

Supporting Information:

**Degradation of selected perfluoroalkyl  
substances (PFAS) using  $\text{AlF}_3$  in water**

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The Cartesian coordinates of the global minima of PFBA<sup>-</sup> (C<sub>3</sub>F<sub>7</sub>COO<sup>-</sup>), PFHxA<sup>-</sup> (C<sub>5</sub>F<sub>11</sub>COO<sup>-</sup>), PFBS<sup>-</sup> (C<sub>4</sub>F<sub>9</sub>SO<sub>3</sub><sup>-</sup>), and PFPeS<sup>-</sup> (C<sub>5</sub>F<sub>11</sub>SO<sub>3</sub><sup>-</sup>) systems calculated at the B3LYP/aug-cc-pVDZ/PCM level of theory:

| PFBA <sup>-</sup> |              |              |              | PFHxA <sup>-</sup> |              |              |              |
|-------------------|--------------|--------------|--------------|--------------------|--------------|--------------|--------------|
| F                 | 2.653533000  | 0.852984000  | -0.326005000 | C                  | 1.664066000  | 0.553137000  | 0.061194000  |
| C                 | 1.745063000  | -0.106363000 | -0.058899000 | C                  | 0.402031000  | -0.375800000 | 0.104206000  |
| F                 | 1.926018000  | -1.102822000 | -0.940374000 | F                  | 0.537893000  | -1.322782000 | -0.860760000 |
| F                 | 1.982309000  | -0.575699000 | 1.179547000  | F                  | 0.390100000  | -0.994844000 | 1.313377000  |
| C                 | 0.309982000  | 0.496300000  | -0.160710000 | C                  | -0.958560000 | 0.373435000  | -0.108446000 |
| F                 | 0.322714000  | 1.659619000  | 0.541935000  | F                  | -0.900907000 | 1.550179000  | 0.572541000  |
| F                 | 0.105441000  | 0.797282000  | -1.477249000 | F                  | -1.063709000 | 0.658587000  | -1.438781000 |
| C                 | -0.857792000 | -0.404254000 | 0.336025000  | C                  | -2.234502000 | -0.411631000 | 0.324955000  |
| F                 | -0.579412000 | -1.688310000 | -0.065418000 | F                  | -2.044016000 | -1.727019000 | -0.018233000 |
| F                 | -0.819612000 | -0.414955000 | 1.710587000  | F                  | -2.307228000 | -0.374838000 | 1.696962000  |
| C                 | -2.277374000 | 0.075973000  | -0.170360000 | C                  | -3.561282000 | 0.173425000  | -0.309687000 |
| O                 | -2.647773000 | 1.155582000  | 0.340072000  | O                  | -3.878502000 | 1.293311000  | 0.146413000  |
| O                 | -2.832000000 | -0.670934000 | -1.000515000 | O                  | -4.106388000 | -0.546025000 | -1.169655000 |
|                   |              |              |              | C                  | 3.022484000  | -0.194449000 | -0.139355000 |
|                   |              |              |              | F                  | 1.544605000  | 1.444420000  | -0.955971000 |
|                   |              |              |              | F                  | 1.748118000  | 1.234924000  | 1.229377000  |
|                   |              |              |              | F                  | 3.147498000  | -1.203334000 | 0.738807000  |
|                   |              |              |              | F                  | 4.027851000  | 0.674751000  | 0.060432000  |
|                   |              |              |              | F                  | 3.127983000  | -0.683042000 | -1.383448000 |

| PFBS <sup>-</sup> |              |              |              | PFPeS <sup>-</sup> |              |              |              |
|-------------------|--------------|--------------|--------------|--------------------|--------------|--------------|--------------|
| C                 | -2.814077000 | -0.313094000 | 0.060912000  | C                  | -2.124640000 | -0.498985000 | 0.240196000  |
| C                 | -1.503970000 | 0.502019000  | -0.187098000 | C                  | -0.871546000 | 0.406829000  | -0.015366000 |
| F                 | -1.542971000 | 0.948940000  | -1.466537000 | F                  | -0.991247000 | 0.973548000  | -1.243455000 |
| F                 | -1.536137000 | 1.572855000  | 0.647925000  | F                  | -0.879142000 | 1.395156000  | 0.915546000  |
| C                 | -0.173430000 | -0.298136000 | 0.029845000  | C                  | 0.499414000  | -0.357492000 | 0.050568000  |
| F                 | -0.306650000 | -1.046868000 | 1.156435000  | F                  | 0.452839000  | -1.226475000 | 1.094435000  |
| F                 | -0.027502000 | -1.137991000 | -1.026931000 | F                  | 0.628275000  | -1.069576000 | -1.097390000 |
| C                 | 1.098990000  | 0.592028000  | 0.171428000  | C                  | 1.741712000  | 0.568648000  | 0.230249000  |
| F                 | 1.038128000  | 1.604826000  | -0.737891000 | F                  | 1.597958000  | 1.667471000  | -0.562442000 |
| F                 | 1.096956000  | 1.142860000  | 1.413416000  | F                  | 1.780555000  | 0.985165000  | 1.522742000  |
| S                 | 2.780340000  | -0.308064000 | -0.071352000 | S                  | 3.443103000  | -0.227069000 | -0.182015000 |
| O                 | 2.658771000  | -1.539462000 | 0.780575000  | O                  | 3.411240000  | -1.544241000 | 0.539406000  |
| O                 | 2.856637000  | -0.558765000 | -1.549460000 | O                  | 3.457878000  | -0.319709000 | -1.680198000 |
| F                 | -2.794412000 | -1.470671000 | -0.620643000 | C                  | -3.487154000 | 0.126646000  | -0.203566000 |
| F                 | -2.980703000 | -0.577559000 | 1.364930000  | F                  | -1.984862000 | -1.672788000 | -0.426649000 |
| O                 | 3.749765000  | 0.720924000  | 0.438801000  | F                  | -2.212518000 | -0.759118000 | 1.566769000  |
| F                 | -3.863587000 | 0.413669000  | -0.360506000 | F                  | -3.632033000 | 1.362420000  | 0.303214000  |
|                   |              |              |              | F                  | -4.486019000 | -0.645382000 | 0.255427000  |
|                   |              |              |              | F                  | -3.579311000 | 0.188611000  | -1.539425000 |
|                   |              |              |              | O                  | 4.395029000  | 0.784942000  | 0.390892000  |

The Cartesian coordinates of the remaining stationary point structures (reactant complexes, transition states, and product complexes) calculated at the B3LYP/aug-cc-pVDZ/PCM level of theory:

| RC(1) |              |              |              | TS(1) |              |              |              |
|-------|--------------|--------------|--------------|-------|--------------|--------------|--------------|
| F     | 1.408420000  | -0.168442000 | 0.543575000  | F     | 0.339285000  | -2.593813000 | -0.089835000 |
| C     | 0.283501000  | 0.614408000  | 0.074625000  | C     | 1.241333000  | -1.665086000 | 0.240569000  |
| F     | 0.273551000  | 1.695701000  | 0.820680000  | F     | 1.273349000  | -1.516576000 | 1.564091000  |
| F     | 0.543656000  | 0.907075000  | -1.185927000 | F     | 2.454300000  | -2.080724000 | -0.184370000 |
| C     | -0.971761000 | -0.293546000 | 0.251075000  | C     | 0.958707000  | -0.337773000 | -0.493217000 |
| F     | -0.677180000 | -1.481071000 | -0.326585000 | F     | 0.483944000  | -0.485666000 | -1.687518000 |
| F     | -1.128182000 | -0.481572000 | 1.588518000  | F     | -0.707138000 | -0.139141000 | 0.421012000  |
| C     | -2.286635000 | 0.289987000  | -0.343976000 | C     | 1.661795000  | 0.911876000  | -0.220690000 |
| F     | -2.316392000 | 1.620277000  | -0.006615000 | F     | 2.664268000  | 0.721658000  | 0.679230000  |
| F     | -2.175075000 | 0.238524000  | -1.711801000 | F     | 2.189071000  | 1.428446000  | -1.368353000 |
| C     | -3.583562000 | -0.481802000 | 0.140250000  | C     | 0.581431000  | 2.168494000  | 0.395030000  |
| O     | -3.659457000 | -1.644407000 | -0.309784000 | O     | -0.108327000 | 2.599252000  | -0.517652000 |
| O     | -4.337688000 | 0.164654000  | 0.891209000  | O     | 0.799503000  | 2.361677000  | 1.579326000  |
| Al    | 3.338969000  | -0.241777000 | -0.026615000 | Al    | -2.456368000 | -0.102023000 | 0.013657000  |
| F     | 3.938181000  | -0.931602000 | 1.376496000  | F     | -2.560509000 | 0.144292000  | -1.661399000 |
| F     | 3.587336000  | 1.396651000  | -0.276218000 | F     | -3.114151000 | 1.162642000  | 0.932535000  |
| F     | 3.203610000  | -1.217002000 | -1.381814000 | F     | -3.050889000 | -1.621807000 | 0.483375000  |

| PC(1) |              |              |              | RC(2) |              |              |              |
|-------|--------------|--------------|--------------|-------|--------------|--------------|--------------|
| F     | -3.011115000 | 1.519178000  | -0.824473000 | F     | 2.767001000  | -0.320568000 | 0.347963000  |
| C     | -3.244142000 | 0.457950000  | -0.010449000 | C     | 1.671551000  | 0.523416000  | -0.022556000 |
| F     | -3.119374000 | 0.876418000  | 1.262098000  | F     | 1.743340000  | 1.589744000  | 0.747043000  |
| F     | -4.539434000 | 0.101667000  | -0.208570000 | F     | 1.853198000  | 0.834753000  | -1.289571000 |
| C     | -2.322295000 | -0.676485000 | -0.328883000 | C     | 0.385644000  | -0.329504000 | 0.230860000  |
| F     | -2.443078000 | -1.115955000 | -1.602569000 | F     | 0.408448000  | -1.351912000 | -0.653411000 |
| F     | 1.065254000  | 0.211752000  | 0.008340000  | F     | 0.473368000  | -0.819939000 | 1.485629000  |
| C     | -1.430299000 | -1.259401000 | 0.473331000  | C     | -0.943414000 | 0.491695000  | 0.078495000  |
| F     | -1.211530000 | -0.940313000 | 1.729231000  | F     | -1.046948000 | 1.295982000  | 1.165606000  |
| F     | -0.674314000 | -2.261379000 | 0.075721000  | F     | -0.825299000 | 1.272571000  | -1.026317000 |
| C     | 3.142270000  | -2.171580000 | -0.139856000 | C     | -2.229966000 | -0.395644000 | -0.050519000 |
| O     | 3.083224000  | -2.158632000 | -1.305217000 | F     | -2.249750000 | -0.899003000 | -1.317231000 |
| O     | 3.205863000  | -2.209891000 | 1.024748000  | F     | -2.105476000 | -1.436029000 | 0.816868000  |
| Al    | 2.199283000  | 1.499022000  | -0.032576000 | Al    | 4.764171000  | -0.255887000 | -0.110187000 |
| F     | 3.778564000  | 0.834426000  | -0.117977000 | F     | 5.319431000  | -0.869629000 | 1.343173000  |
| F     | 2.047089000  | 2.446470000  | 1.387625000  | F     | 4.856060000  | 1.394708000  | -0.375596000 |
| F     | 1.910540000  | 2.478625000  | -1.409160000 | F     | 4.761902000  | -1.266106000 | -1.443909000 |
|       |              |              |              | C     | -3.579498000 | 0.340517000  | 0.208550000  |
|       |              |              |              | C     | -4.831378000 | -0.459639000 | -0.340790000 |
|       |              |              |              | O     | -5.383506000 | 0.033648000  | -1.343394000 |
|       |              |              |              | O     | -5.089848000 | -1.490043000 | 0.317645000  |
|       |              |              |              | F     | -3.697117000 | 0.540003000  | 1.562369000  |
|       |              |              |              | F     | -3.478715000 | 1.585718000  | -0.361036000 |

| TS(2) |              |              |              | PC(2) |              |              |              |
|-------|--------------|--------------|--------------|-------|--------------|--------------|--------------|
| C     | 1.853431000  | 0.496322000  | -0.043716000 | C     | -2.261450000 | 0.330420000  | -0.291645000 |
| C     | 1.039059000  | -0.851805000 | -0.087096000 | C     | -2.148263000 | -1.161306000 | 0.162153000  |
| F     | 0.913635000  | -1.221843000 | -1.374551000 | F     | -2.247893000 | -1.191337000 | 1.519276000  |
| F     | 1.760668000  | -1.806619000 | 0.578303000  | F     | -3.215704000 | -1.840201000 | -0.360411000 |
| C     | -0.340360000 | -0.908702000 | 0.603621000  | C     | -0.880457000 | -1.833860000 | -0.284782000 |
| F     | -0.410878000 | -0.373727000 | 1.782020000  | F     | -0.880746000 | -2.205635000 | -1.585175000 |
| F     | -1.010217000 | 0.601241000  | -0.345938000 | F     | 2.117799000  | 0.122449000  | 0.076137000  |
| C     | -1.300006000 | -1.979512000 | 0.322859000  | C     | 0.202176000  | -2.097972000 | 0.451086000  |
| F     | -0.707149000 | -3.046439000 | -0.282636000 | F     | 0.353105000  | -1.794121000 | 1.720412000  |
| F     | -1.878449000 | -2.402777000 | 1.479901000  | F     | 1.247081000  | -2.731543000 | -0.036438000 |
| C     | -2.626516000 | -1.458806000 | -0.741052000 | C     | 4.934272000  | -1.135415000 | -0.269925000 |
| O     | -3.18016000  | -0.962381000 | -0.071055000 | O     | 4.837657000  | -1.052406000 | -1.429912000 |
| O     | -2.369658000 | -1.755176000 | -1.895522000 | O     | 5.047486000  | -1.237224000 | 0.887041000  |
| Al    | -1.978620000 | 2.079034000  | 0.013922000  | Al    | 2.529214000  | 1.787987000  | 0.065906000  |
| F     | -2.622541000 | 1.878107000  | 1.569919000  | F     | 4.238538000  | 1.927076000  | 0.018763000  |
| F     | -3.133922000 | 2.199902000  | -1.220803000 | F     | 1.927657000  | 2.540646000  | 1.483496000  |
| F     | -0.858213000 | 3.354551000  | -0.043581000 | F     | 1.852063000  | 2.542412000  | -1.316093000 |
| C     | 3.405429000  | 0.291226000  | -0.099685000 | C     | -3.601129000 | 1.063452000  | 0.022384000  |
| F     | 3.735169000  | -0.535362000 | -1.106368000 | F     | -3.493328000 | 2.346816000  | -0.365763000 |
| F     | 3.871624000  | -0.209333000 | 1.052199000  | F     | -3.869920000 | 1.037607000  | 1.337315000  |
| F     | 3.987134000  | 1.481686000  | -0.311936000 | F     | -4.624474000 | 0.505008000  | -0.642008000 |
| F     | 1.577210000  | 1.183214000  | 1.090591000  | F     | -2.075548000 | 0.390415000  | -1.636375000 |
| F     | 1.513398000  | 1.250806000  | -1.109116000 | F     | -1.265500000 | 1.026105000  | 0.314704000  |

| RC(3) |              |              |              | TS(3) |              |              |              |
|-------|--------------|--------------|--------------|-------|--------------|--------------|--------------|
| F     | 2.591337000  | 0.106018000  | -0.527011000 | C     | 2.724573000  | -0.431961000 | 0.239224000  |
| C     | 1.455423000  | -0.603664000 | -0.017159000 | C     | 1.431685000  | -1.325978000 | 0.189875000  |
| F     | 1.400770000  | -1.740741000 | -0.677741000 | F     | 1.802806000  | -2.521467000 | -0.361917000 |
| F     | 1.690070000  | -0.805827000 | 1.264102000  | F     | 1.016798000  | -1.537642000 | 1.451030000  |
| C     | 0.225748000  | 0.323168000  | -0.287112000 | C     | 0.239816000  | -0.905016000 | -0.693618000 |
| F     | 0.384889000  | 1.424671000  | 0.481581000  | F     | 0.120761000  | 0.889060000  | 0.280132000  |
| F     | 0.270925000  | 0.677834000  | -1.589505000 | F     | 0.501411000  | -0.316282000 | -1.812561000 |
| C     | -1.152903000 | -0.360185000 | 0.023225000  | C     | -1.036632000 | -1.561396000 | -0.595584000 |
| F     | -1.378216000 | -1.268421000 | -0.957878000 | F     | -1.639038000 | -1.713120000 | -1.790164000 |
| F     | -1.031377000 | -1.021061000 | 1.203924000  | F     | -1.015192000 | -2.726819000 | 0.083211000  |
| C     | -2.351441000 | 0.632135000  | 0.118784000  | S     | -2.559820000 | -0.461982000 | 0.522670000  |
| F     | -2.266869000 | 1.283437000  | 1.307365000  | O     | -1.985199000 | -0.387338000 | 1.891594000  |
| F     | -2.241659000 | 1.555316000  | -0.876566000 | O     | -2.691207000 | 0.796122000  | -0.261852000 |
| Al    | 4.544625000  | 0.191508000  | 0.077638000  | F     | 2.617789000  | 0.540184000  | 1.144187000  |
| F     | 5.155313000  | 0.761261000  | -1.371696000 | F     | 3.751796000  | -1.223399000 | 0.593733000  |
| F     | 4.737560000  | -1.429304000 | 0.449980000  | O     | -3.603573000 | -1.502963000 | 0.290603000  |
| F     | 4.385277000  | 1.269448000  | 1.347752000  | F     | 2.991587000  | 0.100032000  | -0.963432000 |
| S     | -4.096833000 | -0.164895000 | -0.002736000 | Al    | -0.099924000 | 2.612120000  | -0.087313000 |
| O     | -4.976460000 | 0.968374000  | 0.442029000  | F     | -1.124793000 | 3.291060000  | 1.087464000  |
| O     | -4.025602000 | -1.324650000 | 0.949073000  | F     | -0.668625000 | 2.763165000  | -1.683440000 |
| O     | -4.232180000 | -0.532935000 | -1.451189000 | F     | 1.460180000  | 3.292303000  | 0.035113000  |

| PC(3) |              |              |              | RC(4) |              |              |              |
|-------|--------------|--------------|--------------|-------|--------------|--------------|--------------|
| C     | 3.622125000  | -0.553642000 | 0.100605000  | F     | 3.253962000  | -0.153571000 | 0.458532000  |
| C     | 3.206259000  | 0.912400000  | -0.227694000 | C     | 2.162663000  | 0.535028000  | -0.155935000 |
| F     | 4.220994000  | 1.714298000  | 0.226436000  | F     | 2.242387000  | 1.790174000  | 0.234844000  |
| F     | 3.159065000  | 1.015073000  | -1.583187000 | F     | 2.337476000  | 0.428246000  | -1.457653000 |
| C     | 1.911780000  | 1.357311000  | 0.386301000  | C     | 0.872123000  | -0.185419000 | 0.356827000  |
| F     | -0.896617000 | -0.887725000 | -0.196631000 | F     | 0.871899000  | -1.427260000 | -0.176458000 |
| F     | 1.974301000  | 1.525685000  | 1.727878000  | F     | 0.966513000  | -0.274191000 | 1.700003000  |
| C     | 0.753731000  | 1.604061000  | -0.231092000 | C     | -0.449337000 | 0.570490000  | -0.025198000 |
| F     | -0.311297000 | 2.025981000  | 0.416682000  | F     | -0.544498000 | 1.656493000  | 0.780383000  |
| F     | 0.535391000  | 1.484941000  | -1.520892000 | F     | -0.336674000 | 0.993462000  | -1.309915000 |
| S     | -4.259790000 | 1.459674000  | 0.025965000  | C     | -1.745979000 | -0.305579000 | 0.111394000  |
| O     | -4.268686000 | 1.286746000  | -1.433813000 | F     | -1.777865000 | -1.152799000 | -0.946735000 |
| O     | -4.795062000 | 0.401956000  | 0.895095000  | F     | -1.641051000 | -1.038473000 | 1.250371000  |
| F     | 3.727648000  | -0.732387000 | 1.429066000  | Al    | 5.229044000  | -0.355885000 | -0.068768000 |
| F     | 2.706011000  | -1.412814000 | -0.378417000 | F     | 5.813017000  | -0.580138000 | 1.482096000  |
| O     | -3.717751000 | 2.691956000  | 0.616402000  | F     | 5.401224000  | 1.146288000  | -0.787340000 |
| F     | 4.808793000  | -0.836318000 | -0.463934000 | F     | 5.101747000  | -1.691857000 | -1.067660000 |
| Al    | -1.509488000 | -2.477566000 | 0.002294000  | C     | -3.069313000 | 0.518511000  | 0.164503000  |
| F     | -2.755631000 | -2.757187000 | -1.141802000 | S     | -4.678649000 | -0.470730000 | -0.194560000 |
| F     | -2.137284000 | -2.651993000 | 1.588428000  | F     | -2.996212000 | 1.534178000  | -0.740763000 |
| F     | -0.245972000 | -3.611162000 | -0.240900000 | F     | -3.180238000 | 1.065942000  | 1.402335000  |
|       |              |              |              | O     | -4.539833000 | -1.704263000 | 0.651576000  |
|       |              |              |              | O     | -4.643777000 | -0.704714000 | -1.676750000 |
|       |              |              |              | O     | -5.734554000 | 0.495419000  | 0.262553000  |



| TS(4) |              |              |              | PC(4) |              |              |              |
|-------|--------------|--------------|--------------|-------|--------------|--------------|--------------|
| C     | -2.185502000 | 0.260547000  | -0.079729000 | C     | -2.958400000 | 0.193103000  | 0.170689000  |
| C     | -1.158344000 | -0.936580000 | -0.057360000 | C     | -2.512834000 | -1.291104000 | -0.036080000 |
| F     | -1.769684000 | -2.007882000 | 0.542750000  | F     | -3.439102000 | -2.095004000 | 0.571696000  |
| F     | -0.862019000 | -1.268625000 | -1.325135000 | F     | -2.536889000 | -1.549399000 | -1.372156000 |
| C     | 0.144516000  | -0.804491000 | 0.758825000  | C     | -1.156434000 | -1.600412000 | 0.533396000  |
| F     | 0.593125000  | 0.919902000  | -0.244074000 | F     | 1.462163000  | 0.850716000  | -0.109782000 |
| F     | 0.088538000  | -0.186273000 | 1.890165000  | F     | -1.145736000 | -1.767739000 | 1.875386000  |
| C     | 1.236062000  | -1.727873000 | 0.591818000  | C     | -0.006487000 | -1.734226000 | -0.132411000 |
| F     | 1.850106000  | -2.022791000 | 1.753380000  | F     | 1.120284000  | -2.053173000 | 0.466738000  |
| F     | 0.927044000  | -2.851955000 | -0.085389000 | F     | 0.142323000  | -1.595299000 | -1.430461000 |
| S     | 2.905611000  | -0.969580000 | -0.598406000 | S     | 4.947791000  | -1.209207000 | -0.137642000 |
| O     | 2.298731000  | -0.770818000 | -1.940719000 | O     | 4.836027000  | -1.034720000 | -1.592958000 |
| O     | 3.332781000  | 0.230102000  | 0.172683000  | O     | 5.460095000  | -0.113393000 | 0.697397000  |
| F     | -1.933906000 | 1.041635000  | -1.148304000 | F     | -2.839110000 | 0.502963000  | 1.488417000  |
| C     | -3.678317000 | -0.203211000 | -0.196395000 | F     | -2.112249000 | 0.983951000  | -0.537906000 |
| O     | 3.716943000  | -2.207186000 | -0.407131000 | O     | 4.549837000  | -2.481387000 | 0.482247000  |
| F     | -2.081148000 | 0.999107000  | 1.049917000  | C     | -4.411354000 | 0.558643000  | -0.260863000 |
| Al    | 1.226504000  | 2.547187000  | 0.076139000  | Al    | 1.967773000  | 2.476802000  | 0.096524000  |
| F     | 2.338154000  | 2.957983000  | -1.143436000 | F     | 3.169701000  | 2.852959000  | -1.067148000 |
| F     | 1.864994000  | 2.580981000  | 1.652704000  | F     | 2.612873000  | 2.677449000  | 1.672634000  |
| F     | -0.134707000 | 3.572322000  | -0.019730000 | F     | 0.624630000  | 3.522891000  | -0.109066000 |
| F     | -4.439204000 | 0.872157000  | -0.451622000 | F     | -4.591299000 | 1.881820000  | -0.099416000 |
| F     | -3.820457000 | -1.080841000 | -1.204035000 | F     | -5.315710000 | -0.085954000 | 0.491914000  |
| F     | -4.106667000 | -0.764306000 | 0.942040000  | F     | -4.623025000 | 0.254802000  | -1.551341000 |