

Rung	Description	HFX	local DFX	non-local DFX	local DFC	non-local DFC	spin/spin scale	spin/orbit scale	RMS error kJ mol ⁻¹	Time H:M	Disk Gb
double hybrid	B2PLYP	53%	47%	47%	73%	73%	27%	27%	10.1	10:55	2.3
	B2PLYP-D	53%	47%	47%	73%	73%	27%	27%	10.3	10:40	2.3
	mPW2PLYP	55%	45%	45%	75%	75%	25%	25%	10.3	11:58	2.3
	mPW2PLYP-D	55%	45%	45%	75%	75%	25%	25%	10.4	09:51	2.3
	B2PLYP-D3	53%	47%	47%	73%	73%	27%	27%	10.5	12:00	2.5
	PBE0-DH	50%	50%	50%	88%	88%	13%	13%	11.6	08:12	2.3
	DSD-PBEP86-D3	69%	31%	31%	44%	44%	22%	52%	12.4	09:41	2.3
	PBE-QIDH	69%	31%	31%	67%	67%	33%	33%	12.6	11:25	2.3
hyper-GGA	M06-2X	54%	100%	100%	100%	100%	100%	100%	2.1	14:13	2.3
	M08-HX	52%	100%	100%	100%	100%	100%	100%	2.5	16:10	2.9
	MN12-SX	25%	100%	100%	100%	100%	100%	100%	4.7	17:32	2.3
	MN15	44%	100%	100%	100%	100%	100%	100%	5.1	12:07	2.5
	M06-HF	100%	100%	100%	100%	100%	100%	100%	6.1	16:15	2.9
	M052X	56%	44%	44%	100%	100%	100%	100%	6.6	16:28	2.3
	PW6B95	28%	72%	72%	100%	100%	100%	100%	7.6	13:40	2.3
	PW6B95-D3	28%	72%	72%	100%	100%	100%	100%	7.9	15:28	2.5
	B1B95	28%	72%	72%	100%	100%	100%	100%	8.3	13:57	2.3
	M11	100%	100%	100%	100%	100%	100%	100%	8.5	18:55	2.5
	O3LYP	12%	100%	100%	100%	81%	100%	100%	8.9	12:03	2.3
	B1LYP	25%	75%	75%	100%	100%	100%	100%	9.5	10:42	2.3
	mPW1LYP	25%	75%	75%	100%	100%	100%	100%	9.5	10:59	2.3
	OmPW1LYP	25%	75%	75%	100%	100%	100%	100%	9.6	12:22	2.3
	DFX: Becke3 DFC: VWN/LYP	20%	80%	72%	100%	81%	100%	100%	10.2	10:45	2.5
	X3LYP	22%	78%	71%	100%	87%	100%	100%	10.3	10:51	2.3
	B97-2	21%	100%	100%	100%	100%	100%	100%	10.4	11:28	2.3
	N12-SX	25%	100%	100%	100%	100%	100%	100%	10.6	11:45	2.5
	B97-1	21%	100%	100%	100%	100%	100%	100%	10.6	11:33	2.6
	DFX: Becke "Half and Half" DFC: LYP/VWN	50%	50%	50%	100%	100%	100%	100%	10.7	10:39	2.3
	B98	22%	100%	100%	100%	100%	100%	100%	10.7	11:45	2.3
	M06	27%	100%	100%	100%	100%	100%	100%	10.8	16:09	2.5
	DFX: X (0765*B88+0235*PW91) DFC: LYP+VWN5	0%	100%	100%	100%	100%	100%	100%	11.1	08:29	2.3
	SOGA11X	40%	100%	100%	100%	100%	100%	100%	11.4	09:31	2.6
	DFX: HSE + Henderson DFC: LYP+VWN5	0%	100%	100%	100%	100%	100%	100%	11.4	08:24	2.3
	HISSbPBE	100%	100%	100%	100%	100%	100%	100%	11.4	12:03	2.9
	OAPF	23%	100%	100%	100%	100%	100%	100%	11.5	10:10	2.3
	mPW91PW91	25%	75%	75%	100%	100%	100%	100%	12.2	10:04	2.3
	PBE1PBE	25%	75%	75%	100%	100%	100%	100%	12.2	10:51	2.3
	OmPW1PW91	25%	75%	75%	100%	100%	100%	100%	12.2	11:35	2.3
	APF	23%	100%	100%	100%	100%	100%	100%	12.3	11:41	2.3
	HSEH1PBE	25%	100%	100%	100%	100%	100%	100%	12.3	15:13	2.3
	DFX: Becke3 DFC: Perdew 91	20%	80%	72%	100%	81%	100%	100%	12.3	10:55	2.3
	BMK	42%	100%	100%	100%	100%	100%	100%	12.3	12:44	2.3
	mPW1PBE	25%	75%	75%	100%	100%	100%	100%	12.4	10:34	2.3
	OmPW1PBE	25%	75%	75%	100%	100%	100%	100%	12.5	12:23	2.3
	PBE3PBE	20%	80%	72%	100%	81%	100%	100%	12.5	11:00	2.3
	mPW3PBE	20%	80%	72%	100%	81%	100%	100%	12.7	10:52	2.3
	OmPW3PBE	20%	80%	72%	100%	81%	100%	100%	12.7	12:33	2.6
	APF-D	23%	100%	100%	100%	100%	100%	100%	13.7	11:16	2.3
	t-HCTH hybrid	15%	100%	100%	100%	100%	100%	100%	13.9	17:36	2.6
	DFX: Becke3 DFC: Perdew 86	20%	80%	72%	100%	81%	100%	100%	13.9	11:24	2.3
	CAM-B3LYP	100%	100%	100%	100%	81%	100%	100%	14.0	13:46	3.1
	M05	28%	72%	72%	100%	100%	100%	100%	15.0	15:31	2.3
	TPSSh	10%	90%	90%	100%	100%	100%	100%	15.3	17:04	2.3
	wB97X-D	100%	100%	100%	100%	100%	100%	100%	15.4	14:39	2.5
	HISSaPBE	100%	100%	100%	100%	100%	100%	100%	17.0	14:15	2.6
	wB97X	100%	100%	100%	100%	100%	100%	100%	17.6	15:24	2.3
	LC-wHPBE	100%	100%	100%	100%	100%	100%	100%	19.6	12:47	2.3
	wB97	100%	100%	100%	100%	100%	100%	100%	20.5	13:45	2.8
	BA1PBE	25%	75%	75%	100%	100%	100%	100%	32.0	11:04	2.3
	BA3PBE	20%	80%	72%	100%	81%	100%	100%	32.1	11:37	3.1
metaGGA	MN15-L	0%	100%	100%	100%	100%	100%	100%	4.4	11:25	2.5
	SOGA11	0%	100%	100%	100%	100%	100%	100%	5.7	11:14	2.7
	M11L	0%	100%	100%	100%	100%	100%	100%	6.3	11:29	2.8
	MN12-L	0%	100%	100%	100%	100%	100%	100%	7.5	12:23	2.3
	Becke-Roussel88	0%	100%	100%	100%	100%	100%	100%	7.9	03:05	2.4
	M06-L	0%	100%	100%	100%	100%	100%	100%	12.7	12:57	2.5
	t-HCTH	0%	100%	100%	100%	100%	100%	100%	14.4	15:01	2.3
	N12	0%	100%	100%	100%	100%	100%	100%	15.1	08:33	2.3
	DFX: TPSSX DFC: TPSSc	0%	100%	100%	100%	100%	100%	100%	16.7	13:42	2.3
	DFX: revTPSSX DFC: revTPSSc	0%	100%	100%	100%	100%	100%	100%	17.7	13:37	2.3
GGA	DFX: VSXC DFC: VSXC	0%	100%	100%	100%	100%	100%	100%	3.8	13:03	2.3
	HCTH407	0%	100%	100%	100%	100%	100%	100%	8.2	09:13	2.3
	DFX: Becke 1988 DFC: Perdew 81	0%	100%	100%	100%	100%	100%	100%	8.7	08:13	2.3
	DFX: OPTX DFC: LYP+VWN5	0%	100%	100%	100%	100%	100%	100%	9.3	09:37	2.3
	HCTH93	0%	100%	100%	100%	100%	100%	100%	9.4	08:50	2.5
	DFX: OPTX as in O3LYP DFC: LYP+VWN5	0%	100%	100%	100%	100%	100%	100%	9.9	08:10	2.3
	B97-D	0%	100%	100%	100%	100%	100%	100%	9.9	08:12	2.3
	HCTH147	0%	100%	100%	100%	100%	100%	100%	10.5	08:55	2.3
	DFX: Becke 1988 DFC: Lee-Yang-Parr	0%	100%	100%	100%	100%	100%	100%	10.9	09:27	2.4
	DFX: Becke 1988 DFC: LYP+VWN5	0%	100%	100%	100%	100%	100%	100%	10.9	10:26	2.3
	B97-D (DFT-D3)	0%	100%	100%	100%	100%	100%	100%	13.3	10:34	2.3
	PAPF	0%	100%	100%	100%	100%	100%	100%	14.5	07:41	2.3
	DFX: PBE DFC: PBE	0%	100%	100%	100%	100%	100%	100%	14.6	09:44	2.5
	DFX: PW91 DFC: PW91	0%	100%	100%	100%	100%	100%	100%	15.2	08:08	2.3
	DFX: Becke 1988 DFC: Perdew 81 + Perdew 86	0%	100%	100%	100%	100%	100%	100%	15.5	09:30	2.3
	PAPF-D	0%	100%	100%	100%	100%	100%	100%	15.8	07:50	2.3
	DFX: Becke 1988 DFC: VWN 80 (LSD) + Perdew 86	0%	100%	100%	100%	100%	100%	100%	16.3	10:29	2.3
	DFX: CVDFT DFC: CCDFT	0%	100%	100%	100%	100%	100%	100%	36.3	06:16	2.4
	DFX: CVDFT DFC: CVDFT	0%	100%	100%	100%	100%	100%	100%	37.7	05:31	2.4