|  |  |  |  |
| --- | --- | --- | --- |
| **35 / 37Cl *trans* to H2O** | **Pt(IV) isotopologue** | **Percent isotopomers** | **Sum percent of isotopomers to yield isotopologue amount** |
|  |  | Experimental | Statistical | Experimental | Statistical |
|  |  |  |  |  |  |
| 35Cl | [Pt35Cl5(H216O)]- | 25.2 (± 0.3)  | 24.97 | 25.2 (± 0.3) | 24.97 |
| 35Cl37Cl | [Pt35Cl437Cl(H216O)]- | 32.0 (± 0.5)8.00 (± 0.4) | 31.947.99 | 40.0 (± 0.6) | 39.93 |
| 35Cl37Cl | [Pt35Cl337Cl2(H216O)]- | 15.1 (± 0.2)10.2 (± 0.3) | 15.3210.22 | 25.3 (± 0.4) | 25.54 |
| 35Cl37Cl | [Pt35Cl237Cl3(H216O)]- | 3.2 (± 0.2)4.6 (± 0.3) | 3.274.9 | 7.8 (± 0.4) | 8.17 |
| 35Cl37Cl | [Pt35Cl37Cl4(H216O)]- | 0.3 (± 0.2)1.4 (± 0.3) | 0.261.05 | 1.7 (± 0.4) | 1.31 |
| 37Cl | [Pt37Cl5(H216O)]- | n.r.m | 0.08 | n.r.m | 0.08 |
| 35Cl | [Pt35Cl5(H218O)]- | 23.1 (± 0.3)  | 24.97 | 23.1 | 24.97 |
| 35Cl37Cl | [Pt35Cl437Cl(H218O)]- | 32.8 (± 0.4)7.9 (± 0.4) | 31.947.99 | 40.7 (± 0.6) | 39.93 |
| 35Cl37Cl | [Pt35Cl337Cl2(H218O)]- | 15.3 (± 0.3)10.8 (± 0.4) | 15.3210.22 | 26.1 (± 0.5) | 25.54 |
| 35Cl,35Cl,35Cl | *fac-*[Pt35Cl3(H216O)3]+ | -b | - | 43.1 (± 0.2) | 43.50 |
| 35Cl,35Cl,37Cl | *fac-*[Pt35Cl237Cl(H216O)3]+ | - | - | 43.0 (± 0.2) | 41.73 |
| 35Cl,37Cl,37Cl | *fac-*[Pt35Cl37Cl2(H216O)3]+ | - | - | 12.9 (± 0.2) | 13.35 |
| 37Cl,37Cl,37Cl | *fac-*[Pt37Cl3(H216O)3]+ | - | - | 1.0 (± 0.4) | 1.42 |
|  |  | - | - |  |  |
| 35Cl,35Cl,35Cl | *fac-*[Pt35Cl3(H216O)2(H218O)]+ | -a | - | 43.9 (± 0.2) | 43.50 |
| 35Cl,35Cl,37Cl | *fac-*[Pt35Cl237Cl(H216O)2(H218O)]+ | - | - | 42.5 (± 0.3) | 41.73 |
| 35Cl,37Cl,37Cl | *fac-*[Pt35Cl37Cl2(H216O)2(H218O)]+ | - | - | 12.6 (± 0.2) | 13.35 |
| 37Cl,37Cl,37Cl | *fac-*[Pt37Cl3(H216O)2(H218O)]+ | - | - | 1.1 (± 0.4) | 1.42 |
|  |  |  |  |  |  |
| 35Cl,35Cl,35Cl | *fac-*[Pt35Cl3(H216O)(H218O)2]+ | - | - | 43.4 (± 0.2) | 43.50 |
| 35Cl,35Cl,37Cl | *fac-*[Pt35Cl237Cl(H216O)(H218O)2]+ | - | - | 41.2 (± 0.2) | 41.73 |
| 35Cl,37Cl,37Cl | *fac-*[Pt35Cl37Cl2(H216O)(H218O)2]+ | - | - | 14.2 (± 0.3) | 13.35 |
| 37Cl,37Cl,37Cl | *fac-*[Pt37Cl3(H216O)(H218O)2]+ | - | - | 1.1 (± 0.4) | 1.42 |
|  |  | - |  |  |  |
| 35Cl,35Cl,35Cl | *fac-*[Pt35Cl3(H218O)3]+ | - | - | 43.1 (± 0.2)c | 43.50 |
| 35Cl,35Cl,37Cl | *fac-*[Pt35Cl237Cl(H218O)3]+ | - | - | 37.5 (± 0.5) | 41.73 |
| 35Cl,37Cl,37Cl | *fac-*[Pt35Cl37Cl2(H218O)3]+ | - | - | 18.3 (± 0.5) | 13.35 |
| 37Cl,37Cl,37Cl | *fac-*[Pt37Cl3(H218O)3]+ | - | - | 1.0 (± 0.4) | 1.42 |
|  |  |  |  |  |  |

1. ‘not reliably measurable’
2. No magnetically non-equivalent isotopomers possible, together with some overlap of 37Cl isotopologues e.g. *fac-*[Pt37Cl3(H216O)3]+ peaks with 18O isotopologues *fac-*[Pt35Cl3(H216O)2(H218O)]+ is seen in Figure 3
3. Relatively low intensity 195Pt NMR signals result in larger relative errors.