Complexity of Synthetic Routes: Linear, Convergent and Reflexive Syntheses. (Supplementary Information)

Steven H. Bertz

Complexity Study Center, Mendham, NJ 07945

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Table III Selected complexity indices for routes 1-3.

compound[a]	N_T	ΔN_T	N_S	ΔN_S	T_T	ΔT_T	η	Δη	$C(\eta,\varepsilon)$	$\Delta C(\eta,\varepsilon)$	S	ΔS
route 1												
1	9	—	4	—	5	—	3	—	4.8	—	4	—
H_2	0	—	0	—	0	—	0	—	0.0	—	0	—
4	261	252	25	21	105	100	15	12	69.4	64.6	10	6
3	37	–224	7	–18	36	–69	6	–9	15.5	–53.9	4	–6
route 2												
1	9	—	4	—	5	—	3	—	4.8	—	4	—
H_2	0	—	0	—	0	—	0	—	0.0	—	0	—
5	26	17	8	4	17	12	6	3	21.0	16.2	4	0
6	5	–4	3	–1	4	–1	1	–2	0.0	–4.8	2	–2
7	69	38	17	9	51	30	9	2	45.1	24.1	6	0
3	37	–32	7	–10	36	–15	6	–3	15.5	–29.6	4	–2
route 3												
1	9	—	4	—	5	—	3	—	4.8	—	4	—
2	9	—	5	—	5	—	3	—	6.8	—	5	—
H_2	0	—	0	—	0	—	0	—	0.0	—	0	—
IPA[b]	0	—	0	—	0	—	0	—	0.0	—	0	—
HBr[c]	1	—	1	—	1	—	0	—	0.0	—	1	—
R_3P:	19	—	9	—	11	—	6	—	24.8	—	1	—
MeLi	3	—	3	—	3	—	0	—	0.0	—	1	—
8	26	8	14	6	17	7	6	0	30.3	18.7	5	–4
9	16	–10	10	–4	13	–4	4	–2	17.2	–13.1	3	–2
10	16	0	10	0	13	0	4	0	17.2	0.0	3	0
11	62	27	27	8	52	28	10	0	65.1	23.1	4	0
12[d]	141	79	42	15	83	31	15	5	103.1	38.0	5	2
13[e]	95	–36	19	–23	48	–24	11	0	58.1	–22.3	6	0
14	133	38	23	4	73	25	12	1	66.0	7.9	8	2
3	37	–96	7	–16	36	–37	6	–6	15.5	–50.5	4	–4

[a] Note that only intermediates are included in C_x, but starting materials and reagents are also included in the calculation of ΔC_m. [b]Isopropyl alcohol, used as a H-source in the reduction of **8**;[36] therefore, we set $C = 0$. [c]The complexities of HBr and H_2O are equal and cancel out. [d]By-products are methane ($N_T = N_S = T_T = 1$, $\eta = C(\eta) = S = 0$) and LiBr ($N_T = N_S = T_T = S = 2$, $\eta = C(\eta) = 0$). The latter is ionic, and does not have a covalent Li-Br bond. [e]By-product is R_3PO ($N_T = 36$, $N_S = 14$, $T_T = 28$, $\eta = 10$, $C(\eta,\varepsilon) = 53.0$, $S = 4$).