SUPPORTING INFORMATION

Performance of DFT for C_{60} Isomerization Energies: A Noticeable Exception to Jacob's Ladder

(Tables S1–S3, 8 pages)

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Table S1. Minimum and maximum relative errors for the isomerization energies in the iso-C60 database. The isomerization energy for which the minimum and maximum errors are obtained are given in parenthesis.

Type	Method	Min	Max
GGA	BLYP	0.4 (8)	6.2 (5)
	BLYP-D3	1.8 (8)	6.3 (5)
	BLYP-D3BJ	0.6 (3)	5.1 (5)
	B97D	2.3 (8)	7.1 (5)
	HCTH407	0.3 (8)	5.4 (5)
	PBE	1.5 (8)	6.7 (5)
	PBE-D3	1.8 (3)	6.6 (5)
	PBE-D3BJ	1.2 (3)	6.1 (5)
	BP86	1.0 (8)	6.5 (5)
	BPW91	0.7 (8)	6.2 (5)
	SOGGA11	4.7 (3)	10.0 (7)
	N12	0.2 (3)	4.6 (5)
MGGA	M06L	0.2 (7)	4.1 (8)
	M06L-D3	0.1 (7)	4.6 (8)
	TPSS	0.4 (3)	4.6 (5)
	TPSS-D3	0.3 (3)	4.6 (5)
	TPSS-D3BJ	0.6 (3)	3.9 (5)
	tHCTH	0.3 (3)	4.9 (5)
	VSXC	0.3 (3)	4.6 (8)
	BB95	3.5 (3)	8.4 (5)
	M11L	0.0 (5)	4.2 (8)
	MN12L	4.0 (5)	9.1 (8)
	MN15L	0.3 (7)	4.5 (3)
HGGA	BH&HLYP	16.5 (3)	28.4 (8)
	BH&HLYP-D3	16.4 (3)	27.3 (8)
	BH&HLYP-D3BJ	17.5 (3)	27.0 (8)
	B3LYP	5.6 (2)	11.8 (8)
	B3LYP-D3	5.6 (2)	10.1 (8)
	B3LYP-D3BJ	6.6 (6)	9.8 (8)
	X3LYP	6.3 (2)	12.7 (8)
	B3P86	5.9 (2)	10.8 (8)
	B3PW91	5.7 (2)	10.7 (8)
	B3PW91-D3	5.5 (6)	8.7 (8)
	B3PW91-D3BJ	6.5 (6)	8.5 (8)
	PBE0	7.4 (2)	12.6 (8)
	PBE0-D3	7.4 (2)	11.6 (8)
	PBE0-D3BJ	8.1 (2)	11.4 (8)
	PBEh1PBE	7.4 (2)	12.8 (8)
	B971	4.8 (2)	10.7 (8)
	B98	5.4 (2)	11.7 (8)
	SOGGA11X	12.0 (3)	20.1 (8)
	APF	6.7 (2)	11.8 (8)

	APFD	5.9 (2)	9.2 (8)
	mPW1PW91	7.7 (2)	13.2 (8)
	mPW1LYP	7.5 (2)	14.6 (8)
	mPW1PBE	7.6 (2)	13.0 (8)
	mPW3PBE	5.6 (2)	10.5 (8)
	HSEH1PBE	6.2 (2)	10.9 (8)
	OHSE2PBE	6.6 (2)	11.4 (8)
HMGGA	PW6B95	7.1 (2)	12.5 (8)
	PW6B95-D3	7.0 (2)	12.1 (8)
	PW6B95-D3BJ	7.5 (2)	11.8 (8)
	M05	5.0 (2)	9.0 (8)
	M05-D3	5.0 (2)	8.5 (8)
	M052X	13.6 (3)	22.8 (8)
	M052X-D3	13.7 (3)	23.0 (8)
	M06	4.9 (2)	9.2 (8)
	M06-D3	5.1 (2)	9.2 (8)
	M062X	11.8 (3)	20.2 (8)
	M062X-D3	11.9 (3)	20.7 (8)
	M06HF	16.2 (3)	34.7 (5)
	M06HF-D3	16.3 (3)	34.8 (5)
	M08HX	12.4 (3)	21.0 (8)
	MN15	6.4 (3)	13.7 (8)
	BMK	9.6 (2)	17.3 (8)
	BMK-D3	9.4 (2)	15.6 (8)
	BMK-D3BJ	10.6 (2)	15.7 (8)
	B1B95	7.0 (2)	11.9 (8)
	B1B95-D3	6.8 (2)	10.7 (8)
	B1B95-D3BJ	8.0 (2)	10.4 (8)
	TPSSh	1.4 (5)	6.5 (8)
	TPSSh-D3	1.4 (5)	5.1 (8)
	TPSSh-D3BJ	2.8 (5)	5.4 (3)
	tHCTHh	2.6 (6)	7.8 (8)
RS	CAM-B3LYP	13.1 (3)	24.8 (8)
	CAM-B3LYP-D3	13.1 (3)	23.8 (8)
	CAM-B3LYP-D3BJ	13.8 (3)	23.6 (8)
	LC-wPBE	17.1 (3)	33.8 (5)
	LC-wPBE-D3	17.1 (3)	33.7 (5)
	LC-wPBE-D3BJ	17.9 (3)	34.3 (5)
	LC-wHPBE	17.1 (3)	33.8 (5)
	wB97	15.7 (3)	32.7 (8)
	wB97X	15.3 (3)	31.1 (8)
	wB97XD	13.0 (3)	24.8 (8)
	N12SX	6.6 (6)	11.2 (8)
	M11	16.2 (3)	29.8 (5)
	MN12SX	6.9 (2)	11.2 (8)
	LC-BLYP	19.8 (3)	38.5 (8)

	LC-PBE	20.2 (3)	37.9 (5)
	LC-BP86	19.9 (3)	37.7 (5)
	LC-BPW91	20.3 (3)	38.1 (5)
DH	B2PLYP	0.9 (4)	4.0 (5)
	B2PLYP-D3	1.2 (4)	4.1 (5)
	B2PLYP-D3BJ	0.7 (4)	3.9 (8)
	mPW2PLYP	0.1 (5)	5.2 (3)
	B2GPPLYP	0.3 (4)	4.7 (3)
	B2GPPLYP-D3	0.2 (4)	4.7 (3)
	B2GPPLYP-D3BJ	0.4 (6)	5.2 (3)
	B2KPLYP	0.1 (6)	5.5 (3)
	B2TPLYP	0.3 (6)	4.6 (3)
	DSDBLYP	1.8 (4)	6.7 (8)
	DSDPBEP86	0.8 (4)	7.0 (8)
	PBE0DH	8.8 (6)	10.8 (8)
	PBEQIDH	2.1 (8)	8.0 (3)
Ab initio	HF	28.4 (3)	54.2 (8)
	HF-D3	28.5 (3)	52.2 (8)
	HF-D3BJ	34.9 (3)	55.9 (5)
	MP2	1.1 (3)	28.9 (8)
	SCS-MP2	0.4 (3)	19.8 (8)
	SCS-MP2opt	0.4 (7)	9.9 (3)
	SOS-MP2	0.7 (2)	15.2 (8)
	SCS(MI)-MP2	0.9 (6)	9.1 (3)
	SCSN-MP2	0.4 (7)	13.5 (3)
	SCS-MP2-vdW	2.7 (3)	29.0 (8)
	S2-MP2	2.1 (3)	29.5 (8)

Table S2. Statistical analysis for the performance of conventional DFT and DHDFT procedures for the isomerization energies in the iso-C_{60} database (in kJ mol^{-1}). The G4(MP2) reference values are given in Figure 1 of the main text.

Type	Method	RMSD	MAD	MSD	LND	LPD
GGA	BLYP	24.3	20.9	-19.6	-35.2 (7)	4.3 (8)
	BLYP-D3	26.7	24.1	-24.1	-37.9 (7)	N/A
	BLYP-D3BJ	21.8	19.2	-19.2	-30.1 (7)	N/A
	B97D	31.8	29.1	-29.1	-45.6 (7)	N/A
	HCTH407	20.3	16.4	-15.6	-31.4 (7)	2.8 (8)
	PBE	27.5	24.5	-24.5	-40.7 (7)	N/A
	PBE-D3	29.0	26.2	-26.2	-41.6 (7)	N/A
	PBE-D3BJ	27.0	24.2	-24.2	-38.2 (7)	N/A
	BP86	26.6	23.4	-23.4	-39.4 (7)	N/A
	BPW91	24.6	21.1	-21.1	-36.7 (7)	N/A
	SOGGA11	52.6	48.5	-48.5	-69.6 (7)	N/A
	N12	17.5	14.7	-11.6	-26.3 (7)	10.1 (8)
MGGA	M06L	17.7	10.6	8.7	-5.3 (5)	44.4 (8)
	M06L-D3	19.4	11.4	9.9	-4.8 (5)	49.0 (8)
	TPSS	17.9	15.4	-12.3	-26.2 (7)	11.1 (8)
	TPSS-D3	18.3	15.1	-15.1	-27.8 (7)	N/A
	TPSS-D3BJ	15.3	12.8	-12.3	-23.2 (7)	1.8 (3)
	tHCTH	18.5	15.9	-11.7	-27.3 (5)	14.6 (8)
	VSXC	26.6	22.1	-22.1	-49.2 (8)	N/A
	BB95	38.3	35.3	-35.3	-52.8 (7)	N/A
	M11L	18.1	10.8	10.7	-0.3 (5)	45.0 (8)
	MN12L	44.2	35.9	35.9	N/A	98.1 (8)
	MN15L	18.8	11.9	11.9	N/A	46.4 (8)
HGGA	BH&HLYP	158.4	137.3	137.3	N/A	305.3 (8)
	BH&HLYP-D3	154.0	134.4	134.4	N/A	292.7 (8)
	BH&HLYP-D3BJ	156.2	138.0	138.0	N/A	289.6 (8)
	B3LYP	57.3	45.9	45.9	N/A	126.7 (8)
	B3LYP-D3	50.8	42.0	42.0	N/A	108.4 (8)
	B3LYP-D3BJ	53.1	46.3	46.3	N/A	105.5 (8)
	X3LYP	62.7	51.0	51.0	N/A	136.3 (8)
	B3P86	54.1	44.6	44.6	N/A	116.4 (8)
	B3PW91	53.2	43.7	43.7	N/A	114.8 (8)
	B3PW91-D3	45.6	39.3	39.3	N/A	92.9 (8)
	B3PW91-D3BJ	48.5	43.7	43.7	N/A	90.9 (8)
	PBE0	65.4	55.4	55.4	N/A	134.9 (8)
	PBE0-D3	62.1	53.5	53.5	N/A	125.0 (8)
	PBE0-D3BJ	63.1	55.5	55.5	N/A	122.7 (8)
	PBEh1PBE	66.5	56.2	56.2	N/A	137.5 (8)
	B971	51.6	40.9	40.9	N/A	115.0 (8)
	B98	57.1	45.7	45.7	N/A	125.8 (8)
	SOGGA11X	110.6	95.7	95.7	N/A	215.5 (8)
	APF	60.4	50.6	50.6	N/A	126.8 (8)

	APFD	49.0	42.1	42.1	N/A	99.2 (8)
	mPW1PW91	68.8	58.2	58.2	N/A	142.0 (8)
	mPW1LYP	73.6	60.7	60.7	N/A	156.5 (8)
	mPW1PBE	67.7	57.3	57.3	N/A	139.4 (8)
	mPW3PBE	52.1	42.8	42.8	N/A	112.5 (8)
	HSEH1PBE	55.2	46.0	46.0	N/A	117.5 (8)
	OHSE2PBE	58.2	48.7	48.7	N/A	122.9 (8)
HMGGA	PW6B95	65.3	55.2	55.2	N/A	134.4 (8)
	PW6B95-D3	63.8	54.2	54.2	N/A	130.2 (8)
	PW6B95-D3BJ	64.0	55.4	55.4	N/A	126.8 (8)
	M05	46.4	39.1	39.1	N/A	96.2 (8)
	M05-D3	44.9	38.3	38.3	N/A	91.8 (8)
	M052X	131.8	115.7	115.7	N/A	244.3 (8)
	M052X-D3	132.6	116.4	116.4	N/A	246.6 (8)
	M06	48.1	40.4	40.4	N/A	99.2 (8)
	M06-D3	48.4	40.9	40.9	N/A	99.3 (8)
	M062X	117.3	102.8	102.8	N/A	217.4 (8)
	M062X-D3	119.0	104.0	104.0	N/A	222.2 (8)
	M06HF	194.0	169.2	169.2	N/A	348.1 (8)
	M06HF-D3	195.0	169.9	169.9	N/A	350.9 (8)
	M08HX	121.2	106.2	106.2	N/A	225.6 (8)
	MN15	74.8	63.3	63.3	N/A	147.5 (8)
	BMK	94.7	81.2	81.2	N/A	186.0 (8)
	BMK-D3	88.1	76.7	76.7	N/A	167.1 (8)
	BMK-D3BJ	91.7	81.2	81.2	N/A	168.3 (8)
	B1B95	62.9	53.6	53.6	N/A	128.3 (8)
	B1B95-D3	58.1	50.3	50.3	N/A	115.0 (8)
	B1B95-D3BJ	60.2	53.9	53.9	N/A	111.5 (8)
	TPSSh	28.0	18.9	18.9	N/A	69.3 (8)
	TPSSh-D3	22.5	16.0	16.0	N/A	54.4 (8)
	TPSSh-D3BJ	26.3	22.9	22.9	N/A	54.1 (8)
	tHCTHh	35.0	25.2	25.2	N/A	84.1 (8)
RS	CAM-B3LYP	139.5	120.7	120.7	N/A	266.1 (8)
	CAM-B3LYP-D3	136.0	118.4	118.4	N/A	255.8 (8)
	CAM-B3LYP-D3BJ	137.3	120.6	120.6	N/A	253.4 (8)
	LC-wPBE	198.2	173.3	173.3	N/A	358.8 (8)
	LC-wPBE-D3	194.5	170.8	170.8	N/A	347.3 (8)
	LC-wPBE-D3BJ	196.0	173.2	173.2	N/A	344.5 (8)
	LC-wHPBE	198.2	173.3	173.3	N/A	358.8 (8)
	wB97	191.7	166.5	166.5	N/A	351.0 (8)
	wB97X	179.9	156.0	156.0	N/A	333.9 (8)
	wB97XD	142.3	123.7	123.7	N/A	266.3 (8)
	N12SX	57.0	47.9	47.9	N/A	119.8 (8)
	M11	176.0	154.7	154.7	N/A	317.8 (8)
	MN12SX	58.7	50.0	50.0	N/A	120.7 (8)
	LC-BLYP	226.7	197.8	197.8	N/A	413.5 (8)

	LC-PBE	219.7	193.2	193.2	N/A	393.1 (8)
	LC-BP86	218.9	192.2	192.2	N/A	393.6 (8)
	LC-BPW91	221.5	194.8	194.8	N/A	397.3 (8)
DH	B2PLYP	17.6	15.1	-10.7	-31.6 (8)	9.9 (3)
	B2PLYP-D3	20.3	17.0	-12.7	-39.9 (8)	9.8 (3)
	B2PLYP-D3BJ	19.9	16.1	-10.5	-42.0 (8)	11.9 (3)
	mPW2PLYP	10.9	9.8	9.7	-0.5 (5)	16.2 (3)
	B2GPPLYP	14.8	12.3	-4.5	-29.2 (8)	14.7 (3)
	B2GPPLYP-D3	16.4	13.1	-5.6	-34.0 (8)	14.6 (3)
	B2GPPLYP-D3BJ	16.9	13.1	-4.0	-36.3 (8)	16.3 (3)
	B2KPLYP	15.3	12.1	-1.8	-30.8 (8)	17.2 (3)
	B2TPLYP	10.6	9.3	-1.1	-16.5 (8)	14.3 (3)
	DSDBLYP	32.7	25.1	-20.1	-72.0 (8)	11.0 (3)
	DSDPBEP86	30.6	20.2	-14.8	-75.3 (8)	11.1 (3)
	PBE0DH	63.3	57.2	57.2	N/A	116.2 (8)
	PBEQIDH	23.3	23.1	23.1	N/A	25.9 (4)
Ab initio	HF	308.7	267.4	267.4	N/A	582.3 (8)
	HF-D3	301.6	263.0	263.0	N/A	560.2 (8)
	HF-D3BJ	322.6	288.4	288.4	N/A	566.9 (8)
	MP2	141.7	105.1	-105.1	-309.9 (8)	N/A
	SCS-MP2	88.2	57.6	-57.3	-212.5 (8)	1.1 (3)
	SCS-MP2opt	20.9	18.3	5.5	-29.2 (8)	30.7 (3)
	SOS-MP2	63.9	34.9	-33.4	-163.8 (8)	3.3 (3)
	SCS(MI)-MP2	29.1	23.9	-7.2	-57.9 (8)	28.3 (3)
	SCSN-MP2	25.9	22.3	19.0	-11.4 (5)	42.1 (3)
	SCS-MP2-vdW	136.9	99.3	-99.3	-311.4 (8)	N/A
	S2-MP2	142.0	104.5	-104.5	-316.4 (8)	N/A

Table S3. Full references for the Molpro [92] and Gaussian [94] program suites.

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[94] Gaussian 09, Revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.