPR-III	31.77	-2.03	-0.59	34.05	-2.03	22.39	32.39	-2.05	0.01	31.86	-2.03	6.57
	TPSS/EPR-II	28.56	-1.34	-0.44	30.85	-1.34	21.13	29.32	-1.59	0.47	28.80	-1.57	7.46
	TPSS/EPR-III	30.54	-1.25	-0.51	32.87	-1.27	22.18	31.20	-1.54	0.32	30.70	-1.51	7.39
	B2PLYP/EPR-II	30.16	0.19	3.52	31.98	0.58	29.77	31.20	0.22	3.81	31.24	-0.06	9.50
	B2PLYP/EPR-III	30.02	0.35	3.60	31.67	0.73	29.43	30.94	0.34	3.85	31.00	0.05	9.22
	OO-SCS-RI-MP2/EPR-II	32.83	-1.19	-0.23	36.63	-1.24	21.92	33.53	-0.99	0.34	32.52	-0.91	7.07
	OO-SCS-RI-MP2/EPR-III	32.41	-0.94	-0.19	35.86	-0.98	21.04	33.00	-0.81	0.37	32.04	-0.75	6.65
	QCISD/EPR-II	30.50	-2.77	1.38	33.66	-3.15	20.96	31.32	-2.47	1.91	30.40	-2.11	9.38
	EXP	32.40	1.50	10.60	32.40	1.50	10.60	32.40	1.50	10.60	32.40	1.50	10.60

* Experimental values determined in benzene

Relative energies between *anti* and *syn* rotamers for *E* and *Z* isomers ($\Delta E^{anti/syn}$, in kcal/mol), molar fractions of the rotamers determined from Boltzmann distribution (x), and hyperfine coupling constants for *E* and *Z* isomers averaged according to molar fractions of rotamers ($\bar{A}$, in Gauss). The $\Delta E^{anti/syn}$ values at the B2PLYP/TZVP and QCISD/TZVP theory levels were calculated using geometries and the ZPE corrections from B3LYP/TZVP calculations.

VACUUM $\epsilon = 1.00$		B3LYP/TZVP			B2PLYP/TZVP			QCISD/TZVP			B3LYP/TZVP			B2PLYP/TZVP			QCISD/TZVP		
		E^{anti}	E^{syn}		E^{anti}	E^{syn}		E^{anti}	E^{syn}		Z^{anti}	Z^{syn}		Z^{anti}	Z^{syn}		Z^{anti}	Z^{syn}	
$\Delta E^{anti/syn}$		0.00	0.73		0	1.21		0.00	1.11		0.00	1.90		0.00	1.62		0.00	1.96	
x		0.774	0.226		0.886	0.114		0.866	0.134		0.961	0.039		0.939	0.061		0.965	0.035	
		$\bar{A}_N$	$\bar{A}_F$	$\bar{A}_{CH3}$	$\bar{A}_N$	$\bar{A}_F$	$\bar{A}_{CH3}$	$\bar{A}_N$	$\bar{A}_F$	$\bar{A}_{CH3}$	$\bar{A}_N$	$\bar{A}_F$	$\bar{A}_{CH3}$	$\bar{A}_N$	$\bar{A}_F$	$\bar{A}_{CH3}$	$\bar{A}_N$	$\bar{a}_F$	$\bar{a}_{CH3}$
BP/EPR-II		29.59	4.76	-1.52	29.25	2.22	-1.52	29.31	2.66	-1.52	31.66	0.72	-1.52	31.59	0.89	-1.52	31.67	0.69	-1.52
BP/EPR-III		29.72	4.67	-1.48	29.39	2.16	-1.48	29.45	2.60	-1.48	29.91	0.61	-0.98	29.88	0.78	-0.99	29.91	0.58	-0.98
B3LYP/EPR-II		31.51	4.35	-2.18	31.15	1.86	-2.18	31.21	2.29	-2.18	31.95	-0.07	-2.08	31.92	0.08	-2.08	31.95	-0.10	-2.08
B3LYP/EPR-III		29.72	4.67	-1.48	29.39	2.16	-1.48	29.45	2.60	-1.48	29.91	0.61	-0.98	29.88	0.78	-0.99	29.91	0.58	-0.98
TPSS/EPR-II		28.82	4.17	-1.43	28.47	1.86	-1.43	28.53	2.26	-1.43	29.13	0.42	-1.52	29.10	0.57	-1.52	29.13	0.39	-1.52
TPSS/EPR-III		30.63	4.34	-1.35	30.28	1.90	-1.35	30.34	2.32	-1.35	30.84	0.20	-1.46	30.82	0.36	-1.47	30.85	0.17	-1.46
B2PLYP/EPR-II		29.62	10.41	0.63	29.29	7.57	0.59	29.35	8.06	0.60	30.10	5.93	0.90	30.09	6.02	0.89	30.10	5.92	0.91
B2PLYP/EPR-III		29.30	10.37	0.79	28.99	7.57	0.75	29.05	8.05	0.76	29.67	5.92	1.04	29.67	6.00	1.02	29.67	5.90	1.04
OO-SCS-RI-MP2/EPR-II		33.81	4.75	-1.22	33.40	2.27	-1.22	33.47	2.70	-1.22	34.06	0.27	-0.98	34.03	0.43	-0.98	34.07	0.24	-0.98
OO-SCS-RI-MP2/EPR-III		33.28	4.58	-0.97	32.90	2.21	-0.96	32.97	2.62	-0.96	33.44	0.30	-0.80	33.42	0.45	-0.79	33.45	0.28	-0.80
QCISD/EPR-II		31.27	5.47	-3.14	30.82	3.29	-3.11	30.90	3.66	-3.11	31.85	0.74	-2.89	31.81	0.88	-2.87	31.86	0.72	-2.89
PhCH ₃ $\epsilon = 2.40$		B3LYP/TZVP			B2PLYP/TZVP			QCISD/TZVP			B3LYP/TZVP			B2PLYP/TZVP			QCISD/TZVP		
		E^{anti}	E^{syn}		E^{anti}	E^{syn}		E^{anti}	E^{syn}		Z^{anti}	Z^{syn}		Z^{anti}	Z^{syn}		Z^{anti}	Z^{syn}	
$\Delta E^{anti/syn}$		0.00	0.34		0.00	0.48		0.00	0.83		0.00	1.72		0.00	1.38		0.00	1.49	
x		0.638	0.362		0.812	0.188		0.803	0.197		0.948	0.052		0.911	0.089		0.926	0.074	
		$\bar{A}_N$	$\bar{A}_F$	$\bar{A}_{CH3}$	$\bar{A}_N$	$\bar{A}_F$	$\bar{A}_{CH3}$	$\bar{A}_N$	$\bar{A}_F$	$\bar{A}_{CH3}$	$\bar{A}_N$	$\bar{A}_F$	$\bar{A}_{CH3}$	$\bar{A}_N$	$\bar{A}_F$	$\bar{A}_{CH3}$	$\bar{A}_N$	$\bar{a}_F$	$\bar{a}_{CH3}$
BP/EPR-II		30.06	7.99	-1.49	29.59	3.99	-1.48	29.61	4.18	-1.48	29.89	0.94	-1.55	29.85	1.23	-1.55	29.86	1.12	-1.55
BP/EPR-III		30.23	7.85	-1.45	29.78	3.90	-1.45	29.80	4.09	-1.45	29.99	0.83	-1.51	29.96	1.11	-1.51	29.97	1.00	-1.51
B3LYP/EPR-II		32.17	7.56	-2.15	31.67	3.62	-2.15	31.69	3.81	-2.15	32.03	0.18	-2.10	31.99	0.44	-2.10	32.00	0.34	-2.10
B3LYP/EPR-III		32.19	7.47	-2.08	31.72	3.57	-2.08	31.74	3.76	-2.08	31.99	0.13	-2.03	31.95	0.37	-2.03	31.97	0.28	-2.03
TPSS/EPR-II		29.31	7.14	-1.39	28.83	3.48	-1.39	28.85	3.66	-1.39	29.15	0.64	-1.56	29.12	0.89	-1.56	29.13	0.79	-1.56
TPSS/EPR-III		31.19	7.46	-1.31	30.71	3.60	-1.31	30.74	3.79	-1.31	30.93	0.44	-1.50	30.90	0.71	-1.50	30.91	0.61	-1.50
B2PLYP/EPR-II		30.34	13.47	0.53	29.92	8.99	0.47	29.94	9.21	0.47	30.49	5.11	0.60	30.49	5.29	0.58	30.49	5.22	0.59
B2PLYP/EPR-III		30.05	13.39	1.01	29.66	8.98	0.80	29.68	9.19	0.81	30.16	5.10	0.72	30.16	5.26	0.70	30.16	5.20	0.71
OO-SCS-RI-MP2/EPR-II		34.26	7.75	-1.22	33.61	3.90	-1.22	33.64	4.09	-1.22	33.79	0.50	-0.98	33.75	0.75	-0.98	33.77	0.65	-0.98
OO-SCS-RI-MP2/EPR-III		33.70	7.47	-0.97	33.10	3.78	-0.96	33.13	3.96	-0.96	33.22	0.52	-0.80	33.18	0.75	-0.79	33.20	0.66	-0.79
QCISD/EPR-II		31.79	8.23	-3.06	31.17	4.84	-3.01	31.20	5.00	-3.01	31.54	0.82	-2.70	31.49	1.04	-2.68	31.51	0.96	-2.69
EXP (BENZENE)		31.95	6.60	1.50	31.95	6.60	1.50	31.95	6.60	1.50	31.95	6.60	1.50	31.95	6.60	1.50	31.95	6.60	1.50
CH ₂ Cl ₂ $\epsilon = 9.08$		B3LYP/TZVP			B2PLYP/TZVP			QCISD/TZVP			B3LYP/TZVP			B2PLYP/TZVP			QCISD/TZVP		
		E^{anti}	E^{syn}		E^{anti}	E^{syn}		E^{anti}	E^{syn}		Z^{anti}	Z^{syn}		Z^{anti}	Z^{syn}		Z^{anti}	Z^{syn}	
$\Delta E^{anti/syn}$		0.10	0.00		0.00	0.48		0.00	0.55		0.00	1.30		0.00	1.13		0.00	1.49	
x		0.456	0.544		0.692	0.308		0.717	0.283		0.900	0.100		0.871	0.129		0.926	0.074	
		$\bar{A}_N$	$\bar{A}_F$	$\bar{A}_{CH3}$	$\bar{A}_N$	$\bar{A}_F$	$\bar{A}_{CH3}$	$\bar{A}_N$	$\bar{A}_F$	$\bar{A}_{CH3}$	$\bar{A}_N$	$\bar{A}_F$	$\bar{A}_{CH3}$	$\bar{A}_N$	$\bar{A}_F$	$\bar{A}_{CH3}$	$\bar{A}_N$	$\bar{a}_F$	$\bar{a}_{CH3}$
BP/EPR-II		30.52	12.40	-1.45	29.96	6.88	-1.44	29.91	6.31	-1.44	29.94	1.44	-1.58	29.92	1.66	-1.58	29.96	1.24	-1.58
BP/EPR-III		30.75	12.18	-1.41	30.20	6.74	-1.41	30.15	6.18	-1.41	30.11	1.32	-1.53	30.09	1.53	-1.53	30.12	1.13	-1.53

	B3LYP/EPR-II	32.82	11.94	-2.11	32.23	6.50	-2.12	32.17	5.93	-2.12	32.17	0.67	-2.11	32.15	0.86	-2.11	32.19	0.50	-2.12
	B3LYP/EPR-III	32.91	11.79	-2.05	32.34	6.41	-2.05	32.28	5.84	-2.05	32.21	0.60	-2.04	32.19	0.79	-2.04	32.22	0.43	-2.04
	TPSS/EPR-II	29.80	11.19	-1.67	29.23	6.14	-1.83	29.17	5.61	-1.85	29.22	1.11	-1.58	29.20	1.31	-1.58	29.23	0.93	-1.58
	TPSS/EPR-III	31.77	11.72	-1.70	31.19	6.40	-1.93	31.13	5.85	-1.95	31.06	0.97	-1.51	31.04	1.17	-1.51	31.07	0.78	-1.51
	B2PLYP/EPR-II	31.03	17.89	0.46	30.57	11.73	0.37	30.52	11.08	0.36	30.98	4.65	0.31	30.98	4.81	0.30	30.98	4.51	0.31
	B2PLYP/EPR-III	30.77	17.74	0.62	30.34	11.67	0.53	30.30	11.04	0.52	30.70	4.65	0.43	30.70	4.80	0.42	30.70	4.52	0.44
	OO-SCS-RI-MP2/EPR-II	34.91	11.80	-1.22	34.01	6.57	-1.21	33.92	6.03	-1.21	33.52	0.96	-0.98	33.49	1.15	-0.98	33.55	0.79	-0.98
	OO-SCS-RI-MP2/EPR-III	34.29	11.34	-0.97	33.48	6.33	-0.96	33.39	5.81	-0.96	32.98	0.95	-0.81	32.95	1.13	-0.81	33.00	0.78	-0.81
	QCISD/EPR-II	32.30	11.93	-3.02	31.52	7.32	-2.94	31.44	6.84	-2.93	31.29	1.14	-2.50	31.25	1.31	-2.49	31.31	0.99	-2.52
	EXP	32.25	7.50	1.50	32.25	7.50	1.50	32.25	7.50	1.50	32.25	7.50	1.50	32.25	7.50	1.50	32.25	7.50	1.50
CH ₃ CN ε = 36.6		B3LYP/TZVP			B2PLYP/TZVP			QCISD/TZVP			B3LYP/TZVP			B2PLYP/TZVP			QCISD/TZVP		
		<i>E^{anti}</i>	<i>E^{syn}</i>		<i>E^{anti}</i>	<i>E^{syn}</i>		<i>E^{anti}</i>	<i>E^{syn}</i>		<i>Z^{anti}</i>	<i>Z^{syn}</i>		<i>Z^{anti}</i>	<i>Z^{syn}</i>		<i>Z^{anti}</i>	<i>Z^{syn}</i>	
	Δ <i>E^{anti/syn}</i>	0.24	0.00		0.00	0.36		0.00	0.49		0.00	1.24		0.00	1.02		0.00	1.46	
	x	0.402	0.598		0.646	0.354		0.695	0.305		0.890	0.110		0.849	0.151		0.922	0.078	
		<i>A_N</i>	<i>A_F</i>	<i>A_{CH3}</i>	<i>A_N</i>	<i>A_F</i>	<i>A_{CH3}</i>	<i>A_N</i>	<i>A_F</i>	<i>A_{CH3}</i>	<i>A_N</i>	<i>A_F</i>	<i>A_{CH3}</i>	<i>A_N</i>	<i>A_F</i>	<i>A_{CH3}</i>	<i>A_N</i>	<i>a_F</i>	<i>a_{CH3}</i>
	BP/EPR-II	30.63	13.78	-1.71	30.09	8.04	-1.88	29.98	6.89	-1.91	29.97	1.56	-1.59	29.94	1.87	-1.59	29.99	1.31	-1.59
	BP/EPR-III	30.89	13.52	-1.40	30.35	7.87	-1.39	30.24	6.74	-1.39	30.17	1.45	-1.54	30.15	1.75	-1.54	30.19	1.21	-1.54
	B3LYP/EPR-II	33.01	13.32	-2.10	32.43	7.65	-2.10	32.31	6.52	-2.10	32.26	0.81	-2.12	32.23	1.08	-2.12	32.27	0.59	-2.12
	B3LYP/EPR-III	33.12	13.14	-2.03	32.57	7.54	-2.03	32.45	6.42	-2.03	32.32	0.73	-2.05	32.30	1.00	-2.05	32.34	0.52	-2.05
	TPSS/EPR-II	29.93	12.45	-1.34	29.37	7.19	-1.35	29.26	6.15	-1.35	29.26	1.24	-1.59	29.24	1.52	-1.59	29.28	1.01	-1.59
	TPSS/EPR-III	31.93	13.05	-1.26	31.36	7.52	-1.26	31.24	6.41	-1.26	31.13	1.11	-1.52	31.11	1.39	-1.52	31.15	0.88	-1.52
B2PLYP/EPR-II	31.24	19.23	0.43	30.79	12.84	0.33	30.70	11.56	0.32	31.19	4.46	0.20	31.19	4.69	0.18	31.18	4.28	0.21	
B2PLYP/EPR-III	31.00	19.04	1.13	30.59	12.75	0.82	30.51	11.50	0.75	30.93	4.47	0.32	30.93	4.69	0.31	30.93	4.30	0.33	
OO-SCS-RI-MP2/EPR-II	35.13	13.04	-1.23	34.22	7.65	-1.23	34.04	6.58	-1.23	33.43	1.08	-0.98	33.39	1.35	-0.98	33.46	0.86	-0.98	
OO-SCS-RI-MP2/EPR-III	34.47	12.49	-0.97	33.63	7.31	-0.96	33.46	6.28	-0.96	32.90	1.06	-0.81	32.86	1.31	-0.80	32.93	0.85	-0.81	
QCISD/EPR-II	32.40	13.07	-3.01	31.63	8.29	-2.91	31.47	7.34	-2.90	31.22	1.20	-1.13	31.18	1.44	-1.18	31.25	1.01	-1.10	
EXP	32.35	9.25	1.50	32.35	9.25	1.50	32.35	9.25	1.50	32.35	9.25	1.50	32.35	9.25	1.50	32.35	9.25	1.50	
DMF ε = 38.3		B3LYP/TZVP			B2PLYP/TZVP			QCISD/TZVP			B3LYP/TZVP			B2PLYP/TZVP			QCISD/TZVP		
		<i>E^{anti}</i>	<i>E^{syn}</i>		<i>E^{anti}</i>	<i>E^{syn}</i>		<i>E^{anti}</i>	<i>E^{syn}</i>		<i>Z^{anti}</i>	<i>Z^{syn}</i>		<i>Z^{anti}</i>	<i>Z^{syn}</i>		<i>Z^{anti}</i>	<i>Z^{syn}</i>	
	Δ <i>E^{anti/syn}</i>	0.27	0.00		0.00	0.33		0.00	0.46		0.00	1.22		0.00	0.98		0.00	1.41	
	x	0.389	0.611		0.635	0.365		0.687	0.313		0.887	0.113		0.840	0.160		0.916	0.084	
		<i>A_N</i>	<i>A_F</i>	<i>A_{CH3}</i>	<i>A_N</i>	<i>A_F</i>	<i>A_{CH3}</i>	<i>A_N</i>	<i>A_F</i>	<i>A_{CH3}</i>	<i>A_N</i>	<i>A_F</i>	<i>A_{CH3}</i>	<i>A_N</i>	<i>A_F</i>	<i>A_{CH3}</i>	<i>A_N</i>	<i>a_F</i>	<i>a_{CH3}</i>
	BP/EPR-II	30.66	14.10	-1.43	30.11	8.31	-1.43	30.00	7.08	-1.43	29.98	1.59	-1.59	29.96	1.95	-1.58	30.00	1.37	-1.59
	BP/EPR-III	30.92	13.84	-1.40	30.38	8.14	-1.39	30.26	6.93	-1.39	30.17	1.47	-1.54	30.15	1.82	-1.54	30.18	1.25	-1.54
	B3LYP/EPR-II	33.04	13.64	-2.10	32.45	7.92	-2.10	32.33	6.71	-2.10	32.26	0.82	-2.12	32.23	1.14	-2.12	32.27	0.63	-2.12
	B3LYP/EPR-III	33.16	13.45	-2.03	32.59	7.80	-2.03	32.47	6.61	-2.03	32.32	0.75	-2.05	32.30	1.06	-2.05	32.34	0.56	-2.05
	TPSS/EPR-II	29.96	12.75	-1.34	29.39	7.44	-1.34	29.27	6.32	-1.34	29.26	1.26	-1.59	29.24	1.59	-1.59	29.28	1.06	-1.59
	TPSS/EPR-III	31.95	13.37	-1.25	31.38	7.79	-1.25	31.26	6.61	-1.25	31.13	1.12	-1.51	31.11	1.46	-1.51	31.14	0.92	-1.51
B2PLYP/EPR-II	31.26	19.58	0.43	30.81	13.12	0.34	30.72	11.76	0.32	31.19	4.47	0.19	31.19	4.74	0.18	31.19	4.31	0.20	
B2PLYP/EPR-III	31.03	19.38	0.58	30.61	13.03	0.49	30.53	11.69	0.47	30.93	4.48	0.32	30.93	4.73	0.30	30.93	4.33	0.33	
OO-SCS-RI-MP2/EPR-II	35.18	13.34	-1.23	34.27	7.91	-1.23	34.07	6.76	-1.22	33.43	1.10	-0.98	33.38	1.41	-0.98	33.45	0.91	-0.98	
OO-SCS-RI-MP2/EPR-III	34.52	12.79	-0.97	33.67	7.57	-0.96	33.49	6.46	-0.95	32.89	1.07	-0.80	32.85	1.37	-0.79	32.92	0.89	-0.80	
QCISD/EPR-II	32.44	13.35	-3.01	31.66	8.53	-2.91	31.50	7.51	-2.90	31.22	1.23	-2.43	31.17	1.50	-2.41	31.24	1.06	-2.44	
EXP	32.35	10.00	1.50	32.35	10.00	1.50	32.35	10.00	1.50	32.35	10.00	1.50	32.35	10.00	1.50	32.35	10.00	1.50	

$\varepsilon = 42.7$ [illegible]