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# Zeolite Activation of Organometallics: Revisiting Substitution Kinetics of $[Mo(CO)_6]$ with Chemisorbed $PMe_3$ in Dehydrated $Na_{56}Y$ Zeolite

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**Table S1.** Rate constants[a] for substitution reactions of $[Mo(CO)_6]$ with chemisorbed $PMe_3$ in dehydrated $Na_{56}Y$ under vacuum

| T/(°C) | 1975 $cm^{-1}$ $10^4 k_{obs}$(err, $\chi^2$)[b] | 1865 $cm^{-1}$ $10^4 k_{obs}$(err, $\chi^2$)[b] |
|---|---|---|
| 48 | 0.456 (13, 778) | 0.517 (16, 136) |
| 48 | 0.722 (17, 96) | 0.600 (8, 58) |
| 48 | 0.676 (2, 153) | 0.600 (8, 58) |
| 56 | 2.02 (36, 286) | 1.54 (4, 170) |
| 56 | 1.86 (4, 5) | 1.48 (2, 19) |
| 56 | 2.30 (9, 8) | 1.42 (5, 34) |
| 66 | 2.56 (3, 15) | 2.50 (9, 38) |
| 66 | 2.38 (6, 21) | 2.30 (3, 20) |
| 66 | 3.51 (6, 7) | 3.46 (3, 7) |
| 66 | 4.62 (14, 14) | 3.58 (6,60) |
| 66 | 3.08 (7, 8) | 2.86 (3, 17) |
| 75 | 5.42 (10, 3) | 5.25 (8, 7) |
| 75 | 6.69 (4, 25) | |
| 85 | 9.45 (12, 158) | 9.10 (32, 373) |
| 85 | 10.3 (1, 1) | 11.1 (2, 1) |
| 85 | 14.3 (7, 3) | |
| 85 | 15.5 (1, 1) | 14.4 (2, 3) |

[a]Rate constants obtained by fitting the time-dependent absorbances to single or double exponential functions

[b] err = standard deviation of $k_{obs}$; $\chi^2$ =goodness of fit (the smaller the number the better the fit). Thus 0.456(13, 778) represents $10^4 k_{obs} = 0.456 \pm 0.013\ s^{-1}$ with $\chi^2 = 778$.

**Table S2.** Rate constants[a] for substitution reactions of $[Mo(CO)_6]$ with chemisorbed $PMe_3$ in dehydrated $Na_{56}Y$ under 650 Torr CO

| T/( °C) | 1975 $cm^{-1}$ $10^4 k_{obs}$(err, $\chi^2$)[a] | 1865 $cm^{-1}$ $10^4 k_{obs}$(err, $\chi^2$)[a] |
|---|---|---|
| 48 | 0.373 (9, 9319) | 0.434 (5, 295) |
| 48 | 0.395 (5, 2191) | 0.475 (123, 56) |
| 48 | 0.544 (18, 1090) | 0.343 (4, 129) |
| 48 | 0.420 (7, 708) | 0.508 (4, 37) |
| | | 0.309 (3, 216) |
| 56 | 0.601 (10, 2714) | 0.910 (47, 279) |
| 56 | 0.967 (162, 2087) | |
| 56 | 0.687 (7, 412) | 0.806 (15, 61) |
| 56 | 1.65 (4, 4) | 1.85 (4, 2) |
| 56 | 0.766 (12, 67) | 0.889 (18, 387) |
| 56 | 1.10 (1, 110) | 1.14 (1,15) |
| 66 | 1.92 (9, 10) | 3.86 (8, 23) |
| 66 | 3.08 (15, 5) | 2.01 (3, 5) |
| 66 | 2.55 (2, 8) | |
| 66 | 2.56 (4, 150) | 3.10 (18, 466) |
| 75 | 5.44 (12, 1819) | 5.03 (2, 694) |
| 75 | 6.38 (11, 5) | |
| 85 | 12.0 (2, 1) | |
| 85 | 19.2 (4, 1) | |
| 85 | 12.2 (1, 1) | |
| 85 | 11.6 (1, 2) | |

[a]Rate constants obtained by fitting the time-dependent absorbances to single or double exponential functions

[b] err = standard deviation of $k_{obs}$; $\chi^2$ =goodness of fit (the smaller the number the better the fit). Thus 0.373(9, 9319) represents $10^4 k_{obs} = 0.373 \pm 0.009\ s^{-1}$ with $\chi^2 = 9319$.

[#] Professor Vichi sadly passed away just as this manuscript was being completed. Eduardo Vichi was the originator of the Intrazeolite Kinetics project. He suggested it to A.J.P. in Toronto in 1983 and eventually obtained funding for it through FAPESP and CNPq. He was a great scientific colleague and a warm friend, and he will be deeply missed.

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