

# How does vanadium nitrogenase reduce CO to hydrocarbons?

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## Supplementary information

Cartesian coordinates (Å) for reported structures. TS = transition state.

**Fig 1. fevcocyshishomo.car\_7**

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | -3.805250666 | -4.405327955 | 3.658968633  |
| C2   | -1.185734094 | -6.236486583 | 0.319168085  |
| C3   | -0.094389270 | -4.147381497 | 2.067741308  |
| C4   | -1.671809134 | -4.174755517 | 1.943495428  |
| C5   | -1.868345876 | -7.338082007 | -0.486206721 |
| C6   | -2.206177250 | -5.451419911 | 1.197630664  |
| C7   | -2.280161381 | -4.059088236 | 3.377577118  |
| C8   | 1.436057704  | 10.162841749 | -0.306998323 |
| C9   | 3.075108306  | -3.036097277 | -2.216490510 |
| C10  | 0.906201072  | 8.981944274  | 0.534338273  |
| C11  | 2.050164118  | -3.759409017 | -1.245972204 |
| C12  | 0.114502582  | -4.744744749 | -2.667125348 |
| C13  | -1.505762759 | -3.504101450 | -1.999261438 |
| C14  | 0.639810573  | -3.823884423 | -1.762737449 |
| C15  | 0.520176816  | 11.384901479 | -0.187809960 |
| C16  | 4.461734877  | -3.225936955 | -1.631866217 |
| Fe17 | -0.641084342 | 6.068894800  | 0.183959895  |
| Fe18 | -2.087792586 | 3.712407171  | 0.961149870  |
| Fe19 | 0.604376779  | 3.844872637  | 1.224299158  |
| Fe20 | -0.504259783 | 3.686252743  | -1.249796778 |
| Fe21 | -0.435666854 | 1.007386607  | -1.140339344 |
| Fe22 | -2.051073802 | 1.063488978  | 1.028449652  |
| Fe23 | 0.614631375  | 1.242865605  | 1.289429501  |
| H24  | 1.619001210  | 8.158516071  | 0.421858890  |
| H25  | 2.827433034  | -1.967995434 | -2.217292991 |
| H26  | -0.691186146 | 12.468036402 | -1.149394309 |
| H27  | 3.164669810  | 11.312407080 | -0.417853224 |
| H28  | 2.796193267  | 10.802877337 | 1.096592130  |
| H29  | 0.881117530  | 9.284873592  | 1.591632752  |
| H30  | -2.495252721 | -3.085804162 | -1.854830167 |
| H31  | -2.013891373 | -6.115490439 | -2.058261091 |
| H32  | 0.626506146  | -5.561785018 | -3.172832882 |
| H33  | 2.061149866  | -3.265279303 | -0.269392676 |
| H34  | 2.417072623  | -4.788146733 | -1.100599963 |
| H35  | 1.461504389  | 9.851300877  | -1.356743015 |
| H36  | 5.606914556  | -2.606016489 | -0.268253518 |
| H37  | 3.442130158  | -4.496179672 | -3.592693002 |
| H38  | 2.103840341  | -3.605315514 | -3.902020015 |
| H39  | -2.109016761 | -3.033760223 | 3.733441931  |
| H40  | -1.681721068 | -4.719913637 | 4.018477521  |
| H41  | -3.060744929 | -5.110937378 | 0.604709248  |
| H42  | -2.614343003 | -6.139109815 | 1.943705833  |
| H43  | -0.450999625 | -6.715820276 | 0.976548498  |
| H44  | -0.647215385 | -5.559107286 | -0.348826303 |
| N45  | -0.421381080 | -3.017845628 | -1.336718971 |
| N46  | -1.253177649 | -4.559599399 | -2.805677991 |
| N47  | -0.657078472 | 2.393020535  | 0.365719929  |
| N48  | 2.828038392  | 10.504792975 | 0.116299755  |
| N49  | 3.086468307  | -3.533792809 | -3.613697454 |
| O50  | -4.610181691 | -4.488591139 | 2.686908819  |
| O51  | -4.045869088 | -4.560127741 | 4.901911135  |
| O52  | -2.060812549 | -8.477407675 | -0.060868060 |
| O53  | -2.302995650 | -7.030195408 | -1.748804809 |
| O54  | 0.455526128  | -3.116473859 | 1.470643170  |
| O55  | 0.521237966  | -5.036703388 | 2.677848484  |

|     |              |              |              |
|-----|--------------|--------------|--------------|
| O56 | -1.973711180 | -2.996836459 | 1.169921243  |
| O57 | -0.106075851 | 11.713880845 | -1.376512796 |
| O58 | 0.387526757  | 12.092900699 | 0.806072890  |
| O59 | 5.246136279  | -4.131545221 | -1.915362669 |
| O60 | 4.759221850  | -2.306640409 | -0.658827413 |
| S61 | -2.371800448 | 4.987179944  | -0.993200253 |
| S62 | -2.326523312 | -0.318171157 | -0.791412897 |
| S63 | -0.873174410 | 5.163794845  | 2.350652576  |
| S64 | -3.689038444 | 2.389253528  | 1.766433018  |
| S65 | -0.159148185 | 2.282361863  | -2.954162363 |
| S66 | -0.718032131 | -0.216712797 | 2.416517142  |
| S67 | 1.252292053  | 5.112636516  | -0.616284637 |
| S68 | 1.191480109  | -0.385929050 | -0.174793499 |
| S69 | 2.113484141  | 2.538852174  | 2.235762365  |
| S70 | -0.797026303 | 8.426692141  | 0.000560990  |
| V71 | -0.803803882 | -1.785284410 | 0.511495291  |

### A. v6coen6h2h2bh.car\_2

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 1.469009425  | 8.013502643  | 0.981529888  |
| C2   | 1.390210122  | -3.647032273 | -2.901884180 |
| C3   | 1.017855144  | -4.483024713 | -3.930522251 |
| C4   | -0.674862871 | -4.189698591 | -2.501845885 |
| C5   | -0.382457204 | -4.844688066 | 1.281357161  |
| C6   | 1.144024318  | -4.868720848 | 1.084043324  |
| C7   | -1.698140844 | 0.460754453  | 3.109793421  |
| Fe8  | 0.033406713  | 5.118061843  | 0.267402671  |
| Fe9  | -1.520498594 | 2.844138121  | 0.850528353  |
| Fe10 | 1.305607468  | 2.815629279  | 1.004723076  |
| Fe11 | 0.112516850  | 2.878705904  | -1.354513003 |
| Fe12 | 0.171999192  | 0.296387094  | -1.187129527 |
| Fe13 | -1.459332361 | -0.052791101 | 1.429436346  |
| Fe14 | 1.403403446  | 0.299300447  | 1.054337040  |
| H15  | 2.306045033  | 7.647024862  | 0.376182077  |
| H16  | 1.457176839  | 9.112494816  | 0.958014571  |
| H17  | 1.595665024  | 7.679211966  | 2.018353537  |
| H18  | 2.341940441  | -3.161599493 | -2.726325806 |
| H19  | 1.545211922  | -4.854923912 | -4.800143855 |
| H20  | -1.649720723 | -4.275235628 | -2.039240404 |
| H21  | -0.899310983 | -5.422308934 | -4.232250555 |
| H22  | -0.813927446 | -5.785960457 | 0.895429958  |
| H23  | -0.585717245 | -4.814913865 | 2.370074940  |
| N24  | 0.331452642  | -3.475485531 | -2.026867601 |
| N25  | -0.308667389 | -4.826331487 | -3.663983299 |
| N26  | 0.041948289  | 1.459965810  | 0.367477032  |
| O27  | 1.829584224  | -5.852381325 | 1.410475284  |
| O28  | 1.599397750  | -3.754151334 | 0.555950588  |
| O29  | -0.963696042 | -3.727992368 | 0.651338204  |
| O30  | -1.946888724 | 0.661925220  | 4.237102025  |
| S31  | -0.153122731 | 7.404386184  | 0.287293708  |
| S32  | -1.706172569 | 4.195003336  | -0.927783792 |
| S33  | -0.157107121 | 4.078357044  | 2.282826839  |
| S34  | 0.273007231  | 1.454219852  | -3.048963527 |
| S35  | 1.883885463  | 4.251933313  | -0.731109552 |
| S36  | -1.561765134 | -1.126741257 | -0.751399280 |
| S37  | -3.199567237 | 1.292725387  | 0.610344389  |
| S38  | 0.350029631  | -1.320136875 | 2.238640703  |
| S39  | 1.973014611  | -0.954634948 | -0.715179637 |
| S40  | 2.914418429  | 1.587791094  | 1.952309757  |
| V41  | 0.204018404  | -2.276537215 | 0.176438877  |
| H42  | -2.620525159 | 3.651447579  | 1.521013731  |
| H43  | -3.923018517 | 1.608892023  | 1.719526743  |
| H44  | -2.470329719 | -1.096568051 | 1.847197912  |

### B. v2h2b6hxhncotc.car\_4

|    |              |              |              |
|----|--------------|--------------|--------------|
| C1 | 1.561520387  | 7.873256519  | 1.394965650  |
| C2 | 1.430149537  | -3.397934450 | -3.087005929 |
| C3 | 1.046524501  | -4.128934296 | -4.189867807 |
| C4 | -0.625155032 | -3.991376134 | -2.713746437 |
| C5 | -0.269841793 | -5.009056096 | 0.824118961  |
| C6 | 1.264508896  | -4.922783430 | 0.719442247  |

|      |              |              |              |
|------|--------------|--------------|--------------|
| C7   | -2.469006231 | -0.284904324 | 3.140711873  |
| Fe8  | 0.142757753  | 5.107870893  | 0.327323209  |
| Fe9  | -1.265246065 | 2.622650111  | 1.129405631  |
| Fe10 | 1.521297400  | 2.865181466  | 1.032790637  |
| Fe11 | 0.268335120  | 2.909757851  | -1.331602401 |
| Fe12 | 0.292303982  | 0.325609797  | -1.250319275 |
| Fe13 | -1.794758926 | -0.246754163 | 1.508597795  |
| Fe14 | 1.381706993  | 0.330747755  | 1.127023211  |
| H15  | 2.474820005  | 7.524053016  | 0.899820583  |
| H16  | 1.586997591  | 8.968929159  | 1.474489327  |
| H17  | 1.508029797  | 7.439771431  | 2.400366484  |
| H18  | 2.379281534  | -2.918824115 | -2.882192412 |
| H19  | 1.563281228  | -4.409408513 | -5.099198431 |
| H20  | -1.596429558 | -4.121697005 | -2.253290264 |
| H21  | -0.867688095 | -5.054070119 | -4.551486136 |
| H22  | -0.620320867 | -5.826676135 | 0.165768250  |
| H23  | -0.530353460 | -5.292167460 | 1.862165360  |
| H24  | -2.763598096 | -1.419598299 | 1.479718645  |
| H25  | -1.172899780 | 1.360755269  | 2.146880776  |
| H26  | -3.954271135 | 1.730108381  | 1.643977270  |
| H27  | -2.322811413 | 3.275020578  | 2.030169230  |
| N28  | 0.384348241  | -3.321423658 | -2.183721144 |
| N29  | -0.273722895 | -4.505950025 | -3.939847845 |
| N30  | 0.318124869  | 1.640416928  | 0.222275240  |
| O31  | 1.988586910  | -5.917894599 | 0.892170814  |
| O32  | 1.677894600  | -3.709243839 | 0.436234446  |
| O33  | -0.885536410 | -3.787145352 | 0.479258644  |
| O34  | -2.984788627 | -0.393981093 | 4.189161423  |
| S35  | 0.052393514  | 7.396607518  | 0.401995021  |
| S36  | -1.565691666 | 4.114098586  | -0.782342094 |
| S37  | 0.129449512  | 4.022815742  | 2.372373152  |
| S38  | 0.309525028  | 1.563264878  | -3.085199741 |
| S39  | 2.027903029  | 4.257885820  | -0.691122431 |
| S40  | -1.518047556 | -1.036796141 | -0.782280674 |
| S41  | -3.198376084 | 1.344584871  | 0.583191251  |
| S42  | 0.207598339  | -1.301564534 | 2.221756250  |
| S43  | 2.049044300  | -0.937155691 | -0.587881816 |
| S44  | 2.889253827  | 1.521691658  | 2.144396577  |
| V45  | 0.222906796  | -2.259738756 | 0.160556879  |

### C. v6con6h2h2b3bte.car\_4

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 2.207903367  | 7.928652220  | 0.568518159  |
| C2   | 0.891086762  | -3.787356681 | -2.974636868 |
| C3   | 0.313032109  | -4.567571255 | -3.949023075 |
| C4   | -1.129700144 | -4.212043650 | -2.281210717 |
| C5   | -0.459707427 | -5.039976747 | 1.324006751  |
| C6   | 1.061088573  | -5.142450851 | 1.057851154  |
| C7   | -1.802213238 | 0.234832994  | 3.232632575  |
| Fe8  | 0.492984317  | 5.211541736  | -0.148321905 |
| Fe9  | -1.175733041 | 3.233786257  | 0.791306224  |
| Fe10 | 1.586870157  | 2.839051055  | 0.770076802  |
| Fe11 | 0.171995296  | 2.862320778  | -1.563003971 |
| Fe12 | -0.028930186 | 0.298591728  | -1.121519097 |
| Fe13 | -1.331760328 | 0.119369288  | 1.547403068  |
| Fe14 | 1.574819418  | 0.257941198  | 0.923718552  |
| H15  | 3.060191795  | 7.520979183  | 0.011836719  |
| H16  | 2.283799303  | 9.024159436  | 0.599801926  |
| H17  | 2.223562161  | 7.536182971  | 1.592539923  |
| H18  | 1.881525707  | -3.353150465 | -2.934143111 |
| H19  | 0.684774795  | -4.956551223 | -4.888323650 |
| H20  | -2.025896603 | -4.246079244 | -1.676555343 |
| H21  | -1.692821190 | -5.364167795 | -3.980202520 |
| H22  | -0.964457690 | -5.940376203 | 0.928539521  |
| H23  | -0.620733043 | -5.029616331 | 2.417976701  |
| H24  | -2.355021269 | -0.926336825 | 1.835063523  |
| H25  | -0.939707473 | 1.083660289  | 2.865768361  |
| H26  | -3.571904324 | 2.095495732  | 1.960604946  |
| H27  | -2.128703991 | 4.154453187  | 1.554658221  |
| N28  | -0.015349091 | -3.575812846 | -1.948902437 |
| N29  | -0.979474853 | -4.833766527 | -3.493660778 |
| N30  | 0.183768669  | 1.588084312  | 0.269927340  |
| O31  | 1.691833920  | -6.175614414 | 1.340067172  |

|     |              |              |              |
|-----|--------------|--------------|--------------|
| O32 | 1.541731472  | -4.047321065 | 0.523807723  |
| O33 | -0.996866873 | -3.868912441 | 0.744855183  |
| O34 | -2.247368345 | 0.187343776  | 4.336147296  |
| S35 | 0.602777505  | 7.498180997  | -0.280571304 |
| S36 | -1.409134169 | 4.492442888  | -1.113420113 |
| S37 | 0.418698106  | 4.375716216  | 2.011371022  |
| S38 | -0.195569782 | 1.253753571  | -3.058529190 |
| S39 | 2.169741805  | 4.024081066  | -1.156183592 |
| S40 | -1.667624255 | -1.092311493 | -0.440003490 |
| S41 | -2.943109562 | 1.707140215  | 0.817185101  |
| S42 | 0.473395909  | -1.336452409 | 2.199358014  |
| S43 | 1.780864313  | -1.084357873 | -1.000710150 |
| S44 | 3.190156250  | 1.578898904  | 1.671841561  |
| V45 | 0.195176638  | -2.526444810 | 0.112061930  |

#### D. v6concox2h2b.car\_3

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 1.802490915  | 8.041300650  | 0.870496045  |
| C2   | 1.381588717  | -3.670116068 | -2.900683802 |
| C3   | 0.944681049  | -4.486714324 | -3.919376530 |
| C4   | -0.690789446 | -4.138285815 | -2.437628015 |
| C5   | -0.285437754 | -4.857789878 | 1.270115347  |
| C6   | 1.240154807  | -4.867571767 | 1.054935442  |
| C7   | -1.755282118 | 0.705133083  | 3.052849711  |
| C8   | -2.909296643 | -1.368822046 | 1.888949365  |
| Fe9  | 0.246856923  | 5.212207933  | 0.202870269  |
| Fe10 | -1.263574566 | 2.926318128  | 0.742832142  |
| Fe11 | 1.535092962  | 2.895579493  | 0.834730252  |
| Fe12 | 0.175816937  | 2.985397734  | -1.500790120 |
| Fe13 | 0.246198037  | 0.317687516  | -1.276977146 |
| Fe14 | -1.671279542 | -0.160941743 | 1.452170405  |
| Fe15 | 1.411011758  | 0.374318081  | 1.004516380  |
| H16  | 2.560263309  | 7.639567167  | 0.188463669  |
| H17  | 1.831793852  | 9.139517562  | 0.841644284  |
| H18  | 2.017854966  | 7.703853886  | 1.891718056  |
| H19  | 2.353877617  | -3.217495843 | -2.754527302 |
| H20  | 1.428622317  | -4.873743537 | -4.807174311 |
| H21  | -1.654857866 | -4.181977463 | -1.947779562 |
| H22  | -1.013098915 | -5.355863307 | -4.161358126 |
| H23  | -0.711466369 | -5.789369062 | 0.852623546  |
| H24  | -0.472141839 | -4.880932648 | 2.362804657  |
| N25  | 0.356627688  | -3.463597759 | -1.993062831 |
| N26  | -0.384404597 | -4.781707990 | -3.611823461 |
| N27  | 0.225370881  | 1.624384922  | 0.215213338  |
| O28  | 1.934456214  | -5.858131079 | 1.335256285  |
| O29  | 1.690958012  | -3.730867740 | 0.562499696  |
| O30  | -0.878617996 | -3.721557627 | 0.687644239  |
| O31  | -1.886045807 | 1.155752287  | 4.119427624  |
| O32  | -3.741024208 | -2.127512689 | 2.194693051  |
| S33  | 0.098099129  | 7.496806172  | 0.336605405  |
| S34  | -1.571301765 | 4.361658166  | -0.942172641 |
| S35  | 0.134447233  | 4.116226018  | 2.189447148  |
| S36  | 0.228464366  | 1.509228513  | -3.155310850 |
| S37  | 2.023058707  | 4.309070821  | -0.931214783 |
| S38  | -1.528512001 | -1.118164999 | -0.758675273 |
| S39  | -3.022631356 | 1.439164387  | 0.397916277  |
| S40  | 0.332359270  | -1.216037355 | 2.227894563  |
| S41  | 2.073109564  | -0.937989017 | -0.708144962 |
| S42  | 3.010551733  | 1.585390603  | 1.860455355  |
| V43  | 0.298687532  | -2.272534318 | 0.190792503  |
| H44  | -3.824605383 | 1.903861641  | 1.393484916  |
| H45  | -2.318126322 | 3.635299314  | 1.583649746  |

#### E v6h2h2b6condel.car\_1

|     |              |              |              |
|-----|--------------|--------------|--------------|
| C1  | 1.739415278  | 7.944925183  | 1.254307557  |
| C2  | 0.977550947  | -3.570677910 | -2.913544690 |
| C3  | 0.487379639  | -4.338724942 | -3.945884021 |
| C4  | -1.059086914 | -4.074774574 | -2.355653885 |
| C5  | -0.456773636 | -4.917333575 | 1.307832769  |
| C6  | 1.057044189  | -4.914977430 | 1.011879517  |
| Fe7 | 0.153201010  | 5.144895200  | 0.566135127  |

|      |              |              |              |
|------|--------------|--------------|--------------|
| Fe8  | -1.415240043 | 2.994929386  | 1.211672772  |
| Fe9  | 1.360658713  | 2.767391529  | 1.182991866  |
| Fe10 | -0.008972905 | 2.959503425  | -1.121871873 |
| Fe11 | -0.063506796 | 0.370945497  | -0.964723005 |
| Fe12 | -1.386068018 | -0.073556834 | 1.371292478  |
| Fe13 | 1.309654253  | 0.249286968  | 1.240957422  |
| H14  | 2.532010602  | 7.582327724  | 0.589557997  |
| H15  | 1.765445351  | 9.042897856  | 1.287149935  |
| H16  | 1.905145825  | 7.551020044  | 2.264399997  |
| H17  | 1.952211892  | -3.113398735 | -2.801703842 |
| H18  | 0.924524390  | -4.686760342 | -4.872918094 |
| H19  | -1.997908662 | -4.144768568 | -1.820486487 |
| H20  | -1.478858489 | -5.207590163 | -4.118279291 |
| H21  | -0.915068856 | -5.819415274 | 0.861619565  |
| H22  | -0.583716100 | -4.996403844 | 2.406356599  |
| H23  | -2.432812404 | 3.754537620  | 2.038901385  |
| H24  | -3.652111273 | 1.519858687  | 2.349925674  |
| H25  | -2.367914252 | -0.884195789 | 2.219990472  |
| N26  | 0.009500610  | -3.418394743 | -1.936585037 |
| N27  | -0.820643009 | -4.657596254 | -3.578294603 |
| N28  | -0.027486522 | 1.478832202  | 0.598728492  |
| O29  | 1.754816605  | -5.932457909 | 1.156359939  |
| O30  | 1.484106149  | -3.736692400 | 0.619109824  |
| O31  | -1.066409179 | -3.744608037 | 0.824367059  |
| S32  | 0.063505739  | 7.434038680  | 0.611930832  |
| S33  | -1.722066555 | 4.365847756  | -0.497965640 |
| S34  | 0.068677882  | 4.094265258  | 2.578152248  |
| S35  | -0.066321167 | 1.498475631  | -2.812499100 |
| S36  | 1.883323563  | 4.190345133  | -0.580624212 |
| S37  | -1.733139123 | -1.096198670 | -0.572100860 |
| S38  | -3.112071207 | 1.443493477  | 1.100193565  |
| S39  | 0.205398386  | -1.318962099 | 2.436343798  |
| S40  | 1.739807223  | -0.927594643 | -0.618844428 |
| S41  | 2.930997575  | 1.453478895  | 2.058065186  |
| V42  | 0.061799285  | -2.266213415 | 0.363756994  |

### E-TS-A v6h2h2b6contc\_orig.car

|      |        |        |        |
|------|--------|--------|--------|
| C1   | 1.776  | 7.935  | 0.900  |
| C2   | 1.082  | -3.665 | -3.066 |
| C3   | 0.618  | -4.478 | -4.076 |
| C4   | -0.966 | -4.151 | -2.535 |
| C5   | -0.438 | -4.868 | 1.206  |
| C6   | 1.074  | -4.931 | 0.908  |
| C7   | -1.501 | 0.835  | 4.233  |
| D8   | -2.402 | 3.699  | 1.672  |
| D9   | -3.747 | 1.677  | 1.985  |
| D10  | -2.363 | -1.027 | 2.036  |
| Fe11 | 0.199  | 5.094  | 0.267  |
| Fe12 | -1.368 | 2.901  | 0.909  |
| Fe13 | 1.476  | 2.750  | 0.890  |
| Fe14 | 0.122  | 2.878  | -1.388 |
| Fe15 | 0.103  | 0.315  | -1.235 |
| Fe16 | -1.358 | -0.130 | 1.324  |
| Fe17 | 1.449  | 0.231  | 0.949  |
| H18  | 2.563  | 7.553  | 0.240  |
| H19  | 1.797  | 9.034  | 0.891  |
| H20  | 1.959  | 7.583  | 1.923  |
| H21  | 2.058  | -3.211 | -2.947 |
| H22  | 1.078  | -4.859 | -4.980 |
| H23  | -1.912 | -4.215 | -2.012 |
| H24  | -1.340 | -5.359 | -4.260 |
| H25  | -0.918 | -5.793 | 0.834  |
| H26  | -0.568 | -4.854 | 2.307  |
| N27  | 0.089  | -3.470 | -2.121 |
| N28  | -0.697 | -4.786 | -3.726 |
| N29  | 0.109  | 1.457  | 0.319  |
| O30  | 1.751  | -5.941 | 1.164  |
| O31  | 1.524  | -3.814 | 0.381  |
| O32  | -1.019 | -3.721 | 0.632  |
| O33  | -1.676 | 0.938  | 5.359  |
| S34  | 0.094  | 7.387  | 0.303  |
| S35  | -1.640 | 4.245  | -0.835 |

|     |        |        |        |
|-----|--------|--------|--------|
| S36 | 0.112  | 4.036  | 2.280  |
| S37 | 0.111  | 1.445  | -3.089 |
| S38 | 1.969  | 4.187  | -0.856 |
| S39 | -1.633 | -1.064 | -0.691 |
| S40 | -3.075 | 1.373  | 0.839  |
| S41 | 0.386  | -1.327 | 2.209  |
| S42 | 1.873  | -1.011 | -0.873 |
| S43 | 3.078  | 1.452  | 1.739  |
| V44 | 0.162  | -2.283 | 0.150  |

## F. v2con2h2bhcoxtcdelco.car\_1

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 1.941050830  | 7.882508199  | -0.097906075 |
| C2   | 1.156655108  | -3.903467146 | -2.572530219 |
| C3   | 0.764386116  | -4.874851015 | -3.467019985 |
| C4   | -0.738313302 | -4.665906510 | -1.827047237 |
| C5   | -0.478036826 | -4.805325576 | 1.761109136  |
| C6   | 1.060510897  | -4.747240555 | 1.647905145  |
| C7   | -1.828716135 | 2.241417494  | 2.945186608  |
| Fe8  | 0.065347954  | 5.168221302  | -0.080227434 |
| Fe9  | -1.614485239 | 2.820709828  | 1.281140323  |
| Fe10 | 1.334137749  | 3.010616313  | 0.975381633  |
| Fe11 | -0.065290838 | 2.722699591  | -1.335401517 |
| Fe12 | -0.005756738 | 0.088694596  | -1.321315797 |
| Fe13 | -1.418785625 | 0.127763919  | 0.804797851  |
| Fe14 | 1.247466830  | 0.373624276  | 1.063612737  |
| H15  | 2.560896137  | 7.311448806  | -0.797226503 |
| H16  | 2.068318772  | 8.957770668  | -0.285833207 |
| H17  | 2.253985601  | 7.657938649  | 0.928297533  |
| H18  | 2.039606821  | -3.276268787 | -2.581859529 |
| H19  | 1.211042007  | -5.254832721 | -4.377671199 |
| H20  | -1.619505271 | -4.816180102 | -1.216796144 |
| H21  | -1.026368695 | -6.073488894 | -3.402846788 |
| H22  | -0.821916231 | -5.794056575 | 1.399942414  |
| H23  | -0.743099323 | -4.746476374 | 2.834507705  |
| H24  | -2.697790421 | 3.765490781  | 1.744511879  |
| H25  | -3.951115468 | 1.008592830  | 1.582283911  |
| N26  | 0.215787134  | -3.787619776 | -1.563980506 |
| N27  | -0.451293043 | -5.355939799 | -2.978705339 |
| N28  | -0.107196113 | 1.382971208  | 0.202315114  |
| O29  | 1.776287675  | -5.668867026 | 2.077949607  |
| O30  | 1.476440892  | -3.646226943 | 1.069149839  |
| O31  | -1.092947592 | -3.760086640 | 1.035718424  |
| O32  | -2.103183293 | 1.982877514  | 4.055849632  |
| S33  | 0.137344521  | 7.456203358  | -0.336195754 |
| S34  | -1.801695135 | 4.096749841  | -0.837912885 |
| S35  | -0.013517314 | 4.404775898  | 2.113169655  |
| S36  | -0.085568443 | 1.384900632  | -3.116873039 |
| S37  | 1.822143513  | 4.065221716  | -1.028531687 |
| S38  | -1.731846620 | -1.371885446 | -0.848515756 |
| S39  | -3.324936429 | 1.399345236  | 0.435273904  |
| S40  | -0.078246658 | -0.980164628 | 2.309728833  |
| S41  | 1.863653770  | -1.046670673 | -0.572736056 |
| S42  | 2.769788464  | 1.590996571  | 1.964445513  |
| V43  | 0.034774253  | -2.325976239 | 0.414849245  |

## F-TS-G v2con2h2bhcoxtc.car\_1

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 2.110815949  | 7.965562599  | -0.163652113 |
| C2   | 1.249286943  | -3.786579698 | -2.827272292 |
| C3   | 0.828119535  | -4.745227865 | -3.721880507 |
| C4   | -0.614237176 | -4.561218739 | -2.025782817 |
| C5   | -0.236241396 | -4.727141281 | 1.593982958  |
| C6   | 1.289988047  | -4.662453147 | 1.407941822  |
| C7   | -1.602576182 | 2.272065157  | 2.905595820  |
| C8   | -3.247814111 | -1.428029659 | 2.480482975  |
| Fe9  | 0.255383221  | 5.202989844  | -0.107108147 |
| Fe10 | -1.464909280 | 2.937672341  | 1.270484730  |
| Fe11 | 1.456898866  | 2.959639478  | 0.856453347  |
| Fe12 | 0.023602234  | 2.782822007  | -1.390885514 |
| Fe13 | 0.158388012  | 0.199018217  | -1.393490690 |
| Fe14 | -1.317151047 | 0.257816972  | 0.865192357  |

|      |              |              |              |
|------|--------------|--------------|--------------|
| Fe15 | 1.508576522  | 0.394246677  | 0.865902230  |
| H16  | 2.736191127  | 7.433669174  | -0.888463237 |
| H17  | 2.192182184  | 9.048579159  | -0.333489962 |
| H18  | 2.457244476  | 7.735471697  | 0.850804343  |
| H19  | 2.132271274  | -3.162237610 | -2.861911717 |
| H20  | 1.242376490  | -5.112765984 | -4.652230985 |
| H21  | -1.475866483 | -4.724834836 | -1.390114164 |
| H22  | -0.958894304 | -5.948434343 | -3.616224510 |
| H23  | -0.603550818 | -5.690876073 | 1.189636158  |
| H24  | -0.448309662 | -4.733976068 | 2.681425284  |
| H25  | -2.542192105 | 3.844174054  | 1.795643319  |
| H26  | -3.870109780 | 1.226965944  | 1.448230302  |
| N27  | 0.345693432  | -3.685463621 | -1.782876280 |
| N28  | -0.367701171 | -5.238560453 | -3.198217346 |
| N29  | 0.052926710  | 1.413834314  | 0.157355738  |
| O30  | 2.033105808  | -5.595084321 | 1.757610430  |
| O31  | 1.682585964  | -3.534583532 | 0.863636478  |
| O32  | -0.892321887 | -3.637337524 | 0.972609962  |
| O33  | -1.791073578 | 1.976196958  | 4.026608177  |
| O34  | -3.945167470 | -2.208216269 | 2.947542843  |
| S35  | 0.318202989  | 7.485994027  | -0.366940825 |
| S36  | -1.661262156 | 4.204647354  | -0.822250977 |
| S37  | 0.235384022  | 4.410278877  | 2.077449453  |
| S38  | -0.036996310 | 1.468096645  | -3.193561582 |
| S39  | 1.934332550  | 4.076575835  | -1.123145640 |
| S40  | -1.566658851 | -1.228084663 | -0.846678658 |
| S41  | -3.159573765 | 1.578242527  | 0.341352041  |
| S42  | 0.223181447  | -0.886714555 | 2.214142247  |
| S43  | 2.006223753  | -1.021444324 | -0.781728545 |
| S44  | 3.100588329  | 1.640619610  | 1.593072208  |
| V45  | 0.229057631  | -2.195914846 | 0.324751261  |

### G v2con2h2bhcoxtc.car\_4

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 2.085022846  | 7.918334610  | -0.170728340 |
| C2   | 1.231512581  | -3.804282262 | -2.816376857 |
| C3   | 0.797428875  | -4.764174710 | -3.703548054 |
| C4   | -0.631135166 | -4.563128291 | -1.997327972 |
| C5   | -0.227867691 | -4.728581106 | 1.573675877  |
| C6   | 1.303580197  | -4.672371765 | 1.400975502  |
| C7   | -1.657885118 | 2.201120329  | 2.950195890  |
| C8   | -2.665099445 | -0.883582898 | 1.999749116  |
| Fe9  | 0.223570715  | 5.161375693  | -0.051999966 |
| Fe10 | -1.497535452 | 2.800839180  | 1.284463225  |
| Fe11 | 1.401659170  | 2.878617524  | 0.898747396  |
| Fe12 | -0.024879176 | 2.758482424  | -1.314534125 |
| Fe13 | 0.097806942  | 0.232786867  | -1.293934663 |
| Fe14 | -1.494540324 | 0.053520146  | 1.031365885  |
| Fe15 | 1.506659273  | 0.362319048  | 0.853387131  |
| H16  | 2.687167696  | 7.372564884  | -0.905334276 |
| H17  | 2.160590506  | 8.997829764  | -0.362172663 |
| H18  | 2.462824695  | 7.704935098  | 0.835942775  |
| H19  | 2.115920702  | -3.181411942 | -2.858653117 |
| H20  | 1.206718856  | -5.140628727 | -4.632539014 |
| H21  | -1.487997029 | -4.717991159 | -1.353382148 |
| H22  | -0.993028878 | -5.958800233 | -3.574407389 |
| H23  | -0.590748472 | -5.694386634 | 1.170102870  |
| H24  | -0.451945943 | -4.729165043 | 2.659510905  |
| H25  | -2.570257075 | 3.727664572  | 1.824728504  |
| H26  | -4.057034094 | 1.343833417  | 1.323548959  |
| N27  | 0.336870190  | -3.692777091 | -1.767189066 |
| N28  | -0.398454083 | -5.245458409 | -3.168508648 |
| N29  | -0.008426191 | 1.463812781  | 0.193200407  |
| O30  | 2.044084791  | -5.603046739 | 1.754208498  |
| O31  | 1.702976335  | -3.543942012 | 0.849624556  |
| O32  | -0.857091387 | -3.642946752 | 0.935338991  |
| O33  | -1.832263546 | 2.003162005  | 4.094217212  |
| O34  | -3.439733798 | -1.500841840 | 2.619903484  |
| S35  | 0.286782843  | 7.438952697  | -0.307143416 |
| S36  | -1.697496015 | 4.182584532  | -0.772810862 |
| S37  | 0.182242509  | 4.322455365  | 2.120843490  |
| S38  | -0.011601746 | 1.404789534  | -3.103135441 |
| S39  | 1.901838027  | 4.032365446  | -1.049880678 |

|     |              |              |              |
|-----|--------------|--------------|--------------|
| S40 | -1.517731970 | -1.246013099 | -0.847400981 |
| S41 | -3.170093356 | 1.493443429  | 0.300322616  |
| S42 | 0.289941152  | -0.968638998 | 2.239504997  |
| S43 | 1.921417802  | -1.001412380 | -0.864142135 |
| S44 | 3.062348391  | 1.624772963  | 1.682337708  |
| V45 | 0.273880847  | -2.196980189 | 0.319253761  |

## H. v6h2b2h26h.car\_2

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 1.832479447  | 7.878908578  | 1.190662314  |
| C2   | 1.014737345  | -3.720863438 | -2.838418163 |
| C3   | 0.511223896  | -4.425070054 | -3.909410612 |
| C4   | -1.025424357 | -4.223886412 | -2.301295955 |
| C5   | -0.517426231 | -4.904571990 | 1.308696568  |
| C6   | 1.014582837  | -4.861968762 | 1.147746397  |
| Fe7  | 0.255037648  | 5.099221794  | 0.373086690  |
| Fe8  | -1.352774664 | 2.799908198  | 1.316721989  |
| Fe9  | 1.529968997  | 2.820792591  | 1.155055336  |
| Fe10 | 0.105775577  | 2.827108720  | -1.213590527 |
| Fe11 | 0.014287206  | 0.279019562  | -1.181480902 |
| Fe12 | -1.343412750 | 0.172135210  | 1.206521696  |
| Fe13 | 1.332674867  | 0.276433160  | 1.086480978  |
| H14  | 2.682823896  | 7.474249135  | 0.629546728  |
| H15  | 1.893492842  | 8.976028890  | 1.202395810  |
| H16  | 1.869798035  | 7.506675835  | 2.221463866  |
| H17  | 1.994221224  | -3.276999169 | -2.711315257 |
| H18  | 0.938385097  | -4.717656472 | -4.860362241 |
| H19  | -1.968299279 | -4.300458194 | -1.774001768 |
| H20  | -1.470453656 | -5.246573759 | -4.125839704 |
| H21  | -0.909902135 | -5.724183832 | 0.677017153  |
| H22  | -0.754980899 | -5.161226972 | 2.358960937  |
| H23  | -2.373063745 | -0.486568315 | 2.113863231  |
| H24  | -1.307488471 | 1.393950677  | 2.358275940  |
| H25  | -3.850676963 | 1.471904835  | 1.742999673  |
| H26  | -2.398396084 | 3.459502444  | 2.206700859  |
| N27  | 0.051364180  | -3.603875724 | -1.851961646 |
| N28  | -0.798874633 | -4.748467321 | -3.553286387 |
| N29  | 0.106156923  | 1.521548086  | 0.263101278  |
| O30  | 1.715149257  | -5.872693703 | 1.323106342  |
| O31  | 1.447441791  | -3.669389711 | 0.812966427  |
| O32  | -1.104799357 | -3.671658565 | 0.958729428  |
| S33  | 0.220347195  | 7.399149114  | 0.383130801  |
| S34  | -1.596318711 | 4.201475594  | -0.596364227 |
| S35  | 0.203108701  | 4.095186794  | 2.467733508  |
| S36  | -0.013389400 | 1.474138763  | -2.997998887 |
| S37  | 2.014904256  | 4.103532330  | -0.712927542 |
| S38  | -1.678823471 | -1.127880425 | -0.656192278 |
| S39  | -3.151697309 | 1.520718035  | 0.578082669  |
| S40  | 0.136576233  | -1.070962845 | 2.403521167  |
| S41  | 1.749741529  | -1.050773069 | -0.667929395 |
| S42  | 2.954773946  | 1.341282799  | 2.041532617  |
| V43  | 0.027149187  | -2.227142409 | 0.424275089  |

## H-TS-I. v6h2b2h26h2cote.car\_1

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 1.631125183  | 7.849974820  | 1.147863654  |
| C2   | 1.360636996  | -3.746190629 | -3.036548720 |
| C3   | 0.912899568  | -4.447214979 | -4.134068349 |
| C4   | -0.678745557 | -4.323636733 | -2.572310031 |
| C5   | -0.255665612 | -5.022693833 | 1.035848288  |
| C6   | -2.113228072 | 2.198777703  | 3.826378552  |
| C7   | 1.280414331  | -4.923039873 | 0.934989194  |
| Fe8  | 0.195663227  | 5.026651346  | 0.250740724  |
| Fe9  | -1.548326779 | 2.703321874  | 1.338112252  |
| Fe10 | 1.461501606  | 2.733951219  | 1.025605530  |
| Fe11 | 0.154546183  | 2.768460865  | -1.344502844 |
| Fe12 | 0.176497918  | 0.221294168  | -1.332764196 |
| Fe13 | -1.241982552 | 0.011732872  | 0.904730146  |
| Fe14 | 1.485194166  | 0.200577047  | 0.910647826  |
| H15  | 2.517381235  | 7.486096616  | 0.615710721  |
| H16  | 1.649714876  | 8.947931210  | 1.179984661  |
| H17  | 1.637921077  | 7.458121632  | 2.172176684  |



|     |              |              |              |
|-----|--------------|--------------|--------------|
| H18 | 2.320689211  | -3.273033254 | -2.872204650 |
| H19 | 1.377227104  | -4.704366893 | -5.077601876 |
| H20 | -1.634036754 | -4.440250840 | -2.075466497 |
| H21 | -1.033737757 | -5.326678498 | -4.426252076 |
| H22 | -0.590182217 | -5.857185397 | 0.390473503  |
| H23 | -0.521617311 | -5.290001383 | 2.077083373  |
| H24 | -2.284379838 | -0.700048901 | 1.746612311  |
| H25 | -1.304234125 | 0.990765054  | 2.161819627  |
| H26 | -3.914030183 | 1.037557857  | 1.385195033  |
| H27 | -2.724930223 | 3.541048893  | 1.845906688  |
| N28 | 0.363524984  | -3.677350447 | -2.079661241 |
| N29 | -0.396157034 | -4.818096299 | -3.824845472 |
| N30 | 0.175843047  | 1.406634106  | 0.169794890  |
| O31 | 2.010986947  | -5.905120834 | 1.147330570  |
| O32 | 1.681830303  | -3.718207419 | 0.605460319  |
| O33 | -2.851423064 | 1.666854270  | 4.536777834  |
| O34 | -0.873914054 | -3.812756600 | 0.660034443  |
| S35 | 0.077697212  | 7.324540692  | 0.260161882  |
| S36 | -1.641536292 | 4.014195770  | -0.664338589 |
| S37 | 0.170242612  | 4.060024886  | 2.338278653  |
| S38 | 0.154268152  | 1.417264071  | -3.136255425 |
| S39 | 1.993483616  | 4.084288989  | -0.804496191 |
| S40 | -1.484986191 | -1.261019752 | -0.976129199 |
| S41 | -3.118640882 | 1.333857703  | 0.322278714  |
| S42 | 0.255055834  | -1.197592901 | 2.146798147  |
| S43 | 1.944807542  | -1.084070496 | -0.859317467 |
| S44 | 2.996480640  | 1.372647462  | 1.917258393  |
| V45 | 0.226120993  | -2.328015071 | 0.162710154  |

## I. v6h2b2h26h2cotd.car\_2

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 1.616879735  | 7.840990123  | 1.139979269  |
| C2   | 1.367213798  | -3.763751030 | -3.033880319 |
| C3   | 0.919371630  | -4.465487484 | -4.130519341 |
| C4   | -0.675243162 | -4.334058609 | -2.572480796 |
| C5   | -0.244383204 | -5.023895863 | 1.034277103  |
| C6   | -2.230140410 | 2.351691559  | 3.261102251  |
| C7   | 1.291753448  | -4.924069678 | 0.942296026  |
| Fe8  | 0.104984973  | 4.994517275  | 0.336130766  |
| Fe9  | -1.765150007 | 2.763345068  | 1.612889906  |
| Fe10 | 1.393013759  | 2.687083759  | 1.086248936  |
| Fe11 | 0.136946129  | 2.756171515  | -1.226253126 |
| Fe12 | 0.178550665  | 0.199079810  | -1.343625480 |
| Fe13 | -1.182478846 | 0.018817753  | 0.856307629  |
| Fe14 | 1.586492041  | 0.173461172  | 0.858510178  |
| H15  | 2.507862895  | 7.486029877  | 0.608564000  |
| H16  | 1.621329646  | 8.940357591  | 1.160864786  |
| H17  | 1.634016640  | 7.461661199  | 2.168929316  |
| H18  | 2.328368271  | -3.294074060 | -2.867836595 |
| H19  | 1.385050756  | -4.725289340 | -5.072577345 |
| H20  | -1.630359907 | -4.448386531 | -2.074622077 |
| H21  | -1.030615929 | -5.338008567 | -4.425610693 |
| H22  | -0.575036915 | -5.864085464 | 0.394448683  |
| H23  | -0.518811975 | -5.278727632 | 2.075719265  |
| H24  | -2.199902439 | -0.695756635 | 1.715163955  |
| H25  | -1.257881154 | 0.775821856  | 2.198079067  |
| H26  | -3.921170703 | 0.759396722  | 1.383593193  |
| H27  | -2.816283493 | 3.796787571  | 1.890561781  |
| N28  | 0.367998489  | -3.689327321 | -2.079955043 |
| N29  | -0.391508775 | -4.832088062 | -3.823308526 |
| N30  | 0.204319282  | 1.354770334  | 0.180861137  |
| O31  | 2.021695433  | -5.899141906 | 1.185440858  |
| O32  | 1.695173504  | -3.727904369 | 0.585278367  |
| O33  | -2.591286582 | 2.149240600  | 4.357664217  |
| O34  | -0.861117469 | -3.817530554 | 0.645072629  |
| S35  | 0.062099714  | 7.283577198  | 0.268372366  |
| S36  | -1.654816874 | 3.998114226  | -0.638876394 |
| S37  | 0.095259966  | 4.006205933  | 2.435881710  |
| S38  | 0.185626616  | 1.458413442  | -3.083628732 |
| S39  | 1.939744788  | 4.070696296  | -0.650974684 |
| S40  | -1.499164635 | -1.281875186 | -0.985359230 |
| S41  | -3.152127132 | 1.342056815  | 0.423840279  |
| S42  | 0.340130586  | -1.205417630 | 2.101088254  |

|     |             |              |              |
|-----|-------------|--------------|--------------|
| S43 | 1.949298714 | -1.118397082 | -0.935468670 |
| S44 | 3.023502988 | 1.401635691  | 1.905293801  |
| V45 | 0.240783256 | -2.342634041 | 0.132508178  |

### J. v6con6h2h2b3btcas\_car\_3

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 1.451545628  | 8.073507624  | 0.860191976  |
| C2   | 1.261278594  | -3.632145194 | -3.023093138 |
| C3   | 0.807421999  | -4.449211494 | -4.031946887 |
| C4   | -0.778438773 | -4.175996093 | -2.480402454 |
| C5   | -0.260127771 | -4.960126201 | 1.210791528  |
| C6   | 1.269453497  | -5.027018829 | 0.965112999  |
| C7   | -1.655575204 | 0.794478290  | 2.948048472  |
| Fe8  | 0.026656268  | 5.184930327  | 0.199839055  |
| Fe9  | -1.514306383 | 2.973200775  | 1.005806995  |
| Fe10 | 1.331661409  | 2.823529072  | 0.852678355  |
| Fe11 | 0.034203574  | 2.977404406  | -1.429006184 |
| Fe12 | 0.092980408  | 0.334375277  | -1.197025176 |
| Fe13 | -1.508304525 | 0.326385765  | 1.228868823  |
| Fe14 | 1.491701463  | 0.235339921  | 0.954897981  |
| H15  | 2.268879168  | 7.719277627  | 0.223028866  |
| H16  | 1.431453410  | 9.170799093  | 0.853709672  |
| H17  | 1.612158199  | 7.719719167  | 1.884103264  |
| H18  | 2.222014642  | -3.148157384 | -2.906391004 |
| H19  | 1.270074670  | -4.810671795 | -4.941700442 |
| H20  | -1.711754060 | -4.267513147 | -1.941399012 |
| H21  | -1.134785023 | -5.370969739 | -4.207786669 |
| H22  | -0.722181783 | -5.902482576 | 0.861424834  |
| H23  | -0.416061876 | -4.908919844 | 2.306481521  |
| H24  | -2.424187410 | -0.791544660 | 1.753796949  |
| H25  | -0.128491446 | -1.290130673 | 3.035571189  |
| H26  | -3.968233691 | 1.721521690  | 1.684522291  |
| H27  | -2.546388886 | 3.699123495  | 1.851498769  |
| N28  | 0.267148419  | -3.472580149 | -2.069195062 |
| N29  | -0.498066147 | -4.791628320 | -3.673559328 |
| N30  | 0.027696248  | 1.396924673  | 0.332786407  |
| O31  | 1.935057970  | -6.014420056 | 1.320228146  |
| O32  | 1.727332696  | -3.946952412 | 0.372570465  |
| O33  | -0.825519038 | -3.842288855 | 0.580367573  |
| O34  | -1.869412778 | 0.933331295  | 4.093120796  |
| S35  | -0.190280039 | 7.469807747  | 0.208503145  |
| S36  | -1.767652562 | 4.239435332  | -0.858892164 |
| S37  | 0.056495465  | 4.120524202  | 2.243257145  |
| S38  | -0.001101159 | 1.450336085  | -3.045850709 |
| S39  | 1.839637922  | 4.303672971  | -0.886837757 |
| S40  | -1.542568000 | -1.093408928 | -0.636693717 |
| S41  | -3.279036007 | 1.583270738  | 0.522554554  |
| S42  | 0.975090925  | -1.624413063 | 2.313556248  |
| S43  | 1.948968775  | -0.944920877 | -0.993182545 |
| S44  | 3.028210651  | 1.665279486  | 1.682744565  |
| V45  | 0.365350558  | -2.450674772 | -0.027100334 |

### J-TS-K. v6con6h2h2b3btcas\_1\_4444.14

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 1.432923014  | 8.068388282  | 0.862024568  |
| C2   | 1.282964833  | -3.653967602 | -3.058277461 |
| C3   | 0.839370531  | -4.477321389 | -4.066904892 |
| C4   | -0.764386101 | -4.192672631 | -2.537047970 |
| C5   | -0.358431146 | -4.896899044 | 1.232934230  |
| C6   | 1.168743841  | -5.004324590 | 0.990813342  |
| C7   | -1.307261472 | 0.348210108  | 3.157169364  |
| Fe8  | -0.002580761 | 5.173291984  | 0.198147985  |
| Fe9  | -1.463729058 | 2.912536310  | 0.878046870  |
| Fe10 | 1.322366390  | 2.876121018  | 0.939175216  |
| Fe11 | 0.073293555  | 2.956749084  | -1.427338408 |
| Fe12 | 0.040532397  | 0.344405607  | -1.210973294 |
| Fe13 | -1.304026063 | 0.150728212  | 1.308552031  |
| Fe14 | 1.555928205  | 0.299240912  | 0.882564957  |
| H15  | 2.260830229  | 7.702449056  | 0.244190180  |
| H16  | 1.419755726  | 9.166904494  | 0.840824344  |
| H17  | 1.574417658  | 7.729486805  | 1.894766633  |
| H18  | 2.240756699  | -3.166681276 | -2.934908273 |

|     |              |              |              |
|-----|--------------|--------------|--------------|
| H19 | 1.313715873  | -4.848752652 | -4.966381755 |
| H20 | -1.706513639 | -4.279035237 | -2.013254344 |
| H21 | -1.098181103 | -5.405835037 | -4.256189558 |
| H22 | -0.841329069 | -5.853599171 | 0.958491225  |
| H23 | -0.516408213 | -4.747782558 | 2.319678650  |
| H24 | -2.290391752 | -0.875944632 | 1.856689393  |
| H25 | -0.314882238 | -0.522393271 | 3.157770545  |
| H26 | -3.784102200 | 1.641094038  | 1.840222945  |
| H27 | -2.541824127 | 3.681754949  | 1.616871649  |
| N28 | 0.277943313  | -3.487083235 | -2.118128182 |
| N29 | -0.469605704 | -4.817476024 | -3.721360686 |
| N30 | 0.069218796  | 1.470206811  | 0.305557474  |
| O31 | 1.813439809  | -5.992630908 | 1.382469866  |
| O32 | 1.644386113  | -3.957461746 | 0.360141252  |
| O33 | -0.914591972 | -3.814419260 | 0.515172405  |
| O34 | -1.751359897 | 0.672756740  | 4.219342370  |
| S35 | -0.200971681 | 7.460114339  | 0.190726505  |
| S36 | -1.758108214 | 4.226484573  | -0.934963899 |
| S37 | -0.070635028 | 4.153360591  | 2.247631331  |
| S38 | 0.045877063  | 1.454763629  | -3.066840029 |
| S39 | 1.853070529  | 4.307358564  | -0.820727485 |
| S40 | -1.575165492 | -1.097070926 | -0.739511121 |
| S41 | -3.137543020 | 1.393388281  | 0.669000939  |
| S42 | 0.753581636  | -1.427661690 | 2.141781751  |
| S43 | 1.908966454  | -0.920693086 | -1.057998632 |
| S44 | 2.991640592  | 1.703624416  | 1.821854460  |
| V45 | 0.288304691  | -2.453712839 | -0.101806492 |

### K. v6con6h2h2b3btcab.car\_2

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 2.057971415  | 7.943418521  | 0.578927295  |
| C2   | 0.908427274  | -3.832639410 | -3.020170937 |
| C3   | 0.369416418  | -4.653078900 | -3.985448627 |
| C4   | -1.136769540 | -4.217949830 | -2.393843281 |
| C5   | -0.593169505 | -4.766747519 | 1.363773290  |
| C6   | 0.899782987  | -4.943046553 | 1.017925364  |
| C7   | -1.366452994 | 0.444897683  | 3.290426232  |
| Fe8  | 0.450406342  | 5.128839016  | 0.043505248  |
| Fe9  | -1.169842476 | 3.027154314  | 0.815668430  |
| Fe10 | 1.610394971  | 2.762057734  | 0.792709597  |
| Fe11 | 0.221261747  | 2.829808977  | -1.484956924 |
| Fe12 | 0.022240971  | 0.247985237  | -1.233560296 |
| Fe13 | -1.161066414 | 0.039848329  | 1.308780371  |
| Fe14 | 1.602457919  | 0.222237739  | 0.786981018  |
| H15  | 2.837303989  | 7.509177921  | -0.057197572 |
| H16  | 2.111506071  | 9.040058000  | 0.525721451  |
| H17  | 2.218626250  | 7.626460851  | 1.616149003  |
| H18  | 1.904807471  | -3.413791121 | -2.956593298 |
| H19  | 0.774595720  | -5.077007364 | -4.895430586 |
| H20  | -2.060034022 | -4.223002502 | -1.829496580 |
| H21  | -1.632285560 | -5.453297420 | -4.061460415 |
| H22  | -1.149238403 | -5.677892435 | 1.078562924  |
| H23  | -0.674759462 | -4.651494189 | 2.463588355  |
| H24  | -2.187133128 | -0.705510130 | 2.188206322  |
| H25  | -0.867946905 | -0.250424662 | 4.007318767  |
| H26  | -3.396202813 | 1.817685606  | 1.952544386  |
| H27  | -2.186148336 | 3.884953743  | 1.540620529  |
| N28  | -0.037499548 | -3.571383056 | -2.043388333 |
| N29  | -0.941874141 | -4.895092000 | -3.573306194 |
| N30  | 0.203992690  | 1.453638140  | 0.275080881  |
| O31  | 1.513351522  | -5.984482927 | 1.307945311  |
| O32  | 1.400585381  | -3.891260318 | 0.414106763  |
| O33  | -1.134481574 | -3.636696522 | 0.721013425  |
| O34  | -1.973850213 | 1.395660841  | 3.772853284  |
| S35  | 0.370007815  | 7.415520522  | -0.014653779 |
| S36  | -1.442467220 | 4.326745643  | -0.962861330 |
| S37  | 0.340551618  | 4.197081135  | 2.111676728  |
| S38  | 0.010031368  | 1.339244153  | -3.124008411 |
| S39  | 2.144337047  | 4.079436998  | -1.056645619 |
| S40  | -1.695146373 | -1.095363943 | -0.712766950 |
| S41  | -2.905357443 | 1.532246400  | 0.717086904  |
| S42  | 0.598820394  | -1.324310465 | 2.068381306  |
| S43  | 1.820709786  | -1.099357068 | -1.016370456 |

|     |             |              |             |
|-----|-------------|--------------|-------------|
| S44 | 3.225798471 | 1.413357547  | 1.582955528 |
| V45 | 0.094346098 | -2.313698896 | 0.079677668 |

### I-TS-L. v2chon2h6h2bhth\_1\_4463.43

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 1.880935969  | 8.034875917  | -0.164145192 |
| C2   | 1.175488209  | -3.802617352 | -2.892803966 |
| C3   | 0.783681252  | -4.746680870 | -3.815335780 |
| C4   | -0.739021818 | -4.558279740 | -2.191842341 |
| C5   | -0.554289173 | -4.871243983 | 1.429659577  |
| C6   | 0.981078726  | -4.926786861 | 1.283011860  |
| C7   | -1.554619751 | 2.241184749  | 3.247398776  |
| Fe8  | 0.290738068  | 5.078894724  | -0.029510828 |
| Fe9  | -1.320547897 | 2.754393142  | 1.480236851  |
| Fe10 | 1.530452664  | 2.824677753  | 0.972906266  |
| Fe11 | 0.064253522  | 2.688417705  | -1.299406089 |
| Fe12 | 0.081080541  | 0.156452390  | -1.331475320 |
| Fe13 | -1.311642211 | -0.137293853 | 0.967070405  |
| Fe14 | 1.335013788  | 0.198450524  | 0.943401439  |
| H15  | 2.586825216  | 7.491736183  | -0.802303149 |
| H16  | 1.858750532  | 9.092561676  | -0.462579912 |
| H17  | 2.207680121  | 7.966018489  | 0.880623427  |
| H18  | 2.066865861  | -3.189010185 | -2.877316294 |
| H19  | 1.241193712  | -5.114786851 | -4.724478944 |
| H20  | -1.627360621 | -4.717894490 | -1.593362898 |
| H21  | -1.017470662 | -5.932195480 | -3.799152149 |
| H22  | -0.986774784 | -5.828561913 | 1.083937744  |
| H23  | -0.794273450 | -4.774714061 | 2.506793657  |
| H24  | -2.343109191 | -0.935829409 | 1.752911991  |
| H25  | -3.754584801 | 1.013781469  | 1.810465708  |
| H26  | -2.350185959 | 3.732463037  | 1.954397698  |
| H27  | -0.943437212 | 1.270662007  | 3.031042824  |
| N28  | 0.222676673  | -3.699652377 | -1.893705938 |
| N29  | -0.444497219 | -5.223522050 | -3.356523648 |
| N30  | 0.035194254  | 1.362042231  | 0.192188684  |
| O31  | 1.633697677  | -5.909058771 | 1.675461186  |
| O32  | 1.467977843  | -3.845671883 | 0.722055829  |
| O33  | -1.092820752 | -3.782948311 | 0.711841966  |
| O34  | -1.991500543 | 2.416748093  | 4.363313852  |
| S35  | 0.157425691  | 7.349353581  | -0.361152902 |
| S36  | -1.613178136 | 4.093545060  | -0.681044771 |
| S37  | 0.332348060  | 4.303828398  | 2.179165601  |
| S38  | 0.040538761  | 1.369290628  | -3.116129816 |
| S39  | 2.012300907  | 3.948560410  | -1.011428917 |
| S40  | -1.610335806 | -1.271533568 | -0.926219555 |
| S41  | -3.050013094 | 1.359574758  | 0.699025180  |
| S42  | 0.205543954  | -1.274983935 | 2.201253819  |
| S43  | 1.862776646  | -1.120914895 | -0.789481461 |
| S44  | 2.938575870  | 1.302714766  | 1.861741381  |
| V45  | 0.106568564  | -2.386046852 | 0.169494148  |

### L. v2chon2h6h2bhth.car\_4

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 2.156029666  | 7.823141519  | -0.055565057 |
| C2   | 1.025816603  | -3.834545435 | -2.907689413 |
| C3   | 0.570902159  | -4.735832386 | -3.844401113 |
| C4   | -0.897115912 | -4.527681133 | -2.173127297 |
| C5   | -0.412535823 | -4.954713444 | 1.361514874  |
| C6   | 1.115238299  | -4.913166879 | 1.158501526  |
| C7   | -1.646013622 | 2.205772487  | 3.238334669  |
| Fe8  | 0.335734414  | 5.046818173  | -0.079166830 |
| Fe9  | -1.282850586 | 2.794546747  | 1.408441174  |
| Fe10 | 1.545326964  | 2.779298769  | 0.889198778  |
| Fe11 | 0.017288083  | 2.681569275  | -1.346196958 |
| Fe12 | -0.019346363 | 0.150060667  | -1.326427133 |
| Fe13 | -1.314772309 | -0.026162101 | 1.016826353  |
| Fe14 | 1.287864021  | 0.204202110  | 0.924183157  |
| H15  | 2.830312177  | 7.281087037  | -0.728075902 |
| H16  | 2.236868124  | 8.902110915  | -0.246103881 |
| H17  | 2.438895814  | 7.618719652  | 0.983327934  |
| H18  | 1.944152638  | -3.262709635 | -2.899547621 |
| H19  | 0.987091239  | -5.096239483 | -4.776168499 |

|     |              |              |              |
|-----|--------------|--------------|--------------|
| H20 | -1.777063007 | -4.670486444 | -1.556545362 |
| H21 | -1.280761308 | -5.843052881 | -3.811301428 |
| H22 | -0.805170390 | -5.880932175 | 0.900592112  |
| H23 | -0.615011907 | -5.021964750 | 2.448143642  |
| H24 | -2.333783415 | -0.719947605 | 1.910632343  |
| H25 | -3.684146914 | 1.304457865  | 1.894685506  |
| H26 | -2.217965236 | 3.805311784  | 2.020195517  |
| H27 | -0.660519978 | 2.152033350  | 3.773901123  |
| N28 | 0.106190447  | -3.716620633 | -1.880978708 |
| N29 | -0.663134234 | -5.175515481 | -3.363362305 |
| N30 | -0.003547436 | 1.388514093  | 0.165217871  |
| O31 | 1.836052277  | -5.888211432 | 1.428428063  |
| O32 | 1.523006895  | -3.757416778 | 0.687585770  |
| O33 | -1.033573706 | -3.810652402 | 0.819135394  |
| O34 | -2.665398552 | 1.951574804  | 3.871548205  |
| S35 | 0.384565331  | 7.320512291  | -0.359371217 |
| S36 | -1.605883688 | 4.139420987  | -0.768667856 |
| S37 | 0.403972884  | 4.283703558  | 2.126508209  |
| S38 | -0.079718196 | 1.324108195  | -3.136406758 |
| S39 | 2.002939579  | 3.888948322  | -1.097813831 |
| S40 | -1.685510666 | -1.278218305 | -0.803296532 |
| S41 | -3.046804526 | 1.455212750  | 0.699111940  |
| S42 | 0.171094142  | -1.209799359 | 2.251283865  |
| S43 | 1.765190616  | -1.107419159 | -0.830242107 |
| S44 | 2.964570242  | 1.283694165  | 1.760991424  |
| V45 | 0.081533239  | -2.353543571 | 0.252144865  |

## M. v2con2h6h2bhti.car\_2

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 2.404848601  | 7.908165662  | 0.061065782  |
| C2   | 0.930961666  | -3.860151266 | -2.805234771 |
| C3   | 0.470306205  | -4.757086623 | -3.743909578 |
| C4   | -1.054797742 | -4.439191740 | -2.142703454 |
| C5   | -1.001243250 | -4.722259856 | 1.469982225  |
| C6   | 0.525080272  | -4.923565888 | 1.366359434  |
| C7   | -1.410144159 | 2.155919874  | 3.058323115  |
| Fe8  | 0.573370939  | 5.081977718  | 0.166641567  |
| Fe9  | -1.184024764 | 2.833275278  | 1.438368761  |
| Fe10 | 1.681538737  | 2.735083480  | 1.062276570  |
| Fe11 | 0.244359096  | 2.757862185  | -1.241630953 |
| Fe12 | 0.174549556  | 0.217496442  | -1.282951676 |
| Fe13 | -1.292612661 | 0.075260292  | 0.980556485  |
| Fe14 | 1.369792159  | 0.154296618  | 1.017049075  |
| H15  | 3.050731282  | 7.312344848  | -0.594488359 |
| H16  | 2.462513938  | 8.965731502  | -0.233305575 |
| H17  | 2.749375426  | 7.807269448  | 1.097694529  |
| H18  | 1.874962333  | -3.331623290 | -2.770098611 |
| H19  | 0.908151597  | -5.158565944 | -4.649212678 |
| H20  | -1.970341462 | -4.515367194 | -1.569786707 |
| H21  | -1.430781262 | -5.773926148 | -3.767587749 |
| H22  | -1.512322717 | -5.611102202 | 1.053755312  |
| H23  | -1.268712315 | -4.667686285 | 2.544383916  |
| H24  | -2.409221278 | -0.637320527 | 1.733220265  |
| H25  | -3.512676131 | 1.388108579  | 1.970677928  |
| H26  | -2.211502340 | 3.803551823  | 1.980416968  |
| N27  | -0.023994345 | -3.675113361 | -1.820651880 |
| N28  | -0.804308477 | -5.121795546 | -3.309573825 |
| N29  | 0.163169813  | 1.423893617  | 0.225130084  |
| O30  | 1.067261022  | -5.982352606 | 1.723193819  |
| O31  | 1.134448828  | -3.867878045 | 0.877518855  |
| O32  | -1.402255356 | -3.551203040 | 0.799731117  |
| O33  | -1.794939578 | 1.809722050  | 4.110267308  |
| S34  | 0.624126078  | 7.370286286  | -0.092453568 |
| S35  | -1.380032427 | 4.198092641  | -0.641679479 |
| S36  | 0.529118912  | 4.235267263  | 2.310605999  |
| S37  | 0.193097316  | 1.439431871  | -3.062447772 |
| S38  | 2.240305768  | 3.914586722  | -0.855550728 |
| S39  | -1.625934205 | -1.070388553 | -0.893424873 |
| S40  | -3.026015875 | 1.567309434  | 0.710348277  |
| S41  | 0.072536966  | -1.147836857 | 2.300661560  |
| S42  | 1.818329036  | -1.224048939 | -0.700240361 |
| S43  | 3.100143899  | 1.172318693  | 1.828644689  |
| V44  | -0.047244701 | -2.288781249 | 0.290064845  |

### M-TS-N. v2con2h6h2bhtk.car\_1

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 2.279444356  | 7.950799646  | 0.097079176  |
| C2   | 0.993736859  | -3.825000902 | -2.826776599 |
| C3   | 0.549322840  | -4.728257170 | -3.769187500 |
| C4   | -0.981064100 | -4.440654126 | -2.167615738 |
| C5   | -0.933881673 | -4.726314789 | 1.451890184  |
| C6   | 0.589382012  | -4.921860903 | 1.340550739  |
| C7   | -1.384897817 | 1.864387805  | 2.948033972  |
| Fe8  | 0.502929300  | 5.089046363  | 0.172862025  |
| Fe9  | -1.270537750 | 2.794589275  | 1.343687800  |
| Fe10 | 1.597156835  | 2.719268764  | 1.072652170  |
| Fe11 | 0.183692711  | 2.748384091  | -1.186657883 |
| Fe12 | 0.172167100  | 0.206527508  | -1.233790695 |
| Fe13 | -1.384897817 | 0.120742529  | 1.039943545  |
| Fe14 | 1.462729620  | 0.168587149  | 0.990976123  |
| H15  | 2.944896911  | 7.372675855  | -0.554421980 |
| H16  | 2.316052578  | 9.011022454  | -0.194224714 |
| H17  | 2.614344881  | 7.854760770  | 1.136118928  |
| H18  | 1.927812655  | -3.281420438 | -2.789235939 |
| H19  | 0.995518063  | -5.117050205 | -4.674797346 |
| H20  | -1.896929127 | -4.537112966 | -1.594660773 |
| H21  | -1.332186786 | -5.777853756 | -3.796360893 |
| H22  | -1.443226324 | -5.606850339 | 1.016304263  |
| H23  | -1.200682414 | -4.696020169 | 2.526944142  |
| H24  | -2.538867075 | -0.665747990 | 1.658219048  |
| H25  | -2.955333526 | 1.355938559  | 2.263714161  |
| H26  | -2.245102294 | 3.739623204  | 2.045092371  |
| N27  | 0.034280069  | -3.660416113 | -1.843067724 |
| N28  | -0.719579855 | -5.117686173 | -3.336465984 |
| N29  | 0.171861451  | 1.434647201  | 0.277740989  |
| O30  | 1.142011206  | -5.979512667 | 1.703120008  |
| O31  | 1.197474363  | -3.869863759 | 0.839631560  |
| O32  | -1.339230411 | -3.545095368 | 0.805744079  |
| O33  | -1.836426543 | 1.792490379  | 4.129245237  |
| S34  | 0.513588403  | 7.371381766  | -0.075645735 |
| S35  | -1.426777701 | 4.219379449  | -0.611596672 |
| S36  | 0.406524891  | 4.143924719  | 2.330843914  |
| S37  | 0.167340563  | 1.440804666  | -3.003074084 |
| S38  | 2.163060355  | 3.936272707  | -0.829775709 |
| S39  | -1.599583038 | -1.084867058 | -0.853922362 |
| S40  | -3.104008986 | 1.586530314  | 0.528346635  |
| S41  | 0.118065729  | -1.126431013 | 2.280415187  |
| S42  | 1.858682366  | -1.214476174 | -0.740121699 |
| S43  | 3.152029619  | 1.284564241  | 1.781562549  |
| V44  | 0.022574575  | -2.283857334 | 0.300681222  |

### N. v2con2h6h2bhtj\_3\_4399.68

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 2.420912861  | 7.894197687  | 0.067412077  |
| C2   | 0.941293705  | -3.876204081 | -2.790406408 |
| C3   | 0.475482520  | -4.764967650 | -3.733935859 |
| C4   | -1.049019009 | -4.449341657 | -2.132716637 |
| C5   | -0.994200850 | -4.733645270 | 1.462679804  |
| C6   | 0.536684899  | -4.918747506 | 1.371795024  |
| C7   | -2.060411333 | 2.048294115  | 3.034063092  |
| Fe8  | 0.581122795  | 5.083276972  | 0.151001725  |
| Fe9  | -1.251202819 | 2.706317686  | 1.325789550  |
| Fe10 | 1.576468534  | 2.687137536  | 1.054795306  |
| Fe11 | 0.277688682  | 2.812192735  | -1.330889709 |
| Fe12 | 0.225664586  | 0.221217142  | -1.272570296 |
| Fe13 | -1.385066686 | 0.152310585  | 0.777655075  |
| Fe14 | 1.406158057  | 0.129814515  | 1.022794322  |
| H15  | 3.050166201  | 7.293497490  | -0.598788659 |
| H16  | 2.482998672  | 8.951404455  | -0.225347919 |
| H17  | 2.779377307  | 7.788149727  | 1.098056507  |
| H18  | 1.886398316  | -3.350265401 | -2.751894159 |
| H19  | 0.911769598  | -5.164244727 | -4.640120316 |
| H20  | -1.967434956 | -4.518313981 | -1.563323916 |
| H21  | -1.432388500 | -5.769208725 | -3.764003471 |
| H22  | -1.493126870 | -5.632207832 | 1.055260826  |

|     |              |              |              |
|-----|--------------|--------------|--------------|
| H23 | -1.273382161 | -4.662541501 | 2.532921147  |
| H24 | -2.427133110 | -0.480833307 | 1.664952983  |
| H25 | -3.093985799 | 1.650150048  | 2.906935471  |
| H26 | -2.234322339 | 3.604821897  | 2.033535064  |
| N27 | -0.013147712 | -3.693393286 | -1.806185132 |
| N28 | -0.801168338 | -5.125021122 | -3.302562973 |
| N29 | 0.183313685  | 1.413962361  | 0.311477420  |
| O30 | 1.087189158  | -5.970689784 | 1.737577481  |
| O31 | 1.137528358  | -3.857297821 | 0.883657514  |
| O32 | -1.405810581 | -3.576802064 | 0.770824992  |
| O33 | -1.521731362 | 2.056263925  | 4.129250539  |
| S34 | 0.635681163  | 7.372421533  | -0.062737602 |
| S35 | -1.357180472 | 4.215623006  | -0.718266823 |
| S36 | 0.385807576  | 4.155099502  | 2.272033368  |
| S37 | 0.281578619  | 1.408061062  | -3.087870786 |
| S38 | 2.263706426  | 3.908567566  | -0.812387910 |
| S39 | -1.607366564 | -1.106468999 | -1.026731290 |
| S40 | -2.963472822 | 1.548102505  | 0.265191555  |
| S41 | -0.014350221 | -1.119715690 | 2.220672239  |
| S42 | 1.845367935  | -1.246051862 | -0.692460520 |
| S43 | 3.035453941  | 1.219852441  | 1.911169383  |
| V44 | -0.061911091 | -2.304774223 | 0.251697921  |

## O. v2chob6h2bh\_car\_2

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 2.009042420  | 8.070123567  | 0.675394065  |
| C2   | 1.374369891  | -3.560805833 | -2.892494927 |
| C3   | 1.087994329  | -4.437670585 | -3.915836873 |
| C4   | -0.622929274 | -4.305904568 | -2.485174193 |
| C5   | -0.756101123 | -4.942205292 | 1.094996332  |
| C6   | 0.784792576  | -4.972095443 | 1.070863423  |
| C7   | -1.885882122 | 2.070779986  | 2.800762109  |
| Fe8  | 0.333366127  | 5.194833117  | 0.326413202  |
| Fe9  | -1.410245800 | 2.715071572  | 1.086571187  |
| Fe10 | 1.421470624  | 2.771529685  | 1.213535918  |
| Fe11 | 0.203991860  | 2.933468411  | -1.223387818 |
| Fe12 | 0.085356838  | 0.348761300  | -1.022925968 |
| Fe13 | -1.677765123 | -0.142939712 | 1.206285075  |
| Fe14 | 1.168870853  | 0.221628313  | 1.321315811  |
| H15  | 2.737139298  | 7.563197889  | 0.032777672  |
| H16  | 2.057597534  | 9.153723373  | 0.498533491  |
| H17  | 2.251221402  | 7.866184835  | 1.725413849  |
| H18  | 2.269842679  | -2.974607810 | -2.726266463 |
| H19  | 1.652851651  | -4.764373105 | -4.780229109 |
| H20  | -1.584822208 | -4.482746272 | -2.019929617 |
| H21  | -0.718798100 | -5.580548040 | -4.199179091 |
| H22  | -1.147179996 | -5.829193675 | 0.562800766  |
| H23  | -1.085521505 | -5.023050845 | 2.149998178  |
| H24  | -2.775810248 | -1.104126233 | 1.604355493  |
| H25  | -4.033737211 | 1.498024865  | 1.424550062  |
| H26  | -2.120397141 | 2.720749709  | 3.680123617  |
| N27  | 0.305734150  | -3.490098888 | -2.015550798 |
| N28  | -0.196349430 | -4.911285538 | -3.645076590 |
| N29  | 0.031350337  | 1.560830135  | 0.531851236  |
| O30  | 1.420356913  | -6.003663806 | 1.345748718  |
| O31  | 1.297451981  | -3.808894506 | 0.742086091  |
| O32  | -1.247722664 | -3.753625572 | 0.522408939  |
| O33  | -1.999919078 | 0.833586988  | 3.011855354  |
| S34  | 0.278755303  | 7.499826736  | 0.277075499  |
| S35  | -1.532149029 | 4.328987518  | -0.691241475 |
| S36  | 0.100740985  | 4.183378581  | 2.386558949  |
| S37  | 0.204235094  | 1.455970620  | -2.884057420 |
| S38  | 2.116741731  | 4.094859928  | -0.597513322 |
| S39  | -1.631081140 | -1.097639533 | -0.866991085 |
| S40  | -3.248321028 | 1.433219682  | 0.316511423  |
| S41  | -0.111743515 | -1.369207634 | 2.342213359  |
| S42  | 1.795250028  | -0.992988263 | -0.453984823 |
| S43  | 2.823202042  | 1.327771286  | 2.192477696  |
| V44  | -0.025250906 | -2.298836941 | 0.276362057  |

## P. v26och2h6h2bha.car\_2

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 2.160102226  | 7.747955934  | 1.126443998  |
| C2   | 1.165091788  | -3.651565308 | -3.024455427 |
| C3   | 0.765367683  | -4.429460619 | -4.088153088 |
| C4   | -0.925714906 | -4.114070549 | -2.663322301 |
| C5   | -0.608425319 | -4.978281443 | 0.896351044  |
| C6   | 0.929923568  | -4.962938013 | 0.798152160  |
| C7   | -1.659197801 | 0.723272808  | 3.042953550  |
| Fe8  | 0.439139098  | 5.117230632  | 0.226097044  |
| Fe9  | -1.271398212 | 2.889992146  | 1.061356033  |
| Fe10 | 1.448663299  | 2.717140263  | 1.090570699  |
| Fe11 | 0.294795500  | 2.903507736  | -1.356394355 |
| Fe12 | 0.040573826  | 0.333892292  | -1.173011009 |
| Fe13 | -1.406128848 | 0.076026670  | 1.130522885  |
| Fe14 | 1.364838109  | 0.176828289  | 1.076781530  |
| H15  | 2.996539923  | 7.280566518  | 0.593462534  |
| H16  | 2.312445325  | 8.835707027  | 1.161777097  |
| H17  | 2.120349813  | 7.356290507  | 2.149827895  |
| H18  | 2.133255570  | -3.210607857 | -2.825231709 |
| H19  | 1.284925419  | -4.793580289 | -4.965279126 |
| H20  | -1.910957105 | -4.170440453 | -2.217571087 |
| H21  | -1.186169514 | -5.275319517 | -4.438320047 |
| H22  | -0.989760238 | -5.800641584 | 0.261939037  |
| H23  | -0.890284796 | -5.212605861 | 1.940452748  |
| H24  | -0.689491102 | 0.832948018  | 3.594879924  |
| H25  | -3.698664158 | 1.610350261  | 1.753694413  |
| H26  | -2.502405411 | -0.800513197 | 1.667069806  |
| H27  | -2.313698080 | 3.613035613  | 1.904966321  |
| N28  | 0.107231844  | -3.465439369 | -2.151942186 |
| N29  | -0.577835098 | -4.720328840 | -3.847551338 |
| N30  | 0.114925994  | 1.470840430  | 0.358623007  |
| O31  | -2.691952180 | 0.921689113  | 3.678455617  |
| O32  | 1.604324666  | -5.980604159 | 1.026229677  |
| O33  | 1.398026294  | -3.785858638 | 0.453105716  |
| O34  | -1.157935754 | -3.742115187 | 0.504076831  |
| S35  | 0.550116626  | 7.410082238  | 0.242268907  |
| S36  | -1.422197317 | 4.278374485  | -0.790795378 |
| S37  | 0.181300248  | 4.133557273  | 2.329323209  |
| S38  | 0.195206901  | 1.416485812  | -3.032413847 |
| S39  | 2.217300565  | 4.020774027  | -0.682979107 |
| S40  | -1.683176664 | -1.041390598 | -0.888513717 |
| S41  | -3.101703223 | 1.590174588  | 0.528936425  |
| S42  | 0.137361331  | -1.365055108 | 2.166030069  |
| S43  | 1.787111469  | -1.003703252 | -0.779668724 |
| S44  | 2.922951862  | 1.336821480  | 2.055872161  |
| V45  | 0.015218733  | -2.289014946 | 0.105392100  |

## P-TS-Q. v26och2h6h2bhb\_1\_4462.08

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 2.106872502  | 7.683761621  | 1.181152260  |
| C2   | 1.248494311  | -3.621083845 | -3.026946055 |
| C3   | 0.898884593  | -4.392015380 | -4.113607728 |
| C4   | -0.826733445 | -4.170485529 | -2.713640438 |
| C5   | -0.746986801 | -4.970265883 | 0.909962920  |
| C6   | 0.789091759  | -5.042883765 | 0.808078079  |
| C7   | -1.510258868 | 1.293729247  | 2.975490545  |
| Fe8  | 0.357379429  | 5.082070071  | 0.259796932  |
| Fe9  | -1.344360694 | 2.659467628  | 1.167882264  |
| Fe10 | 1.444402307  | 2.717220413  | 1.104144411  |
| Fe11 | 0.194420884  | 2.868236677  | -1.322063727 |
| Fe12 | 0.169633580  | 0.272995898  | -1.195502274 |
| Fe13 | -1.395146204 | 0.118171416  | 1.010764133  |
| Fe14 | 1.420684899  | 0.183388968  | 1.074470977  |
| H15  | 2.946694218  | 7.223058627  | 0.646805200  |
| H16  | 2.266405435  | 8.769462801  | 1.243941052  |
| H17  | 2.053208366  | 7.268619361  | 2.194505807  |
| H18  | 2.194577396  | -3.143408021 | -2.804361794 |
| H19  | 1.449052118  | -4.712938710 | -4.989027516 |
| H20  | -1.820680546 | -4.268463144 | -2.294648772 |
| H21  | -1.010023681 | -5.308422227 | -4.515435720 |
| H22  | -1.183356735 | -5.731006696 | 0.235629135  |
| H23  | -1.045856565 | -5.238363012 | 1.941277165  |



|     |              |              |              |
|-----|--------------|--------------|--------------|
| H24 | -0.517610618 | 1.312732001  | 3.487071581  |
| H25 | -3.866320561 | 1.462944268  | 1.586604930  |
| H26 | -2.466218444 | -0.714582881 | 1.692685584  |
| H27 | -2.349829731 | 3.423608960  | 1.990560410  |
| N28 | 0.170361489  | -3.495051733 | -2.168454665 |
| N29 | -0.435488870 | -4.740121013 | -3.904127015 |
| N30 | 0.185709703  | 1.433343318  | 0.322873227  |
| O31 | -2.528608665 | 1.254783021  | 3.661138100  |
| O32 | 1.403852378  | -6.108909683 | 0.970385258  |
| O33 | 1.327434828  | -3.873581925 | 0.537096119  |
| O34 | -1.215809782 | -3.684926280 | 0.581701059  |
| S35 | 0.503153187  | 7.378589307  | 0.273451973  |
| S36 | -1.516322492 | 4.210930991  | -0.680751333 |
| S37 | 0.134988456  | 4.061461901  | 2.349235591  |
| S38 | 0.190315337  | 1.399964745  | -3.039186210 |
| S39 | 2.115874679  | 4.017797582  | -0.716280932 |
| S40 | -1.596440997 | -1.091206565 | -0.902735272 |
| S41 | -3.177408681 | 1.498890710  | 0.409745447  |
| S42 | 0.086885509  | -1.237118322 | 2.223313701  |
| S43 | 1.877114286  | -1.111869167 | -0.688704457 |
| S44 | 2.973133979  | 1.365372703  | 2.032606227  |
| V45 | 0.044836751  | -2.303898455 | 0.203103821  |

### Q. v26och2h6h2bh.car\_2

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 2.336033879  | 7.635739582  | 1.169064527  |
| C2   | 1.146233782  | -3.710429299 | -3.054668794 |
| C3   | 0.720527730  | -4.429514052 | -4.148991112 |
| C4   | -0.949054299 | -4.156737553 | -2.690618357 |
| C5   | -0.778188809 | -4.999511425 | 0.845273394  |
| C6   | 0.763255086  | -5.030920747 | 0.798140543  |
| C7   | -1.580020962 | 1.838946729  | 3.211537887  |
| Fe8  | 0.536298100  | 5.061830983  | 0.294676908  |
| Fe9  | -1.232122684 | 2.653011202  | 1.465383268  |
| Fe10 | 1.567165855  | 2.679187051  | 1.166819282  |
| Fe11 | 0.245520333  | 2.813113885  | -1.181481579 |
| Fe12 | 0.110181890  | 0.276731158  | -1.375540189 |
| Fe13 | -1.375208574 | -0.030945698 | 0.854234464  |
| Fe14 | 1.234561966  | 0.110871427  | 0.966823962  |
| H15  | 3.162340210  | 7.150739898  | 0.635922703  |
| H16  | 2.519665679  | 8.718254548  | 1.220808740  |
| H17  | 2.274376169  | 7.231438007  | 2.186308011  |
| H18  | 2.122349931  | -3.291324611 | -2.847653342 |
| H19  | 1.223105435  | -4.754514131 | -5.050956994 |
| H20  | -1.929335736 | -4.210894690 | -2.234604826 |
| H21  | -1.252209796 | -5.218078467 | -4.517715001 |
| H22  | -1.164992641 | -5.825124126 | 0.218311999  |
| H23  | -1.100222413 | -5.204284240 | 1.884198736  |
| H24  | -0.591838697 | 1.673299222  | 3.720828731  |
| H25  | -3.707907365 | 1.272540642  | 1.761427759  |
| H26  | -2.464440053 | -0.771770686 | 1.617775755  |
| H27  | -2.237229129 | 3.591391082  | 2.096915841  |
| N28  | 0.100512713  | -3.548649677 | -2.162675115 |
| N29  | -0.623919092 | -4.711967967 | -3.904589428 |
| N30  | 0.045329588  | 1.396684436  | 0.209776222  |
| O31  | -2.603054140 | 1.583902651  | 3.837901976  |
| O32  | 1.395236907  | -6.073616609 | 1.037822475  |
| O33  | 1.280412317  | -3.867759442 | 0.483484765  |
| O34  | -1.279200738 | -3.756867889 | 0.408000881  |
| S35  | 0.727082782  | 7.348773677  | 0.264933548  |
| S36  | -1.365786800 | 4.258033098  | -0.638581178 |
| S37  | 0.335860107  | 4.116358834  | 2.408294233  |
| S38  | 0.268536695  | 1.599417652  | -3.074622114 |
| S39  | 2.251005773  | 3.904141516  | -0.661183560 |
| S40  | -1.665205141 | -1.094763375 | -1.086241310 |
| S41  | -3.058520223 | 1.525482228  | 0.589517253  |
| S42  | -0.028590597 | -1.351235440 | 2.100776600  |
| S43  | 1.787936602  | -1.112057796 | -0.833336823 |
| S44  | 2.880234912  | 1.060813523  | 1.996594824  |
| V45  | -0.046713673 | -2.349754341 | 0.011908581  |

## R. v2ch2oa6h2bh.car\_4

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 2.280331077  | 7.900868724  | -0.212681620 |
| C2   | 0.881937408  | -3.848415459 | -2.906623052 |
| C3   | 0.367850699  | -4.732076230 | -3.830804246 |
| C4   | -1.014189435 | -4.513851718 | -2.089571913 |
| C5   | -0.318470737 | -4.988195319 | 1.415852430  |
| C6   | 1.194081975  | -4.957373210 | 1.118327657  |
| C7   | -1.885574851 | 2.475189264  | 3.089840115  |
| Fe8  | 0.402720027  | 5.129595309  | -0.013103766 |
| Fe9  | -1.203450549 | 2.757524482  | 1.188870064  |
| Fe10 | 1.649593992  | 2.795711741  | 0.767601558  |
| Fe11 | -0.066408352 | 2.766144271  | -1.405198893 |
| Fe12 | -0.049026398 | 0.189168945  | -1.176845663 |
| Fe13 | -1.362322123 | -0.053676978 | 1.304022318  |
| Fe14 | 1.446803469  | 0.252330878  | 0.948407924  |
| H15  | 2.801161096  | 7.350652878  | -1.004585538 |
| H16  | 2.336553698  | 8.978954621  | -0.418183917 |
| H17  | 2.766634058  | 7.695905821  | 0.749119392  |
| H18  | 1.808354775  | -3.289073065 | -2.938187427 |
| H19  | 0.734326121  | -5.090886637 | -4.784552324 |
| H20  | -1.871888850 | -4.646004241 | -1.441671976 |
| H21  | -1.498230922 | -5.807435667 | -3.721264504 |
| H22  | -0.757901229 | -5.870311827 | 0.910815914  |
| H23  | -0.458835333 | -5.138175517 | 2.504809836  |
| H24  | -2.393529653 | -0.846492298 | 2.077277443  |
| H25  | -3.844284832 | 1.417846187  | 1.603002777  |
| H26  | -2.966605136 | 2.298351597  | 3.161371494  |
| H27  | -1.457448824 | 3.158643989  | 3.832177776  |
| N28  | 0.015162363  | -3.724408566 | -1.835686417 |
| N29  | -0.848899303 | -5.156097855 | -3.295341850 |
| N30  | 0.191495812  | 1.534873511  | 0.204958016  |
| O31  | 1.910479365  | -5.958907199 | 1.282439282  |
| O32  | 1.591532832  | -3.781502812 | 0.689018035  |
| O33  | -0.943586014 | -3.797328870 | 0.998442288  |
| O34  | -1.078832635 | 1.463731099  | 2.726978721  |
| S35  | 0.474437418  | 7.430580529  | -0.160112859 |
| S36  | -1.644607303 | 4.225352782  | -0.594983800 |
| S37  | 0.538704633  | 4.242658734  | 2.093268470  |
| S38  | -0.378382065 | 1.278446890  | -3.040399369 |
| S39  | 1.932058939  | 3.976094858  | -1.250183613 |
| S40  | -1.668915489 | -1.279747154 | -0.565315668 |
| S41  | -3.062092211 | 1.389891400  | 0.491434579  |
| S42  | 0.362439403  | -1.180726042 | 2.335895639  |
| S43  | 1.762444200  | -1.104200587 | -0.798211151 |
| S44  | 3.177401173  | 1.398233097  | 1.596609854  |
| V45  | 0.146977711  | -2.341864355 | 0.392967984  |

## Q-TS-S. v2chon2h6h2bhotn\_orig

|      |        |        |        |
|------|--------|--------|--------|
| C1   | 2.107  | 7.825  | 0.262  |
| C2   | 1.135  | -3.733 | -3.021 |
| C3   | 0.716  | -4.607 | -4.000 |
| C4   | -0.808 | -4.457 | -2.373 |
| C5   | -0.431 | -5.001 | 1.159  |
| C6   | 1.102  | -4.941 | 1.006  |
| C7   | -1.657 | 2.058  | 3.178  |
| Fe8  | 0.305  | 5.051  | 0.084  |
| Fe9  | -1.327 | 2.673  | 1.399  |
| Fe10 | 1.508  | 2.746  | 1.005  |
| Fe11 | 0.036  | 2.721  | -1.270 |
| Fe12 | 0.018  | 0.194  | -1.325 |
| Fe13 | -1.397 | -0.011 | 0.981  |
| Fe14 | 1.245  | 0.184  | 0.954  |
| H15  | 2.797  | 7.303  | -0.410 |
| H16  | 2.196  | 8.910  | 0.111  |
| H17  | 2.362  | 7.585  | 1.301  |
| H18  | 2.050  | -3.157 | -2.965 |
| H19  | 1.164  | -4.936 | -4.928 |
| H20  | -1.708 | -4.621 | -1.793 |
| H21  | -1.128 | -5.722 | -4.064 |
| H22  | -0.803 | -5.909 | 0.647  |
| H23  | -0.665 | -5.117 | 2.235  |

|     |        |        |        |
|-----|--------|--------|--------|
| H24 | -2.420 | -0.803 | 1.770  |
| H25 | -3.358 | 1.445  | 2.496  |
| H26 | -2.303 | 3.662  | 2.013  |
| H27 | -0.892 | 2.156  | 3.973  |
| N28 | 0.180  | -3.651 | -2.022 |
| N29 | -0.531 | -5.066 | -3.574 |
| N30 | -0.004 | 1.412  | 0.190  |
| O31 | 1.823  | -5.920 | 1.260  |
| O32 | 1.515  | -3.764 | 0.596  |
| O33 | -1.045 | -3.839 | 0.647  |
| O34 | -2.798 | 1.645  | 3.614  |
| S35 | 0.342  | 7.339  | -0.105 |
| S36 | -1.613 | 4.112  | -0.686 |
| S37 | 0.312  | 4.198  | 2.248  |
| S38 | 0.004  | 1.422  | -3.100 |
| S39 | 2.005  | 3.933  | -0.939 |
| S40 | -1.677 | -1.231 | -0.883 |
| S41 | -3.195 | 1.380  | 0.862  |
| S42 | 0.075  | -1.268 | 2.200  |
| S43 | 1.787  | -1.078 | -0.822 |
| S44 | 2.895  | 1.222  | 1.884  |
| V45 | 0.074  | -2.351 | 0.167  |

### S. v2chon2h6h2bhota.car\_2

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 2.318006287  | 7.774219550  | 0.073275538  |
| C2   | 1.000215380  | -3.817225086 | -2.937050755 |
| C3   | 0.540716877  | -4.693881352 | -3.895282820 |
| C4   | -0.960262558 | -4.459895579 | -2.257941556 |
| C5   | -0.548948319 | -4.947474014 | 1.259755871  |
| C6   | 0.985145893  | -4.924008176 | 1.102341637  |
| C7   | -1.425918720 | 2.157747729  | 3.125428499  |
| Fe8  | 0.398947352  | 5.078557925  | -0.090837822 |
| Fe9  | -1.279550248 | 2.668244511  | 1.367068540  |
| Fe10 | 1.524751957  | 2.792554501  | 0.975792153  |
| Fe11 | 0.095608170  | 2.707965456  | -1.360439895 |
| Fe12 | 0.052589815  | 0.186108469  | -1.330852620 |
| Fe13 | -1.460636651 | -0.007133638 | 0.890475959  |
| Fe14 | 1.226939135  | 0.215965015  | 0.977604402  |
| H15  | 2.982715520  | 7.213648949  | -0.593831214 |
| H16  | 2.458914019  | 8.852184525  | -0.089884658 |
| H17  | 2.565539581  | 7.533656804  | 1.114302338  |
| H18  | 1.933479529  | -3.269923418 | -2.901140194 |
| H19  | 0.969325277  | -5.057326056 | -4.820575933 |
| H20  | -1.864017848 | -4.575950970 | -1.672633547 |
| H21  | -1.340275635 | -5.747050279 | -3.918227000 |
| H22  | -0.944489400 | -5.845835795 | 0.749052320  |
| H23  | -0.783319466 | -5.053711260 | 2.336888103  |
| H24  | -2.508933250 | -0.855395413 | 1.568100716  |
| H25  | -3.103233972 | 1.354736199  | 2.979689401  |
| H26  | -2.323926280 | 3.640472621  | 1.862523596  |
| H27  | -0.677688009 | 2.410902893  | 3.894339973  |
| N28  | 0.060251945  | -3.683638692 | -1.930521921 |
| N29  | -0.716922614 | -5.100515743 | -3.449031864 |
| N30  | 0.027326589  | 1.448653260  | 0.154322127  |
| O31  | 1.679483526  | -5.922914221 | 1.357371491  |
| O32  | 1.425780220  | -3.761077084 | 0.687627207  |
| O33  | -1.136338901 | -3.773239970 | 0.743101961  |
| O34  | -2.483409998 | 1.609753602  | 3.738425830  |
| S35  | 0.533053064  | 7.365803163  | -0.290844645 |
| S36  | -1.527308909 | 4.144623861  | -0.848284061 |
| S37  | 0.325347544  | 4.322373871  | 2.098741228  |
| S38  | 0.079214009  | 1.351406263  | -3.147229728 |
| S39  | 2.090726983  | 3.865599738  | -1.018044295 |
| S40  | -1.679113531 | -1.215239338 | -0.950798101 |
| S41  | -3.141581998 | 1.396437069  | 0.816403595  |
| S42  | -0.003220113 | -1.194977228 | 2.215501900  |
| S43  | 1.782531707  | -1.112123743 | -0.747244452 |
| S44  | 2.846192800  | 1.261778870  | 1.954665017  |
| V45  | 0.006297654  | -2.334861492 | 0.207913880  |

## T. v2h6co6hco2btd.car\_2

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 2.337601426  | 7.849967407  | -0.015374960 |
| C2   | 0.936185709  | -3.717952485 | -3.062001393 |
| C3   | 0.427033596  | -4.614564570 | -3.975941598 |
| C4   | -0.991586435 | -4.334750887 | -2.272779968 |
| C5   | -0.354289122 | -4.835440588 | 1.254081205  |
| C6   | 1.161345352  | -4.847184329 | 0.973798196  |
| C7   | -1.222834191 | 0.994786801  | 3.260136997  |
| C8   | -2.612705271 | -1.034051750 | 2.166259117  |
| Fe9  | 0.425118761  | 5.146361878  | 0.045200911  |
| Fe10 | -1.230507645 | 3.039946956  | 0.849186965  |
| Fe11 | 1.556392036  | 2.772890486  | 0.754360284  |
| Fe12 | 0.183999876  | 2.860627014  | -1.490571923 |
| Fe13 | 0.121833829  | 0.306564009  | -1.282196685 |
| Fe14 | -1.382300739 | 0.047638063  | 1.481259397  |
| Fe15 | 1.524785063  | 0.264404836  | 0.840813599  |
| H16  | 2.871564950  | 7.276043615  | -0.780358599 |
| H17  | 2.435432341  | 8.923967159  | -0.226510480 |
| H18  | 2.773787639  | 7.635807924  | 0.967745391  |
| H19  | 1.875695281  | -3.181059753 | -3.082369226 |
| H20  | 0.809313872  | -5.002009715 | -4.911854675 |
| H21  | -1.858255396 | -4.443141663 | -1.632688865 |
| H22  | -1.458252127 | -5.658232900 | -3.880792013 |
| H23  | -0.800951258 | -5.750764820 | 0.821666097  |
| H24  | -0.503455617 | -4.887114105 | 2.350191568  |
| H25  | -3.563585209 | 1.894335274  | 2.004421243  |
| H26  | -2.233448524 | 3.911385234  | 1.576160234  |
| H27  | -0.173604702 | 1.045244342  | 3.659877281  |
| N28  | 0.045757514  | -3.554928054 | -2.015589252 |
| N29  | -0.809207648 | -5.003839718 | -3.459286096 |
| N30  | 0.142921128  | 1.468675297  | 0.278045045  |
| O31  | 1.867296574  | -5.831733789 | 1.248609453  |
| O32  | 1.581309309  | -3.726532994 | 0.432230707  |
| O33  | -0.968533281 | -3.678973128 | 0.730418924  |
| O34  | -2.111868303 | 1.436069197  | 3.986186191  |
| O35  | -3.453718178 | -1.727155248 | 2.585072477  |
| S36  | 0.518849891  | 7.428870585  | -0.039096002 |
| S37  | -1.486307918 | 4.335723137  | -0.953322928 |
| S38  | 0.315215811  | 4.202371739  | 2.111162056  |
| S39  | 0.115234349  | 1.409238448  | -3.170645532 |
| S40  | 2.097811241  | 4.104767708  | -1.062715122 |
| S41  | -1.607909044 | -1.054603651 | -0.740064765 |
| S42  | -3.004410657 | 1.589733556  | 0.797338129  |
| S43  | 0.474773605  | -1.252501141 | 2.150970574  |
| S44  | 1.884805091  | -1.028705548 | -0.957127956 |
| S45  | 3.176290340  | 1.472867197  | 1.566835665  |
| V46  | 0.167389527  | -2.253035424 | 0.119246701  |

## T-TS-U. v2h6co6hco2btf\_orig

|      |        |        |        |
|------|--------|--------|--------|
| C1   | 2.244  | 7.891  | -0.047 |
| C2   | 1.032  | -3.741 | -3.029 |
| C3   | 0.539  | -4.639 | -3.950 |
| C4   | -0.890 | -4.388 | -2.251 |
| C5   | -0.314 | -4.828 | 1.288  |
| C6   | 1.207  | -4.814 | 1.043  |
| C7   | -1.300 | 1.093  | 2.996  |
| C8   | -2.622 | -0.973 | 2.010  |
| Fe9  | 0.378  | 5.134  | 0.037  |
| Fe10 | -1.351 | 2.929  | 0.882  |
| Fe11 | 1.514  | 2.792  | 0.788  |
| Fe12 | 0.130  | 2.826  | -1.435 |
| Fe13 | 0.123  | 0.259  | -1.331 |
| Fe14 | -1.372 | 0.113  | 1.338  |
| Fe15 | 1.528  | 0.278  | 0.805  |
| H16  | 2.816  | 7.325  | -0.791 |
| H17  | 2.321  | 8.966  | -0.265 |
| H18  | 2.657  | 7.698  | 0.950  |
| H19  | 1.964  | -3.191 | -3.043 |
| H20  | 0.929  | -5.015 | -4.888 |
| H21  | -1.759 | -4.510 | -1.615 |
| H22  | -1.336 | -5.704 | -3.872 |

|     |        |        |        |
|-----|--------|--------|--------|
| H23 | -0.730 | -5.755 | 0.850  |
| H24 | -0.489 | -4.881 | 2.381  |
| H25 | -3.107 | 1.604  | 2.600  |
| H26 | -2.286 | 3.834  | 1.654  |
| H27 | -0.388 | 1.253  | 3.602  |
| N28 | 0.135  | -3.596 | -1.985 |
| N29 | -0.694 | -5.049 | -3.441 |
| N30 | 0.114  | 1.445  | 0.227  |
| O31 | 1.925  | -5.785 | 1.336  |
| O32 | 1.623  | -3.690 | 0.506  |
| O33 | -0.940 | -3.685 | 0.746  |
| O34 | -2.372 | 1.527  | 3.579  |
| O35 | -3.469 | -1.629 | 2.465  |
| S36 | 0.438  | 7.422  | -0.113 |
| S37 | -1.552 | 4.281  | -0.901 |
| S38 | 0.240  | 4.178  | 2.116  |
| S39 | 0.117  | 1.437  | -3.176 |
| S40 | 2.052  | 4.082  | -1.056 |
| S41 | -1.608 | -1.112 | -0.797 |
| S42 | -3.174 | 1.607  | 0.881  |
| S43 | 0.466  | -1.191 | 2.131  |
| S44 | 1.915  | -1.029 | -0.963 |
| S45 | 3.141  | 1.487  | 1.592  |
| V46 | 0.198  | -2.256 | 0.126  |

### U. v2h6co6hco2btf.car\_3

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 2.264910043  | 7.896462499  | -0.042521699 |
| C2   | 1.009585904  | -3.699599818 | -3.025749584 |
| C3   | 0.515940353  | -4.609560882 | -3.935133309 |
| C4   | -0.922938877 | -4.321875132 | -2.250131135 |
| C5   | -0.284648580 | -4.862920692 | 1.281370510  |
| C6   | 1.227154070  | -4.874578515 | 0.981823490  |
| C7   | -1.311050086 | 0.944237867  | 3.113800812  |
| C8   | -2.652627730 | -1.040854606 | 2.053528431  |
| Fe9  | 0.353038977  | 5.178570981  | -0.056883634 |
| Fe10 | -1.372688492 | 2.998476105  | 0.667967554  |
| Fe11 | 1.446249721  | 2.812265848  | 0.752193508  |
| Fe12 | 0.152044834  | 2.885422060  | -1.563164724 |
| Fe13 | 0.163965687  | 0.259911950  | -1.264913667 |
| Fe14 | -1.376826486 | 0.045004201  | 1.444161278  |
| Fe15 | 1.514910986  | 0.297731428  | 0.896874878  |
| H16  | 2.815367733  | 7.336999343  | -0.806595803 |
| H17  | 2.363717781  | 8.974438722  | -0.233884352 |
| H18  | 2.684472400  | 7.667317414  | 0.944618392  |
| H19  | 1.945081050  | -3.155578584 | -3.041451155 |
| H20  | 0.910668899  | -5.005383933 | -4.862620367 |
| H21  | -1.795187496 | -4.428421649 | -1.617659217 |
| H22  | -1.361947059 | -5.667980477 | -3.846810792 |
| H23  | -0.735000788 | -5.783288229 | 0.862890976  |
| H24  | -0.418763843 | -4.909826791 | 2.380207643  |
| H25  | -2.987598817 | 1.734623572  | 2.888411364  |
| H26  | -2.401500969 | 3.913678272  | 1.280745363  |
| H27  | -0.472268595 | 0.917957736  | 3.829893459  |
| N28  | 0.107378670  | -3.533601851 | -1.989832986 |
| N29  | -0.723978661 | -5.000960324 | -3.427863193 |
| N30  | 0.127784025  | 1.438071422  | 0.282106035  |
| O31  | 1.936130319  | -5.860373248 | 1.246661375  |
| O32  | 1.644348198  | -3.754607277 | 0.436971558  |
| O33  | -0.910328121 | -3.712215900 | 0.756805178  |
| O34  | -2.319944389 | 1.593296049  | 3.664574747  |
| O35  | -3.511376198 | -1.716713087 | 2.458170033  |
| S36  | 0.447736763  | 7.468677372  | -0.104782316 |
| S37  | -1.540776357 | 4.350745060  | -1.092339344 |
| S38  | 0.088164724  | 4.224352404  | 1.995058673  |
| S39  | 0.188016223  | 1.365889668  | -3.176619922 |
| S40  | 2.063981140  | 4.115819786  | -1.079430135 |
| S41  | -1.597022914 | -1.108391890 | -0.717118296 |
| S42  | -3.066453479 | 1.595218464  | 0.801232719  |
| S43  | 0.500327282  | -1.259033400 | 2.176491700  |
| S44  | 1.981857917  | -1.011620134 | -0.872971520 |
| S45  | 3.082546449  | 1.584728347  | 1.666927752  |
| V46  | 0.227547793  | -2.282510149 | 0.144989722  |

## V. v26hoch2h6hta.car\_2

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 2.096948086  | 7.684354335  | 1.159701584  |
| C2   | 1.234340405  | -3.643372274 | -3.051279407 |
| C3   | 0.875330208  | -4.401839846 | -4.143796648 |
| C4   | -0.843660761 | -4.177989232 | -2.735666404 |
| C5   | -0.742699819 | -4.967435293 | 0.878058084  |
| C6   | 0.796214853  | -5.016787974 | 0.792558187  |
| C7   | -1.475098693 | 1.340802704  | 2.744777168  |
| Fe8  | 0.354378825  | 5.065921312  | 0.279853076  |
| Fe9  | -1.400925228 | 2.595142590  | 1.128782897  |
| Fe10 | 1.470892489  | 2.695217103  | 1.071010800  |
| Fe11 | 0.188998135  | 2.902661210  | -1.360104236 |
| Fe12 | 0.128648860  | 0.300605785  | -1.253179741 |
| Fe13 | -1.376559369 | 0.124628116  | 1.051252132  |
| Fe14 | 1.389161806  | 0.158130017  | 1.045647334  |
| H15  | 2.925460738  | 7.220978645  | 0.610830565  |
| H16  | 2.251495441  | 8.771315093  | 1.205927819  |
| H17  | 2.067693535  | 7.279627463  | 2.178121035  |
| H18  | 2.184369269  | -3.173886839 | -2.828606202 |
| H19  | 1.419270657  | -4.718632326 | -5.024686947 |
| H20  | -1.836940810 | -4.270537413 | -2.313825151 |
| H21  | -1.043421595 | -5.298131203 | -4.547496909 |
| H22  | -1.157727117 | -5.743702925 | 0.207142218  |
| H23  | -1.046417154 | -5.232217264 | 1.909326688  |
| H24  | -0.614842058 | 1.330941982  | 3.423763088  |
| H25  | -3.352099221 | 1.350430352  | 2.889392028  |
| H26  | -2.440183921 | -0.620689858 | 1.815903667  |
| H27  | -2.403865736 | 3.437152142  | 1.892718792  |
| N28  | 0.160358521  | -3.515454166 | -2.188200129 |
| N29  | -0.461361152 | -4.741079053 | -3.932530859 |
| N30  | 0.196076998  | 1.432653434  | 0.271696548  |
| O31  | -2.600881733 | 1.328638187  | 3.528820374  |
| O32  | 1.424358155  | -6.075137437 | 0.955547312  |
| O33  | 1.317555630  | -3.838017610 | 0.535617364  |
| O34  | -1.228172213 | -3.690895378 | 0.537085726  |
| S35  | 0.475290441  | 7.361633754  | 0.293364064  |
| S36  | -1.514246516 | 4.227828976  | -0.687331425 |
| S37  | 0.164336816  | 4.006604491  | 2.343914707  |
| S38  | 0.164720587  | 1.435147024  | -3.084629524 |
| S39  | 2.120629833  | 4.024213199  | -0.732139020 |
| S40  | -1.611398270 | -1.072224545 | -0.906829135 |
| S41  | -3.124160472 | 1.459814814  | 0.374587823  |
| S42  | 0.083496787  | -1.257027310 | 2.207825587  |
| S43  | 1.831281894  | -1.087193200 | -0.756493223 |
| S44  | 2.935971865  | 1.295983499  | 2.037710353  |
| V45  | 0.017381007  | -2.288175081 | 0.175857839  |

## W. v26hoch2h6h3btc.car\_2

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 1.624611016  | 7.870646358  | 1.115410880  |
| C2   | 1.328333591  | -3.462404154 | -3.158747938 |
| C3   | 0.950523065  | -4.266341405 | -4.207841879 |
| C4   | -0.734658235 | -4.046958663 | -2.755414285 |
| C5   | -0.231645964 | -5.098287972 | 0.737808416  |
| C6   | 1.308911940  | -5.063194838 | 0.596882814  |
| C7   | -1.548413210 | 0.823167545  | 2.878422166  |
| Fe8  | -0.002331526 | 5.122558967  | 0.274401370  |
| Fe9  | -1.627579060 | 2.967350396  | 0.896363194  |
| Fe10 | 1.224433271  | 2.781208985  | 0.903805065  |
| Fe11 | -0.003003560 | 3.004508490  | -1.430156295 |
| Fe12 | 0.079523374  | 0.302044028  | -1.184318769 |
| Fe13 | -1.549104685 | 0.437082573  | 1.076652026  |
| Fe14 | 1.475201391  | 0.222334359  | 0.983417878  |
| H15  | 2.465334560  | 7.466174578  | 0.538907082  |
| H16  | 1.691217031  | 8.967561155  | 1.134730422  |
| H17  | 1.676245922  | 7.488945476  | 2.142113441  |
| H18  | 2.272628182  | -2.972306416 | -2.963951446 |
| H19  | 1.476047429  | -4.602160799 | -5.091736562 |
| H20  | -1.698254526 | -4.165230215 | -2.278002128 |
| H21  | -0.958412124 | -5.225308398 | -4.513250673 |

|     |              |              |              |
|-----|--------------|--------------|--------------|
| H22 | -0.609380185 | -5.956340453 | 0.147786868  |
| H23 | -0.492869133 | -5.287422060 | 1.794873731  |
| H24 | -0.209658906 | -1.301236499 | 2.762256307  |
| H25 | -3.402761092 | 1.010845006  | 3.008264792  |
| H26 | -2.461632836 | -0.663526124 | 1.585924451  |
| H27 | -2.693127288 | 3.736049716  | 1.628859747  |
| H28 | -0.633252806 | 0.883673546  | 3.514970291  |
| N29 | 0.274580502  | -3.335268474 | -2.269294501 |
| N30 | -0.368917204 | -4.634513870 | -3.938786776 |
| N31 | 0.041277153  | 1.355152718  | 0.396763826  |
| O32 | -2.642293765 | 0.938363275  | 3.655265825  |
| O33 | 1.991686997  | -6.063696637 | 0.889880634  |
| O34 | 1.751520210  | -3.924209484 | 0.142548538  |
| O35 | -0.837639297 | -3.892367058 | 0.312296362  |
| S36 | -0.002829555 | 7.409282508  | 0.325037629  |
| S37 | -1.788047930 | 4.313863226  | -0.912630405 |
| S38 | -0.136797358 | 4.035839377  | 2.293393965  |
| S39 | 0.020458582  | 1.507916184  | -3.041114770 |
| S40 | 1.832039896  | 4.248900733  | -0.765400850 |
| S41 | -1.627051007 | -1.125941720 | -0.713205202 |
| S42 | -3.367270330 | 1.636299636  | 0.630426526  |
| S43 | 0.935608448  | -1.694923046 | 2.150869200  |
| S44 | 2.011652569  | -0.925626044 | -0.901571821 |
| S45 | 2.899060926  | 1.634775535  | 1.813789943  |
| V46 | 0.296035455  | -2.457303708 | -0.206691692 |

### W-TS-X. v26hoch2h6h3btzg\_orig

|      |        |        |        |
|------|--------|--------|--------|
| C1   | 1.771  | 7.904  | 0.785  |
| C2   | 1.281  | -3.628 | -3.008 |
| C3   | 0.904  | -4.457 | -4.038 |
| C4   | -0.792 | -4.157 | -2.613 |
| C5   | -0.390 | -4.971 | 0.934  |
| C6   | 1.148  | -4.934 | 0.806  |
| C7   | -1.369 | 0.683  | 2.970  |
| Fe8  | 0.187  | 5.156  | 0.019  |
| Fe9  | -1.493 | 2.869  | 0.696  |
| Fe10 | 1.315  | 2.809  | 0.815  |
| Fe11 | 0.100  | 2.946  | -1.561 |
| Fe12 | 0.066  | 0.285  | -1.263 |
| Fe13 | -1.459 | 0.164  | 1.106  |
| Fe14 | 1.412  | 0.287  | 1.006  |
| H15  | 2.617  | 7.455  | 0.247  |
| H16  | 1.867  | 8.998  | 0.768  |
| H17  | 1.780  | 7.558  | 1.824  |
| H18  | 2.234  | -3.147 | -2.828 |
| H19  | 1.433  | -4.833 | -4.904 |
| H20  | -1.771 | -4.236 | -2.161 |
| H21  | -1.016 | -5.387 | -4.345 |
| H22  | -0.764 | -5.826 | 0.341  |
| H23  | -0.649 | -5.171 | 1.991  |
| H24  | -0.637 | -0.550 | 2.977  |
| H25  | -3.243 | 0.774  | 3.053  |
| H26  | -2.498 | -0.827 | 1.589  |
| H27  | -2.522 | 3.762  | 1.349  |
| H28  | -0.552 | 1.168  | 3.493  |
| N29  | 0.220  | -3.452 | -2.132 |
| N30  | -0.425 | -4.791 | -3.776 |
| N31  | 0.067  | 1.440  | 0.287  |
| O32  | -2.515 | 0.796  | 3.720  |
| O33  | 1.846  | -5.927 | 1.079  |
| O34  | 1.596  | -3.772 | 0.385  |
| O35  | -0.987 | -3.768 | 0.504  |
| S36  | 0.159  | 7.449  | -0.035 |
| S37  | -1.658 | 4.293  | -1.046 |
| S38  | -0.066 | 4.146  | 2.062  |
| S39  | 0.087  | 1.419  | -3.157 |
| S40  | 1.983  | 4.154  | -0.969 |
| S41  | -1.682 | -1.118 | -0.898 |
| S42  | -3.182 | 1.523  | 0.719  |
| S43  | 0.561  | -1.398 | 2.222  |
| S44  | 1.940  | -0.945 | -0.829 |
| S45  | 2.915  | 1.610  | 1.818  |

**X. v26hoch2h6h3btze.car\_2**

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 1.807749237  | 7.888024957  | 0.788135723  |
| C2   | 1.268143623  | -3.634956177 | -3.029943116 |
| C3   | 0.867745553  | -4.456556524 | -4.057523106 |
| C4   | -0.808321327 | -4.141027101 | -2.612412041 |
| C5   | -0.376751557 | -4.997478958 | 0.927086712  |
| C6   | 1.153776684  | -5.014251122 | 0.751860410  |
| C7   | -1.408023799 | 0.491227865  | 3.182033881  |
| Fe8  | 0.157250372  | 5.150030727  | 0.026606691  |
| Fe9  | -1.430223822 | 2.985812105  | 0.718816615  |
| Fe10 | 1.327004880  | 2.801291019  | 0.821910616  |
| Fe11 | 0.107876469  | 2.928407160  | -1.568421068 |
| Fe12 | 0.098572691  | 0.239043790  | -1.276467398 |
| Fe13 | -1.404687968 | 0.199231332  | 1.093064062  |
| Fe14 | 1.532449700  | 0.254923973  | 0.866985310  |
| H15  | 2.645943468  | 7.437776471  | 0.244000049  |
| H16  | 1.901602797  | 8.982341244  | 0.763905675  |
| H17  | 1.830131650  | 7.547734336  | 1.830610019  |
| H18  | 2.224801262  | -3.163356238 | -2.848832330 |
| H19  | 1.382745347  | -4.834004239 | -4.931219898 |
| H20  | -1.778757168 | -4.205921466 | -2.136356136 |
| H21  | -1.070472410 | -5.363275229 | -4.339999837 |
| H22  | -0.794874994 | -5.852922757 | 0.359035299  |
| H23  | -0.627661703 | -5.176417348 | 1.990991120  |
| H24  | -1.025797378 | -0.407576292 | 3.686333883  |
| H25  | -3.326287378 | 0.874795188  | 3.135353962  |
| H26  | -2.455844848 | -0.771431847 | 1.554610248  |
| H27  | -2.495656422 | 3.839750089  | 1.361044587  |
| H28  | -0.680420064 | 1.326984377  | 3.243603709  |
| N29  | 0.220563651  | -3.450018945 | -2.148954449 |
| N30  | -0.463791723 | -4.775822212 | -3.779681331 |
| N31  | 0.136929790  | 1.387088903  | 0.268153420  |
| O32  | -2.641551232 | 0.861357698  | 3.828335045  |
| O33  | 1.830410638  | -6.006838063 | 1.069824895  |
| O34  | 1.619029773  | -3.901294272 | 0.230116862  |
| O35  | -0.940710481 | -3.783598587 | 0.483332719  |
| S36  | 0.182762911  | 7.438403896  | -0.012514342 |
| S37  | -1.639864961 | 4.310902806  | -1.116971783 |
| S38  | 0.009088538  | 4.182140522  | 2.103536355  |
| S39  | 0.044290562  | 1.400426598  | -3.154052491 |
| S40  | 1.967437624  | 4.159378563  | -0.951134806 |
| S41  | -1.638064628 | -1.171221758 | -0.850729546 |
| S42  | -3.088307860 | 1.563274548  | 0.764837247  |
| S43  | 0.549915240  | -1.406401803 | 1.975746137  |
| S44  | 2.012788499  | -0.969538257 | -0.969666673 |
| S45  | 2.964017194  | 1.604980632  | 1.766873604  |
| V46  | 0.253042548  | -2.371408085 | -0.051877174 |

**Y. v2chohn2h6h6htca\_1\_4500.78**

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 2.249964734  | 7.776634074  | 0.183230401  |
| C2   | 1.076486778  | -3.748505821 | -3.060732603 |
| C3   | 0.629392478  | -4.614377026 | -4.033405598 |
| C4   | -0.890257748 | -4.408646669 | -2.409738768 |
| C5   | -0.472419697 | -4.983768212 | 1.095397622  |
| C6   | 1.062516922  | -4.978868703 | 0.929024605  |
| C7   | -1.534479379 | 2.168262617  | 3.147333940  |
| Fe8  | 0.367581078  | 5.074349774  | -0.032318656 |
| Fe9  | -1.270585614 | 2.598246426  | 1.372244519  |
| Fe10 | 1.529213521  | 2.785421762  | 0.985373579  |
| Fe11 | 0.117130017  | 2.720386303  | -1.304893869 |
| Fe12 | 0.023592512  | 0.204753017  | -1.351653544 |
| Fe13 | -1.235993199 | -0.089241669 | 1.010780424  |
| Fe14 | 1.392674683  | 0.200885034  | 0.876099318  |
| H15  | 2.927048663  | 7.232390518  | -0.484921618 |
| H16  | 2.387361514  | 8.858461558  | 0.044176223  |
| H17  | 2.483437215  | 7.516598284  | 1.222565086  |
| H18  | 2.009096220  | -3.202177649 | -3.003774182 |
| H19  | 1.066969991  | -4.961567760 | -4.960111123 |



|     |              |              |              |
|-----|--------------|--------------|--------------|
| H20 | -1.794670088 | -4.542927509 | -1.829153576 |
| H21 | -1.248731923 | -5.670024294 | -4.092724874 |
| H22 | -0.884960796 | -5.870677752 | 0.576154497  |
| H23 | -0.708518124 | -5.096624363 | 2.170209948  |
| H24 | -2.369793246 | -0.887761211 | 1.633222496  |
| H25 | -3.266808646 | 1.561416206  | 2.853761322  |
| H26 | -2.385273524 | 3.559551241  | 1.751177090  |
| H27 | -0.794096722 | 2.337229936  | 3.946684315  |
| H28 | -1.512603269 | -0.037029867 | 2.450229272  |
| N29 | 0.124149605  | -3.631994961 | -2.063968386 |
| N30 | -0.630323943 | -5.033064532 | -3.604799218 |
| N31 | 0.058389456  | 1.392898410  | 0.165328875  |
| O32 | 1.740411185  | -5.980889971 | 1.218640761  |
| O33 | 1.514153825  | -3.842442388 | 0.464697474  |
| O34 | -1.045658978 | -3.796782608 | 0.594982879  |
| O35 | -2.675619963 | 1.738543973  | 3.682982726  |
| S36 | 0.472977737  | 7.361243134  | -0.212572698 |
| S37 | -1.522526014 | 4.128250748  | -0.828870874 |
| S38 | 0.310376169  | 4.248052055  | 2.157006742  |
| S39 | 0.046552868  | 1.412582151  | -3.129567273 |
| S40 | 2.087047246  | 3.921654047  | -0.959413418 |
| S41 | -1.635491768 | -1.225253380 | -0.973791640 |
| S42 | -3.060049077 | 1.316986515  | 0.780729433  |
| S43 | 0.359792671  | -1.358087694 | 2.087927171  |
| S44 | 1.820885171  | -1.072339017 | -0.935244264 |
| S45 | 2.985485389  | 1.292551528  | 1.835885930  |
| V46 | 0.096174071  | -2.374296253 | 0.035809538  |

### Y-TS-Z. v2chohn2h6h6htl\_orig

|      |        |        |        |
|------|--------|--------|--------|
| C1   | 2.405  | 7.723  | 0.112  |
| C2   | 0.979  | -3.803 | -3.063 |
| C3   | 0.508  | -4.662 | -4.031 |
| C4   | -0.987 | -4.433 | -2.387 |
| C5   | -0.568 | -4.985 | 1.120  |
| C6   | 0.967  | -4.982 | 0.951  |
| C7   | -1.414 | 2.142  | 3.110  |
| Fe8  | 0.463  | 5.049  | -0.069 |
| Fe9  | -1.241 | 2.626  | 1.310  |
| Fe10 | 1.586  | 2.743  | 0.942  |
| Fe11 | 0.147  | 2.693  | -1.345 |
| Fe12 | 0.020  | 0.175  | -1.363 |
| Fe13 | -1.275 | 0.009  | 1.045  |
| Fe14 | 1.339  | 0.158  | 0.900  |
| H15  | 3.066  | 7.167  | -0.561 |
| H16  | 2.558  | 8.802  | -0.032 |
| H17  | 2.646  | 7.464  | 1.150  |
| H18  | 1.920  | -3.269 | -3.021 |
| H19  | 0.930  | -5.017 | -4.962 |
| H20  | -1.887 | -4.552 | -1.797 |
| H21  | -1.386 | -5.691 | -4.065 |
| H22  | -0.977 | -5.871 | 0.599  |
| H23  | -0.802 | -5.103 | 2.196  |
| H24  | -2.413 | -0.769 | 1.664  |
| H25  | -3.186 | 1.621  | 2.965  |
| H26  | -2.288 | 3.584  | 1.794  |
| H27  | -0.621 | 2.298  | 3.852  |
| H28  | -1.090 | 0.469  | 2.511  |
| N29  | 0.042  | -3.672 | -2.053 |
| N30  | -0.752 | -5.062 | -3.586 |
| N31  | 0.085  | 1.389  | 0.127  |
| O32  | 1.647  | -5.990 | 1.207  |
| O33  | 1.420  | -3.831 | 0.522  |
| O34  | -1.143 | -3.795 | 0.623  |
| O35  | -2.558 | 1.851  | 3.735  |
| S36  | 0.616  | 7.337  | -0.260 |
| S37  | -1.482 | 4.106  | -0.808 |
| S38  | 0.387  | 4.235  | 2.103  |
| S39  | 0.084  | 1.374  | -3.154 |
| S40  | 2.138  | 3.853  | -1.028 |
| S41  | -1.693 | -1.179 | -0.923 |
| S42  | -3.103 | 1.401  | 0.777  |
| S43  | 0.209  | -1.336 | 2.125  |

|     |       |        |        |
|-----|-------|--------|--------|
| S44 | 1.777 | -1.129 | -0.884 |
| S45 | 2.946 | 1.203  | 1.877  |
| V46 | 0.012 | -2.364 | 0.093  |

### Z. v2chohn2h6h6htl.car\_5

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 2.314739801  | 7.658580125  | 0.094559089  |
| C2   | 1.005686369  | -3.834988486 | -3.090898202 |
| C3   | 0.481668252  | -4.632405071 | -4.083342240 |
| C4   | -0.987428495 | -4.388088799 | -2.418624009 |
| C5   | -0.554947324 | -4.989045064 | 1.154475290  |
| C6   | 0.967214299  | -5.056302522 | 0.915797071  |
| C7   | -1.324386326 | 1.998814892  | 3.322336950  |
| Fe8  | 0.416440206  | 4.991161913  | -0.100606065 |
| Fe9  | -1.213182272 | 2.643200036  | 1.291716154  |
| Fe10 | 1.553563385  | 2.759959235  | 0.999683322  |
| Fe11 | 0.252720041  | 2.608185272  | -1.367293810 |
| Fe12 | 0.159555125  | 0.077163073  | -1.426145206 |
| Fe13 | -1.431590929 | -0.069070239 | 0.722335551  |
| Fe14 | 1.408698330  | 0.150241669  | 0.897443486  |
| H15  | 2.994584242  | 7.098171709  | -0.556298389 |
| H16  | 2.473441938  | 8.736233653  | -0.047938176 |
| H17  | 2.520708037  | 7.400569543  | 1.139419241  |
| H18  | 1.973185376  | -3.353570356 | -3.036007416 |
| H19  | 0.875518263  | -4.974157750 | -5.031593595 |
| H20  | -1.887583384 | -4.474095409 | -1.822877776 |
| H21  | -1.473427758 | -5.544449970 | -4.140220670 |
| H22  | -1.027468959 | -5.905911264 | 0.757640173  |
| H23  | -0.728234877 | -4.975501605 | 2.247305018  |
| H24  | -2.477434594 | -1.000119837 | 1.283045078  |
| H25  | -3.245878135 | 1.820595735  | 3.292352345  |
| H26  | -2.259008760 | 3.619939466  | 1.749008712  |
| H27  | -0.591485495 | 2.546355653  | 3.919569636  |
| H28  | -1.066080426 | 0.934003560  | 3.263004016  |
| N29  | 0.083831593  | -3.692139768 | -2.069889219 |
| N30  | -0.794152501 | -4.983423351 | -3.639567080 |
| N31  | 0.157164308  | 1.316664915  | 0.139851123  |
| O32  | 1.614612226  | -6.091405374 | 1.152902459  |
| O33  | 1.450897466  | -3.927984626 | 0.459065544  |
| O34  | -1.117398276 | -3.837826496 | 0.556590899  |
| O35  | -2.598497508 | 2.194974896  | 3.928538128  |
| S36  | 0.539370462  | 7.267910016  | -0.338841668 |
| S37  | -1.427256526 | 4.006172071  | -0.954209908 |
| S38  | 0.269815447  | 4.260884241  | 2.099975710  |
| S39  | 0.175232769  | 1.371549162  | -3.201105987 |
| S40  | 2.170164535  | 3.830413894  | -0.970442081 |
| S41  | -1.643632625 | -1.273198056 | -1.144909590 |
| S42  | -3.032719021 | 1.371164067  | 0.868430675  |
| S43  | 0.076576597  | -1.269460478 | 2.031646193  |
| S44  | 1.963012814  | -1.196607801 | -0.809827963 |
| S45  | 2.914635486  | 1.253435522  | 1.956488678  |
| V46  | 0.068756825  | -2.446591995 | 0.007458511  |

### S-TS-AA. v2choh6h2htg.car\_1

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 2.343108763  | 7.763146599  | 0.223726280  |
| C2   | 0.955660529  | -3.742525388 | -3.065131562 |
| C3   | 0.472822005  | -4.591020659 | -4.036912037 |
| C4   | -0.993915503 | -4.395084571 | -2.364171313 |
| C5   | -0.525371727 | -4.988450773 | 1.124975393  |
| C6   | 1.006153079  | -4.957461723 | 0.942579591  |
| C7   | -1.474252716 | 2.160082168  | 3.230250979  |
| Fe8  | 0.412764296  | 5.089321340  | 0.031079893  |
| Fe9  | -1.230656267 | 2.608951306  | 1.465483527  |
| Fe10 | 1.574179273  | 2.763405521  | 0.992696792  |
| Fe11 | 0.063274842  | 2.751964297  | -1.285585388 |
| Fe12 | 0.021242249  | 0.224228425  | -1.330963343 |
| Fe13 | -1.442107705 | -0.045048290 | 0.906940125  |
| Fe14 | 1.232816992  | 0.193649810  | 0.958851978  |
| H15  | 2.998341709  | 7.216263856  | -0.463695197 |
| H16  | 2.495786090  | 8.844409124  | 0.095054000  |
| H17  | 2.591824292  | 7.487256242  | 1.255574571  |

|     |              |              |              |
|-----|--------------|--------------|--------------|
| H18 | 1.893036664  | -3.202080095 | -3.033592995 |
| H19 | 0.881919348  | -4.932485764 | -4.979240525 |
| H20 | -1.883709864 | -4.525843390 | -1.760641514 |
| H21 | -1.415900676 | -5.631900757 | -4.051714950 |
| H22 | -0.927115364 | -5.877346033 | 0.602345409  |
| H23 | -0.742806032 | -5.119342803 | 2.203054109  |
| H24 | -2.490247526 | -0.889916234 | 1.589739359  |
| H25 | -3.039737734 | 1.152426410  | 3.051877659  |
| H26 | -2.178032739 | 3.475372128  | 2.319883466  |
| H27 | -0.824082965 | 2.565499453  | 4.019502118  |
| N28 | 0.036134107  | -3.631483309 | -2.037144950 |
| N29 | -0.777140676 | -5.005396276 | -3.576032553 |
| N30 | 0.024354789  | 1.450867639  | 0.186451103  |
| O31 | 1.706150230  | -5.960582706 | 1.162673736  |
| O32 | 1.437055585  | -3.784147270 | 0.547289274  |
| O33 | -1.123437029 | -3.804419583 | 0.643873011  |
| O34 | -2.481558618 | 1.494814769  | 3.818442449  |
| S35 | 0.552321158  | 7.380093056  | -0.140397043 |
| S36 | -1.543037962 | 4.174272293  | -0.667957534 |
| S37 | 0.411667506  | 4.257671104  | 2.195143890  |
| S38 | 0.012868602  | 1.444046051  | -3.109565052 |
| S39 | 2.074116453  | 3.899142154  | -0.984454232 |
| S40 | -1.696651575 | -1.199311792 | -0.961398284 |
| S41 | -3.105109496 | 1.378561727  | 0.870722778  |
| S42 | 0.031037904  | -1.259622718 | 2.174720351  |
| S43 | 1.762211789  | -1.083455459 | -0.809758337 |
| S44 | 2.895252464  | 1.197166173  | 1.908505059  |
| V45 | 0.008771455  | -2.345686052 | 0.136919909  |

### AA. v2choh6h2hta.car\_3

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 2.452476927  | 7.740918462  | 0.246706934  |
| C2   | 0.932091858  | -3.743302745 | -3.079077238 |
| C3   | 0.443491308  | -4.580978740 | -4.057457266 |
| C4   | -1.033769282 | -4.365512811 | -2.396538013 |
| C5   | -0.608078154 | -4.987472827 | 1.094501799  |
| C6   | 0.925586489  | -4.970186034 | 0.925905539  |
| C7   | -1.562362914 | 2.302607174  | 3.250659371  |
| Fe8  | 0.514238531  | 5.106729063  | 0.018044196  |
| Fe9  | -1.154124762 | 2.584181013  | 1.369742142  |
| Fe10 | 1.685803507  | 2.771441564  | 0.961420324  |
| Fe11 | 0.128512716  | 2.772267904  | -1.287554055 |
| Fe12 | -0.010654480 | 0.239975053  | -1.326155200 |
| Fe13 | -1.484673298 | -0.068020327 | 0.895717025  |
| Fe14 | 1.179220129  | 0.200906168  | 0.986621540  |
| H15  | 3.106179877  | 7.183530012  | -0.433655366 |
| H16  | 2.631568613  | 8.818973593  | 0.128124778  |
| H17  | 2.677535939  | 7.452006456  | 1.280135373  |
| H18  | 1.878645251  | -3.219798081 | -3.038036737 |
| H19  | 0.853957501  | -4.926966983 | -4.997557738 |
| H20  | -1.931003552 | -4.482274740 | -1.801295711 |
| H21  | -1.463022061 | -5.588702921 | -4.091683085 |
| H22  | -1.015223496 | -5.873895713 | 0.572397134  |
| H23  | -0.837967445 | -5.107977906 | 2.170797986  |
| H24  | -2.564574254 | -0.885381205 | 1.566568574  |
| H25  | -3.055842169 | 1.107232546  | 3.084280637  |
| H26  | -2.067284723 | 3.282481330  | 2.892038773  |
| H27  | -0.825722097 | 2.557476407  | 4.018017121  |
| N28  | 0.006036275  | -3.619917690 | -2.058362952 |
| N29  | -0.816896033 | -4.975803559 | -3.608092024 |
| N30  | 0.028628026  | 1.491789522  | 0.205603821  |
| O31  | 1.612113096  | -5.982199617 | 1.147586101  |
| O32  | 1.371242700  | -3.799377955 | 0.540501255  |
| O33  | -1.189590018 | -3.799913969 | 0.601546060  |
| O34  | -2.489201961 | 1.425585825  | 3.828265479  |
| S35  | 0.661329834  | 7.394925874  | -0.149333773 |
| S36  | -1.455044079 | 4.224469652  | -0.674616585 |
| S37  | 0.505889533  | 4.240111805  | 2.171964443  |
| S38  | 0.034219219  | 1.463222436  | -3.105290441 |
| S39  | 2.158496493  | 3.900897992  | -1.022323654 |
| S40  | -1.732125121 | -1.194237781 | -0.986200427 |
| S41  | -3.037034626 | 1.461397148  | 0.739331552  |
| S42  | -0.032996984 | -1.279505892 | 2.172759351  |

|     |              |              |              |
|-----|--------------|--------------|--------------|
| S43 | 1.724858341  | -1.063649822 | -0.785335614 |
| S44 | 2.900054286  | 1.139131972  | 1.906038884  |
| V45 | -0.044984941 | -2.347181654 | 0.123289687  |

### BB. v6hch22h\_1\_4322.69

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 1.531884961  | 7.904131421  | 1.237757363  |
| C2   | 1.279572827  | -3.508000570 | -2.917315665 |
| C3   | 0.955363334  | -4.315362287 | -3.983029854 |
| C4   | -0.801621879 | -4.065895867 | -2.626392762 |
| C5   | -0.420257321 | -4.975926706 | 0.910213408  |
| C6   | 1.121369529  | -4.892758667 | 0.795245778  |
| C7   | -1.481525500 | 0.392460767  | 3.211240286  |
| Fe8  | -0.004280531 | 5.147318439  | 0.296581983  |
| Fe9  | -1.671859295 | 2.902452758  | 0.725533226  |
| Fe10 | 1.143192988  | 2.841062374  | 1.114335965  |
| Fe11 | 0.007326366  | 2.945814362  | -1.349041558 |
| Fe12 | 0.012262613  | 0.356931092  | -1.157277741 |
| Fe13 | -1.520405941 | 0.039547112  | 1.450951368  |
| Fe14 | 1.303589907  | 0.320800002  | 1.038911992  |
| H15  | 2.389060831  | 7.493601131  | 0.689646841  |
| H16  | 1.585664583  | 9.000860173  | 1.235442534  |
| H17  | 1.562574084  | 7.544043816  | 2.274297617  |
| H18  | 2.218078943  | -3.021225374 | -2.686661547 |
| H19  | 1.528335021  | -4.661933241 | -4.832921148 |
| H20  | -1.800179563 | -4.163859547 | -2.219892938 |
| H21  | -0.938153313 | -5.264552863 | -4.387942340 |
| H22  | -0.776681586 | -5.769425039 | 0.222974156  |
| H23  | -0.687967706 | -5.300288585 | 1.935369471  |
| H24  | -1.539321658 | -0.359751212 | 4.002433352  |
| H25  | -2.516334373 | -1.019791780 | 1.844313343  |
| H26  | -2.820764311 | 3.770928030  | 1.155123737  |
| H27  | -1.334399293 | 1.413196183  | 3.587530989  |
| N28  | 0.182094837  | -3.363797000 | -2.085198921 |
| N29  | -0.380344544 | -4.667702084 | -3.787933642 |
| N30  | -0.053790225 | 1.504175950  | 0.402807888  |
| O31  | 1.849769034  | -5.872630282 | 1.034045786  |
| O32  | 1.535670880  | -3.706232779 | 0.415397616  |
| O33  | -1.042708496 | -3.745185221 | 0.601056526  |
| S34  | -0.077107013 | 7.434725702  | 0.418443840  |
| S35  | -1.736030562 | 4.363856672  | -0.991689445 |
| S36  | -0.444149882 | 4.078118457  | 2.276685384  |
| S37  | -0.008336462 | 1.512302653  | -3.036363327 |
| S38  | 1.856745461  | 4.217844390  | -0.599214641 |
| S39  | -1.729176578 | -1.082742265 | -0.763583180 |
| S40  | -3.212236184 | 1.441774683  | 0.908701743  |
| S41  | 0.318023489  | -1.347136644 | 2.192884380  |
| S42  | 1.834613131  | -0.881634837 | -0.787040666 |
| S43  | 2.714518259  | 1.603017998  | 2.120650745  |
| V44  | 0.067901138  | -2.243131319 | 0.112922055  |

### CC. v6hch22h\_2\_4330.63

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 1.499085712  | 7.873251597  | 1.188241865  |
| C2   | 1.301058491  | -3.546344934 | -2.999448415 |
| C3   | 0.920804576  | -4.348854649 | -4.051974370 |
| C4   | -0.790209419 | -4.018621240 | -2.653711381 |
| C5   | -0.407323456 | -4.955317321 | 0.885962679  |
| C6   | 1.129914872  | -4.907667108 | 0.731106510  |
| C7   | -1.679720685 | 0.503931386  | 3.287762599  |
| Fe8  | -0.018879683 | 5.138107991  | 0.277726772  |
| Fe9  | -1.661417190 | 2.864694480  | 0.815671107  |
| Fe10 | 1.176628543  | 2.827431096  | 1.099250999  |
| Fe11 | 0.064317101  | 2.868973084  | -1.299817351 |
| Fe12 | 0.110446315  | 0.319244143  | -1.161524350 |
| Fe13 | -1.449050894 | 0.161883832  | 1.538863528  |
| Fe14 | 1.365212680  | 0.306413897  | 1.067684100  |
| H15  | 2.353355475  | 7.447552346  | 0.650136327  |
| H16  | 1.592255790  | 8.967780983  | 1.210944691  |
| H17  | 1.498739488  | 7.493954626  | 2.217040847  |
| H18  | 2.261399867  | -3.090202634 | -2.795121504 |
| H19  | 1.457343168  | -4.727755874 | -4.913030346 |

|     |              |              |              |
|-----|--------------|--------------|--------------|
| H20 | -1.778297781 | -4.066339311 | -2.213998629 |
| H21 | -1.022052731 | -5.223653075 | -4.401999220 |
| H22 | -0.792732494 | -5.773186626 | 0.242427228  |
| H23 | -0.643534007 | -5.228070151 | 1.935613206  |
| H24 | -1.168264131 | -0.051126651 | 4.088919508  |
| H25 | -2.493093056 | -0.821506771 | 2.067633909  |
| H26 | -2.778654769 | 3.753397222  | 1.299565715  |
| H27 | -2.452098677 | 1.190057629  | 3.670540648  |
| N28 | 0.230866450  | -3.351749966 | -2.144279513 |
| N29 | -0.424514099 | -4.645975804 | -3.821556856 |
| N30 | -0.045519866 | 1.426863769  | 0.416603302  |
| O31 | 1.829718293  | -5.919840199 | 0.906848420  |
| O32 | 1.565243062  | -3.712691696 | 0.399880363  |
| O33 | -1.007834977 | -3.724550255 | 0.548218072  |
| S34 | -0.098529490 | 7.430680406  | 0.326428774  |
| S35 | -1.720991101 | 4.236583060  | -0.971119390 |
| S36 | -0.361362170 | 4.078692651  | 2.293916921  |
| S37 | 0.272925519  | 1.477014221  | -3.013518174 |
| S38 | 1.845751243  | 4.223061418  | -0.633860094 |
| S39 | -1.636672184 | -1.048547395 | -0.712585226 |
| S40 | -3.233625567 | 1.457150793  | 0.968791197  |
| S41 | 0.321916921  | -1.335412467 | 2.212197795  |
| S42 | 1.919578532  | -0.913229646 | -0.734055929 |
| S43 | 2.801570209  | 1.606104925  | 2.038555617  |
| V44 | 0.146246201  | -2.242181876 | 0.135068235  |

### DD. v6hch2a2hte.car\_3

|      |              |              |               |
|------|--------------|--------------|---------------|
| C1   | 2.309598783  | 7.710479508  | 0.935005586   |
| C2   | 0.626773459  | -3.924133548 | -3.0111108307 |
| C3   | -0.000189111 | -4.554682789 | -4.064904816  |
| C4   | -1.466882669 | -4.053954169 | -2.456781924  |
| C5   | -0.688333779 | -4.936426111 | 1.100113872   |
| C6   | 0.831818472  | -4.977679318 | 0.859208247   |
| C7   | -1.286425068 | 1.470453971  | 2.892374125   |
| Fe8  | 0.459803630  | 5.105430223  | 0.348188936   |
| Fe9  | -1.298739057 | 2.683424969  | 1.319175088   |
| Fe10 | 1.617239004  | 2.710657262  | 0.966754915   |
| Fe11 | 0.207975927  | 2.877740631  | -1.221369177  |
| Fe12 | 0.061738483  | 0.284063210  | -1.267370269  |
| Fe13 | -1.372599664 | 0.305052778  | 1.250332948   |
| Fe14 | 1.492950791  | 0.164498657  | 0.890325981   |
| H15  | 2.961094301  | 7.224792547  | 0.200317582   |
| H16  | 2.484294039  | 8.795571421  | 0.924298700   |
| H17  | 2.534161718  | 7.318793733  | 1.934820322   |
| H18  | 1.672403467  | -3.664061945 | -2.891853307  |
| H19  | 0.364260373  | -4.937407598 | -5.010899895  |
| H20  | -2.403762060 | -3.958240360 | -1.924322939  |
| H21  | -2.095427633 | -5.021214670 | -4.254119931  |
| H22  | -1.161055349 | -5.700413690 | 0.452756143   |
| H23  | -0.892288307 | -5.226916621 | 2.148164416   |
| H24  | -0.359867174 | 1.410568442  | 3.476841903   |
| H25  | -2.373926552 | -0.395864647 | 2.152044299   |
| H26  | -2.243863644 | 3.506943006  | 2.172680862   |
| H27  | -2.177090515 | 1.506926197  | 3.526528419   |
| N28  | -0.295695253 | -3.618108964 | -2.026136426  |
| N29  | -1.342968524 | -4.638528200 | -3.694703892  |
| N30  | 0.204163096  | 1.472609231  | 0.298132298   |
| O31  | 1.490520551  | -6.017006280 | 1.021998507   |
| O32  | 1.307861290  | -3.815260272 | 0.469348221   |
| O33  | -1.216629828 | -3.656714474 | 0.836210416   |
| S34  | 0.521917026  | 7.393521463  | 0.500727772   |
| S35  | -1.449354478 | 4.286842213  | -0.569063276  |
| S36  | 0.425315491  | 4.017528871  | 2.387676572   |
| S37  | 0.115676531  | 1.552088800  | -3.031596639  |
| S38  | 2.145767683  | 4.102562400  | -0.811095940  |
| S39  | -1.718004766 | -1.037580027 | -0.701930411  |
| S40  | -3.107449763 | 1.587275888  | 0.661559245   |
| S41  | 0.239353562  | -1.166794833 | 2.212157691   |
| S42  | 1.720083332  | -1.168626941 | -0.894257630  |
| S43  | 3.191797076  | 1.260262451  | 1.649183995   |
| V44  | -0.036000923 | -2.278458409 | 0.244596102   |

**DE. v6hch2a2hth.car\_1**

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 1.652691932  | 7.833694787  | 0.845843270  |
| C2   | 0.971211445  | -3.749493413 | -2.999692140 |
| C3   | 0.451076088  | -4.515861926 | -4.018053642 |
| C4   | -1.080488140 | -4.165605704 | -2.429680275 |
| C5   | -0.302565483 | -4.986562803 | 1.112537202  |
| C6   | 1.207795602  | -4.938363325 | 0.819122277  |
| C7   | -1.431125045 | 1.049778684  | 3.134829521  |
| Fe8  | 0.002080204  | 5.083845702  | 0.257199784  |
| Fe9  | -1.606656727 | 2.886144638  | 1.061795315  |
| Fe10 | 1.357974793  | 2.817880543  | 0.927489728  |
| Fe11 | -0.036257592 | 2.781854365  | -1.279943949 |
| Fe12 | 0.020002359  | 0.213453305  | -1.237983431 |
| Fe13 | -1.301318557 | 0.337220172  | 1.480876051  |
| Fe14 | 1.525902310  | 0.291912335  | 0.865634209  |
| H15  | 2.411679393  | 7.388936293  | 0.191794882  |
| H16  | 1.740237803  | 8.928532150  | 0.818658770  |
| H17  | 1.812173473  | 7.482361011  | 1.872394427  |
| H18  | 1.964086911  | -3.328781738 | -2.896753949 |
| H19  | 0.871695609  | -4.886135043 | -4.944014377 |
| H20  | -2.021574181 | -4.189651170 | -1.895235939 |
| H21  | -1.547192472 | -5.311454714 | -4.173740966 |
| H22  | -0.750629966 | -5.786572403 | 0.489990818  |
| H23  | -0.445520046 | -5.285622355 | 2.169874070  |
| H24  | -0.673006228 | 0.851535857  | 3.914907426  |
| H25  | -2.288293340 | -0.441125621 | 2.415681288  |
| H26  | -2.652881009 | 3.703268804  | 1.785434644  |
| H27  | -2.292849009 | 1.609910039  | 3.514162362  |
| N28  | 0.011627198  | -3.543112329 | -2.023740980 |
| N29  | -0.867176542 | -4.780059562 | -3.642170932 |
| N30  | 0.053963387  | 1.416213903  | 0.272886631  |
| O31  | 1.930135463  | -5.942327454 | 0.927041690  |
| O32  | 1.607552447  | -3.739961108 | 0.453192927  |
| O33  | -0.919432685 | -3.744407864 | 0.862921532  |
| S34  | -0.058723898 | 7.373769788  | 0.260176839  |
| S35  | -1.802298267 | 4.164586665  | -0.800333432 |
| S36  | 0.015731412  | 4.075984780  | 2.322927627  |
| S37  | -0.013647973 | 1.420894544  | -3.051804998 |
| S38  | 1.763038282  | 4.201852788  | -0.874841975 |
| S39  | -1.646710791 | -1.140486170 | -0.553080457 |
| S40  | -3.185277179 | 1.467646730  | 0.761411294  |
| S41  | 0.480080468  | -1.149439487 | 2.234422866  |
| S42  | 1.823746061  | -1.057136619 | -0.897311187 |
| S43  | 3.071713071  | 1.579528485  | 1.672974234  |
| V44  | 0.177427388  | -2.278644705 | 0.272201502  |

**EE. v6hch2a2htg.car\_3**

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 1.906378761  | 7.831767288  | 0.914031921  |
| C2   | 0.871575963  | -3.774081027 | -3.050736675 |
| C3   | 0.310047095  | -4.520321650 | -4.062461794 |
| C4   | -1.198179007 | -4.092678986 | -2.470783815 |
| C5   | -0.409253989 | -5.000659342 | 1.048322914  |
| C6   | 1.103268752  | -4.982976453 | 0.757767784  |
| C7   | -1.520613145 | 0.621656401  | 3.312805005  |
| Fe8  | 0.131427067  | 5.163612049  | 0.213299615  |
| Fe9  | -1.549443117 | 3.050833297  | 0.887818390  |
| Fe10 | 1.270296366  | 2.795828508  | 1.015016020  |
| Fe11 | 0.048743302  | 2.881183568  | -1.325547625 |
| Fe12 | 0.016005472  | 0.230040853  | -1.206029986 |
| Fe13 | -1.326424456 | 0.300969153  | 1.281748597  |
| Fe14 | 1.483044968  | 0.226563594  | 0.890010646  |
| H15  | 2.673819746  | 7.377819246  | 0.276399234  |
| H16  | 2.037784040  | 8.923032536  | 0.924168606  |
| H17  | 2.013826244  | 7.445220512  | 1.934762336  |
| H18  | 1.884179419  | -3.404802817 | -2.948883631 |
| H19  | 0.707857958  | -4.914344793 | -4.988756782 |
| H20  | -2.131646565 | -4.078593068 | -1.923065895 |
| H21  | -1.728121779 | -5.213517555 | -4.207285584 |
| H22  | -0.860156712 | -5.847408678 | 0.494025824  |

|     |              |              |              |
|-----|--------------|--------------|--------------|
| H23 | -0.552295731 | -5.210612026 | 2.126465373  |
| H24 | -0.565210241 | 0.617668003  | 3.846646287  |
| H25 | -2.132229517 | -0.241633462 | 3.626025304  |
| H26 | -2.630507590 | 3.912290808  | 1.492213201  |
| H27 | -2.064707835 | 1.550918019  | 3.505916874  |
| N28 | -0.075154072 | -3.517270331 | -2.075066676 |
| N29 | -1.017258409 | -4.720921849 | -3.679082981 |
| N30 | 0.028137013  | 1.341610558  | 0.374996370  |
| O31 | 1.812393273  | -5.989896182 | 0.918694468  |
| O32 | 1.520531658  | -3.809992760 | 0.335731390  |
| O33 | -1.024087488 | -3.780336184 | 0.697956063  |
| S34 | 0.205454306  | 7.458629166  | 0.240840852  |
| S35 | -1.643216672 | 4.377559851  | -0.975532406 |
| S36 | -0.050457568 | 4.159428733  | 2.300529111  |
| S37 | 0.097990315  | 1.447248456  | -3.029401714 |
| S38 | 1.918308068  | 4.149121359  | -0.766395379 |
| S39 | -1.746562637 | -1.120820318 | -0.635872547 |
| S40 | -3.121131412 | 1.525483303  | 0.838798636  |
| S41 | 0.385605575  | -1.279215789 | 2.129791205  |
| S42 | 1.833940467  | -1.066260043 | -0.922567020 |
| S43 | 2.979221487  | 1.507889658  | 1.758835853  |
| V44 | 0.106809310  | -2.330024294 | 0.123861033  |

### DD-TS-FF. v2h6h2ch266coti\_1\_4584.04

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 2.536617695  | 7.683004311  | 0.812571949  |
| C2   | 1.071747259  | -3.492613667 | -3.310074867 |
| C3   | 0.662902108  | -4.310326245 | -4.340606583 |
| C4   | -0.953171332 | -4.095951661 | -2.813104178 |
| C5   | -0.722812196 | -4.973543604 | 0.702657384  |
| C6   | 0.808845032  | -5.042215407 | 0.565105848  |
| C7   | -2.247723709 | -0.668734598 | 3.853014878  |
| C8   | -1.587193655 | 1.771003287  | 2.770858951  |
| Fe9  | 0.548732999  | 5.127554649  | 0.176400648  |
| Fe10 | -1.332404830 | 2.637843275  | 1.050006408  |
| Fe11 | 1.577500639  | 2.758751596  | 1.009561678  |
| Fe12 | 0.314818508  | 2.881688182  | -1.382407727 |
| Fe13 | 0.227511057  | 0.296528791  | -1.299831590 |
| Fe14 | -1.729266424 | 0.071193004  | 1.421317140  |
| Fe15 | 1.451959197  | 0.209370069  | 0.934807962  |
| H16  | 3.250155227  | 7.171607367  | 0.155914932  |
| H17  | 2.738244400  | 8.763231160  | 0.802525293  |
| H18  | 2.655342823  | 7.305594805  | 1.835119976  |
| H19  | 2.019796039  | -2.986780819 | -3.174475169 |
| H20  | 1.151780391  | -4.651126996 | -5.244548574 |
| H21  | -1.901667417 | -4.216075749 | -2.304155692 |
| H22  | -1.239665206 | -5.299349971 | -4.557357552 |
| H23  | -1.171674720 | -5.773670367 | 0.082215717  |
| H24  | -0.987028980 | -5.196664879 | 1.753788354  |
| H25  | -2.566999726 | 1.913640581  | 3.243251037  |
| H26  | -2.960786140 | -0.757855716 | 1.520186238  |
| H27  | -0.775240441 | 1.828942270  | 3.506437873  |
| H28  | -2.326865841 | 3.612210642  | 1.673243142  |
| N29  | 0.061230649  | -3.371551561 | -2.372774692 |
| N30  | -0.637648629 | -4.693654414 | -4.011411871 |
| N31  | 0.295387472  | 1.530714117  | 0.241164926  |
| O32  | 1.434799609  | -6.098800264 | 0.748722713  |
| O33  | 1.333846187  | -3.879331289 | 0.245619471  |
| O34  | -1.220655469 | -3.706081886 | 0.337515993  |
| O35  | -2.575713060 | -0.913093790 | 4.933173378  |
| S36  | 0.787581694  | 7.414001846  | 0.216921065  |
| S37  | -1.342726764 | 4.293175299  | -0.795373050 |
| S38  | 0.300318960  | 4.122707847  | 2.242634988  |
| S39  | 0.280460855  | 1.525622886  | -3.133230938 |
| S40  | 2.264749362  | 4.021545389  | -0.817816919 |
| S41  | -1.642144663 | -0.980112022 | -0.845732454 |
| S42  | -3.081853411 | 1.528783404  | 0.374017719  |
| S43  | 0.195745995  | -1.277801827 | 2.071205977  |
| S44  | 1.945782549  | -1.109979371 | -0.807039319 |
| S45  | 3.041247150  | 1.317103422  | 1.905382868  |
| V46  | 0.046138757  | -2.290502096 | 0.024596670  |

**FF. v2h6h2ch266coti.car\_2**

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 2.520718065  | 7.677928488  | 0.801489877  |
| C2   | 1.061769898  | -3.504818419 | -3.268420356 |
| C3   | 0.645423030  | -4.300207880 | -4.311791874 |
| C4   | -0.972581790 | -4.084656103 | -2.786443637 |
| C5   | -0.682684924 | -4.941099893 | 0.758453042  |
| C6   | 0.843576563  | -5.012179621 | 0.606769097  |
| C7   | -2.435079455 | -0.512702694 | 3.275528469  |
| C8   | -1.441697530 | 1.568833019  | 2.781829247  |
| Fe9  | 0.497018673  | 5.155542444  | 0.177909702  |
| Fe10 | -1.256612805 | 2.477131577  | 1.052299114  |
| Fe11 | 1.631463026  | 2.829779477  | 0.982580647  |
| Fe12 | 0.343469395  | 2.879738070  | -1.357425291 |
| Fe13 | 0.203442086  | 0.281694840  | -1.315280334 |
| Fe14 | -2.039030333 | -0.072613074 | 1.593807441  |
| Fe15 | 1.561667843  | 0.244270772  | 0.913241487  |
| H16  | 3.214385825  | 7.162112383  | 0.128893104  |
| H17  | 2.738239596  | 8.754654230  | 0.801869270  |
| H18  | 2.647678356  | 7.284864905  | 1.817191339  |
| H19  | 2.017085432  | -3.017239784 | -3.120351148 |
| H20  | 1.131145073  | -4.625560637 | -5.221865809 |
| H21  | -1.924846651 | -4.201836126 | -2.283103730 |
| H22  | -1.269673570 | -5.257669852 | -4.552390807 |
| H23  | -1.148432445 | -5.683254259 | 0.080222872  |
| H24  | -0.950899952 | -5.235602299 | 1.790052859  |
| H25  | -2.263551150 | 1.986540254  | 3.377530153  |
| H26  | -3.336847018 | -0.862853821 | 1.403825301  |
| H27  | -0.579024700 | 1.339553333  | 3.424670607  |
| H28  | -2.212717040 | 3.416291265  | 1.782264076  |
| N29  | 0.048151385  | -3.379673489 | -2.331423604 |
| N30  | -0.661322500 | -4.670570956 | -3.993414216 |
| N31  | 0.435051294  | 1.568530511  | 0.215532229  |
| O32  | 1.459910259  | -6.082436624 | 0.736763706  |
| O33  | 1.370706080  | -3.835950918 | 0.332677551  |
| O34  | -1.171272257 | -3.647633878 | 0.488004840  |
| O35  | -2.685970916 | -0.804471850 | 4.388799316  |
| S36  | 0.756407532  | 7.443884878  | 0.227386813  |
| S37  | -1.344644239 | 4.243044921  | -0.794736075 |
| S38  | 0.284620748  | 4.100416955  | 2.224491582  |
| S39  | 0.282335556  | 1.565662007  | -3.129052410 |
| S40  | 2.245080322  | 4.103157255  | -0.830646962 |
| S41  | -1.687485297 | -0.945477900 | -0.689465370 |
| S42  | -3.144824991 | 1.619776096  | 0.556696915  |
| S43  | 0.121728977  | -1.091506440 | 2.088980119  |
| S44  | 1.947068961  | -1.127106115 | -0.819569090 |
| S45  | 3.129975186  | 1.429445876  | 1.868092420  |
| V46  | 0.071085027  | -2.235715562 | 0.127515235  |

**FF-TS-GG. v2h26ch26h6contf\_1\_4619.23**

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 1.943430060  | 7.806868084  | 1.005570769  |
| C2   | 1.444838576  | -3.387051868 | -3.257697283 |
| C3   | 1.141979130  | -4.224325306 | -4.308650209 |
| C4   | -0.551187173 | -4.136263984 | -2.854760222 |
| C5   | -0.382208059 | -5.045412549 | 0.679561460  |
| C6   | 1.152016357  | -4.987378907 | 0.598297039  |
| C7   | -2.415580012 | -0.306593103 | 3.048776923  |
| C8   | -1.764257388 | 1.447080061  | 2.710440665  |
| Fe9  | 0.165832034  | 5.148870144  | 0.239166340  |
| Fe10 | -1.509294692 | 2.509636265  | 0.945450734  |
| Fe11 | 1.336897116  | 2.860762109  | 1.134130294  |
| Fe12 | 0.157283156  | 2.894248256  | -1.309286917 |
| Fe13 | 0.212821731  | 0.276418999  | -1.203636174 |
| Fe14 | -1.894968486 | -0.158010292 | 1.375585589  |
| Fe15 | 1.441956109  | 0.298684033  | 1.062389933  |
| H16  | 2.715182266  | 7.354256115  | 0.372914999  |
| H17  | 2.078059027  | 8.897246069  | 1.025325132  |
| H18  | 2.038359384  | 7.414359551  | 2.024902278  |
| H19  | 2.347228983  | -2.814190688 | -3.079619963 |
| H20  | 1.695764045  | -4.522254477 | -5.190630102 |
| H21  | -1.511355964 | -4.325621640 | -2.390527145 |
| H22  | -0.673850837 | -5.344856617 | -4.615522131 |



|     |              |              |              |
|-----|--------------|--------------|--------------|
| H23 | -0.742214350 | -5.841933869 | -0.000612615 |
| H24 | -0.666467692 | -5.345849239 | 1.706343667  |
| H25 | -2.659761709 | 1.897564302  | 3.144409572  |
| H26 | -2.954608914 | -1.217889098 | 1.461805736  |
| H27 | -0.931130108 | 1.433929788  | 3.420092244  |
| H28 | -2.513853601 | 3.510289502  | 1.496790112  |
| N29 | 0.386527639  | -3.343445672 | -2.365371059 |
| N30 | -0.141383882 | -4.701351834 | -4.041111434 |
| N31 | 0.220648091  | 1.524546103  | 0.354504056  |
| O32 | 1.858084060  | -5.996630670 | 0.752224306  |
| O33 | 1.593010181  | -3.769835520 | 0.357026138  |
| O34 | -0.962293269 | -3.801751472 | 0.355230985  |
| O35 | -2.804137595 | -0.709639349 | 4.091931318  |
| S36 | 0.244226209  | 7.443603345  | 0.321729756  |
| S37 | -1.606347139 | 4.195558505  | -0.834606035 |
| S38 | -0.142001377 | 4.097133804  | 2.277168452  |
| S39 | 0.241246945  | 1.516755176  | -3.035756639 |
| S40 | 2.004698998  | 4.156359366  | -0.664721716 |
| S41 | -1.616547279 | -1.112439153 | -0.806115483 |
| S42 | -3.249953866 | 1.375720910  | 0.351537180  |
| S43 | 0.152453386  | -1.241536328 | 2.125044744  |
| S44 | 2.036587883  | -0.992453822 | -0.669785682 |
| S45 | 2.887839315  | 1.556266211  | 2.079660887  |
| V46 | 0.196432712  | -2.289441242 | 0.110399500  |

### GG. v2h26ch26h6conta.car\_4

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 2.325540975  | 7.743401311  | 0.716586690  |
| C2   | 1.106914905  | -3.490772552 | -3.138272137 |
| C3   | 0.702324744  | -4.302020779 | -4.174439081 |
| C4   | -0.927471492 | -4.085780968 | -2.661536118 |
| C5   | -0.578507354 | -4.957468610 | 0.838621015  |
| C6   | 0.951228333  | -4.976166018 | 0.663065114  |
| C7   | -2.294547195 | -0.222276921 | 3.235849503  |
| C8   | -1.570579430 | 0.983153672  | 3.250743161  |
| Fe9  | 0.395034641  | 5.166607063  | 0.085264199  |
| Fe10 | -1.364152700 | 2.798121307  | 0.675123529  |
| Fe11 | 1.459957133  | 2.815102097  | 0.946710082  |
| Fe12 | 0.333414972  | 2.922733462  | -1.501904133 |
| Fe13 | 0.234696312  | 0.313625827  | -1.259768554 |
| Fe14 | -1.586944921 | 0.046982149  | 1.357529350  |
| Fe15 | 1.410884200  | 0.275840444  | 1.014890398  |
| H16  | 3.026625733  | 7.249942276  | 0.034079018  |
| H17  | 2.513288441  | 8.826093428  | 0.719668548  |
| H18  | 2.472696672  | 7.349566320  | 1.729102178  |
| H19  | 2.055169412  | -2.989737477 | -2.990849274 |
| H20  | 1.197586290  | -4.640656833 | -5.075475181 |
| H21  | -1.881707702 | -4.201383741 | -2.163063582 |
| H22  | -1.205232965 | -5.277832082 | -4.412598775 |
| H23  | -1.012782440 | -5.765589332 | 0.220000913  |
| H24  | -0.816371087 | -5.194653542 | 1.892399788  |
| H25  | -2.136734538 | 1.912778595  | 3.320037718  |
| H26  | -2.763532861 | -0.846840310 | 1.524947551  |
| H27  | -0.592940418 | 0.976365704  | 3.734988967  |
| H28  | -2.402537944 | 3.717544377  | 1.299938558  |
| N29  | 0.087451184  | -3.366761665 | -2.210535173 |
| N30  | -0.603240842 | -4.679926732 | -3.858251769 |
| N31  | 0.195121889  | 1.526430686  | 0.276267583  |
| O32  | 1.612456484  | -6.014463828 | 0.831572742  |
| O33  | 1.432556931  | -3.802610206 | 0.325493883  |
| O34  | -1.125950624 | -3.706148104 | 0.482594512  |
| O35  | -2.933836017 | -1.027192687 | 3.869380162  |
| S36  | 0.565777221  | 7.457444747  | 0.156887948  |
| S37  | -1.422597714 | 4.297435250  | -1.051529165 |
| S38  | 0.012559820  | 4.132529246  | 2.111043788  |
| S39  | 0.463059968  | 1.441440945  | -3.141889503 |
| S40  | 2.201676265  | 4.129662912  | -0.823195295 |
| S41  | -1.632543068 | -0.971310934 | -0.845785701 |
| S42  | -3.100359369 | 1.564427749  | 0.577369867  |
| S43  | 0.224184324  | -1.304612522 | 2.127888105  |
| S44  | 1.954570556  | -1.037260884 | -0.722839320 |
| S45  | 2.955772636  | 1.485513188  | 1.942642375  |
| V46  | 0.062020636  | -2.271276026 | 0.071245517  |

## HH. v2h2ch2co6htl.car\_2

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 2.184498564  | 7.764581525  | 0.456366953  |
| C2   | 1.111974922  | -3.650521755 | -3.238204872 |
| C3   | 0.623295688  | -4.441533941 | -4.254488465 |
| C4   | -0.869342874 | -4.266149965 | -2.602515485 |
| C5   | -0.346669515 | -5.052846536 | 0.881496500  |
| C6   | 1.182994592  | -4.966977827 | 0.723165804  |
| C7   | -2.075017172 | 0.439693989  | 3.022085235  |
| C8   | -1.445065415 | 1.770940105  | 3.172474065  |
| Fe9  | 0.241330157  | 5.123082094  | 0.085777990  |
| Fe10 | -1.478789792 | 2.687204086  | 1.286204257  |
| Fe11 | 1.374862612  | 2.766827512  | 0.958105610  |
| Fe12 | 0.056135587  | 2.779280400  | -1.298423884 |
| Fe13 | 0.089608972  | 0.243188716  | -1.263387914 |
| Fe14 | -1.495342441 | -0.027306818 | 1.062777650  |
| Fe15 | 1.355075356  | 0.206530165  | 0.989359890  |
| H16  | 2.868522281  | 7.278793144  | -0.248733488 |
| H17  | 2.336286572  | 8.852619307  | 0.426565091  |
| H18  | 2.394931225  | 7.402118752  | 1.469398758  |
| H19  | 2.067750286  | -3.146492081 | -3.164762210 |
| H20  | 1.039620712  | -4.758001333 | -5.202459550 |
| H21  | -1.777695528 | -4.393078033 | -2.026058303 |
| H22  | -1.298432436 | -5.413398629 | -4.353994698 |
| H23  | -0.717460759 | -5.889773448 | 0.259869711  |
| H24  | -0.576425500 | -5.302344007 | 1.934576390  |
| H25  | -1.961114681 | 2.370990863  | 3.935073184  |
| H26  | -2.527978595 | -1.067016598 | 1.414507263  |
| H27  | -0.382227389 | 1.662580329  | 3.409928703  |
| H28  | -2.592164187 | 3.535010457  | 1.871807601  |
| N29  | 0.176680070  | -3.551459798 | -2.223533441 |
| N30  | -0.648401134 | -4.833629848 | -3.835829419 |
| N31  | 0.040445219  | 1.443581072  | 0.300512576  |
| O32  | 1.915342960  | -5.953760396 | 0.896051057  |
| O33  | 1.583720413  | -3.758067143 | 0.395512752  |
| O34  | -0.969289921 | -3.839682142 | 0.521398099  |
| O35  | -2.842155850 | -0.149505503 | 3.750914134  |
| S36  | 0.409654033  | 7.412457086  | -0.007126599 |
| S37  | -1.647991254 | 4.163873612  | -0.740607754 |
| S38  | 0.165018625  | 4.200774251  | 2.213838082  |
| S39  | 0.095198739  | 1.426142185  | -3.069915343 |
| S40  | 1.966541034  | 4.023591980  | -0.896377109 |
| S41  | -1.590732538 | -1.202235270 | -0.932876627 |
| S42  | -3.126018402 | 1.378509860  | 0.582800497  |
| S43  | 0.169105202  | -1.321314850 | 2.171979395  |
| S44  | 1.860033665  | -1.029515421 | -0.802410019 |
| S45  | 2.927272497  | 1.412424791  | 1.853031670  |
| V46  | 0.132420009  | -2.330180332 | 0.116151352  |

## HH-TS-II. v2h2ch2co6htk\_1\_4593.18

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 2.663116731  | 7.627103672  | 0.392874321  |
| C2   | 0.893310089  | -3.749838790 | -3.223512020 |
| C3   | 0.353375538  | -4.515771301 | -4.233607662 |
| C4   | -1.116741596 | -4.242396247 | -2.573843496 |
| C5   | -0.649002774 | -4.999544500 | 0.932166350  |
| C6   | 0.881592366  | -5.008633927 | 0.761496752  |
| C7   | -1.945255936 | 0.588770987  | 2.868662984  |
| C8   | -1.357901751 | 1.862041416  | 3.197518731  |
| Fe9  | 0.572116815  | 5.104167716  | 0.041260247  |
| Fe10 | -1.335980047 | 2.753874821  | 1.232019196  |
| Fe11 | 1.548920660  | 2.702738688  | 0.942835139  |
| Fe12 | 0.239133686  | 2.785002721  | -1.355411665 |
| Fe13 | 0.107473513  | 0.230476177  | -1.275441884 |
| Fe14 | -1.556670540 | -0.000383175 | 1.085046532  |
| Fe15 | 1.384732425  | 0.151820407  | 0.950356787  |
| H16  | 3.325599450  | 7.097115842  | -0.300893689 |
| H17  | 2.879194559  | 8.703899975  | 0.360084370  |
| H18  | 2.838205448  | 7.256969143  | 1.410198388  |
| H19  | 1.876503117  | -3.298475569 | -3.162813556 |
| H20  | 0.744586910  | -4.859430317 | -5.182702937 |

|     |              |              |              |
|-----|--------------|--------------|--------------|
| H21 | -2.030916364 | -4.304740892 | -1.997131003 |
| H22 | -1.623725553 | -5.372955637 | -4.315873582 |
| H23 | -1.077183156 | -5.800145301 | 0.300812594  |
| H24 | -0.888867019 | -5.252580867 | 1.983515561  |
| H25 | -1.864482876 | 2.487711770  | 3.943921378  |
| H26 | -2.776063137 | -0.819183163 | 2.210633972  |
| H27 | -0.285050390 | 1.748097685  | 3.373675997  |
| H28 | -2.355325778 | 3.715132379  | 1.811199803  |
| N29 | -0.028328098 | -3.589872746 | -2.203803804 |
| N30 | -0.936887710 | -4.829500807 | -3.805398204 |
| N31 | 0.181331497  | 1.450529040  | 0.290520078  |
| O32 | 1.549175479  | -6.044126281 | 0.917772494  |
| O33 | 1.356917321  | -3.827480665 | 0.439786902  |
| O34 | -1.200778970 | -3.747517595 | 0.589264575  |
| O35 | -2.832149591 | -0.115285661 | 3.450302639  |
| S36 | 0.876844959  | 7.378472331  | -0.090732944 |
| S37 | -1.373307362 | 4.259441238  | -0.788722719 |
| S38 | 0.404147108  | 4.210955070  | 2.170364872  |
| S39 | 0.182153907  | 1.423972477  | -3.110010297 |
| S40 | 2.227903218  | 3.892915983  | -0.930163893 |
| S41 | -1.714001718 | -1.135353193 | -0.927877714 |
| S42 | -3.062052617 | 1.589858468  | 0.507468133  |
| S43 | 0.109139870  | -1.292111940 | 2.158281718  |
| S44 | 1.817374405  | -1.152763557 | -0.817809262 |
| S45 | 3.010934917  | 1.261745217  | 1.845305409  |
| V46 | -0.013111001 | -2.324721088 | 0.128404408  |

## II. v2h2ch2co6htk\_3\_4630.30

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 2.641067539  | 7.610192129  | 0.383577681  |
| C2   | 0.889554311  | -3.749192636 | -3.202417568 |
| C3   | 0.353631944  | -4.512184555 | -4.215714366 |
| C4   | -1.124327124 | -4.247002402 | -2.562127716 |
| C5   | -0.655666618 | -4.997579587 | 0.920334563  |
| C6   | 0.876763325  | -5.047938749 | 0.757638840  |
| C7   | -1.832313740 | 0.673986494  | 2.728988950  |
| C8   | -1.318831098 | 1.802971893  | 3.355138042  |
| Fe9  | 0.532383190  | 5.082652470  | 0.055936120  |
| Fe10 | -1.404026349 | 2.784597066  | 1.289136162  |
| Fe11 | 1.499652910  | 2.678274187  | 0.983567344  |
| Fe12 | 0.220462667  | 2.776982951  | -1.348817930 |
| Fe13 | 0.180925796  | 0.202708869  | -1.314876485 |
| Fe14 | -1.294226127 | 0.195868119  | 0.902926909  |
| Fe15 | 1.534114905  | 0.089195738  | 0.875672625  |
| H16  | 3.292611861  | 7.073762082  | -0.315882083 |
| H17  | 2.856769833  | 8.686651780  | 0.336331234  |
| H18  | 2.835110438  | 7.251592926  | 1.401166408  |
| H19  | 1.869152592  | -3.293384194 | -3.132501197 |
| H20  | 0.750308636  | -4.853171837 | -5.163567354 |
| H21  | -2.040755888 | -4.310011321 | -1.988888234 |
| H22  | -1.624212255 | -5.366865026 | -4.310545833 |
| H23  | -1.093496666 | -5.808600898 | 0.306338603  |
| H24  | -0.902960748 | -5.221758882 | 1.976408004  |
| H25  | -1.869214934 | 2.269456698  | 4.179871045  |
| H26  | -3.247765855 | -0.566237897 | 2.609530990  |
| H27  | -0.241983832 | 1.935816719  | 3.368586122  |
| H28  | -2.448515060 | 3.704484623  | 1.878505569  |
| N29  | -0.036747453 | -3.594854179 | -2.186849440 |
| N30  | -0.938526767 | -4.828196125 | -3.794076841 |
| N31  | 0.173510545  | 1.304292969  | 0.295362741  |
| O32  | 1.519192524  | -6.090854355 | 0.967540027  |
| O33  | 1.380590880  | -3.895934073 | 0.381281212  |
| O34  | -1.181535559 | -3.743899060 | 0.544863300  |
| O35  | -2.948385035 | 0.085795054  | 3.276572852  |
| S36  | 0.844917154  | 7.359168363  | -0.064913286 |
| S37  | -1.420372863 | 4.204396449  | -0.747406938 |
| S38  | 0.323128457  | 4.193452541  | 2.184348617  |
| S39  | 0.256904812  | 1.413868766  | -3.112842089 |
| S40  | 2.197698700  | 3.886222280  | -0.892050533 |
| S41  | -1.630031143 | -1.101112154 | -0.968298837 |
| S42  | -3.020359533 | 1.545617917  | 0.396539860  |
| S43  | 0.241921568  | -1.318358620 | 2.050315431  |
| S44  | 1.880080715  | -1.206477415 | -0.935133905 |

|     |             |              |             |
|-----|-------------|--------------|-------------|
| S45 | 3.069371696 | 1.295102825  | 1.809223607 |
| V46 | 0.054427646 | -2.353497944 | 0.041207780 |

### JJ. v26ch22h6chohtb\_car\_3

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 2.378156210  | 7.777780783  | 0.796755162  |
| C2   | 1.276323472  | -3.686164145 | -3.055997346 |
| C3   | 0.851287092  | -4.461967341 | -4.111003306 |
| C4   | -0.806271273 | -4.146141942 | -2.647460832 |
| C5   | -0.536411088 | -4.903871821 | 0.930893495  |
| C6   | 0.997693048  | -4.960351093 | 0.787961593  |
| C7   | -2.671318212 | -0.631811744 | 2.105581072  |
| C8   | -1.248639128 | 1.492621746  | 2.632064943  |
| Fe9  | 0.516344444  | 5.163156330  | 0.096781152  |
| Fe10 | -1.263016047 | 2.658596622  | 1.026556617  |
| Fe11 | 1.604238090  | 2.802994583  | 0.919758769  |
| Fe12 | 0.384777912  | 2.885859876  | -1.434587546 |
| Fe13 | 0.368726960  | 0.295259251  | -1.365088164 |
| Fe14 | -1.364772683 | 0.160120447  | 1.088088835  |
| Fe15 | 1.612671024  | 0.254806854  | 0.875581783  |
| H16  | 3.125598139  | 7.293017797  | 0.158857716  |
| H17  | 2.545084798  | 8.863702719  | 0.798556500  |
| H18  | 2.478230974  | 7.396744589  | 1.820035521  |
| H19  | 2.247207514  | -3.241643285 | -2.879821634 |
| H20  | 1.348717524  | -4.820759115 | -5.002949108 |
| H21  | -1.783935819 | -4.191964695 | -2.183851335 |
| H22  | -1.109797502 | -5.304910343 | -4.417552164 |
| H23  | -0.974738256 | -5.703855751 | 0.302501356  |
| H24  | -0.800158790 | -5.138421003 | 1.980596477  |
| H25  | -3.990192504 | 0.608666353  | 1.688110879  |
| H26  | -2.097048394 | 1.580696596  | 3.318373750  |
| H27  | -0.295994833 | 1.471982601  | 3.171675302  |
| H28  | -2.505313687 | -1.543725357 | 2.704471701  |
| H29  | -2.306824932 | 3.477574743  | 1.768878503  |
| N30  | 0.239048943  | -3.500386685 | -2.158867554 |
| N31  | -0.486234802 | -4.753155776 | -3.839536647 |
| N32  | 0.332111060  | 1.500831850  | 0.165599433  |
| O33  | 1.627577816  | -6.012754004 | 0.988545404  |
| O34  | 1.513058276  | -3.803997310 | 0.441128222  |
| O35  | -1.045595864 | -3.640343991 | 0.564269011  |
| O36  | -3.918225880 | -0.208471859 | 2.305216946  |
| S37  | 0.657696476  | 7.455663789  | 0.147654406  |
| S38  | -1.314816018 | 4.289262801  | -0.894736103 |
| S39  | 0.289471202  | 4.130448575  | 2.175866621  |
| S40  | 0.509662641  | 1.502372328  | -3.183948267 |
| S41  | 2.280743551  | 4.113948454  | -0.872159813 |
| S42  | -1.449552986 | -1.036356917 | -0.974848320 |
| S43  | -2.988044399 | 1.592301154  | 0.165409471  |
| S44  | 0.346345330  | -1.169927535 | 2.085792387  |
| S45  | 2.059772507  | -1.100085202 | -0.844051009 |
| S46  | 3.175096911  | 1.448687592  | 1.773926947  |
| V47  | 0.191261184  | -2.256031518 | 0.080969174  |

### JJ-TS-KK. v26ch22h6chohtd\_1\_4679.09

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 2.510074982  | 7.705014045  | 0.779884829  |
| C2   | 1.189462188  | -3.661358743 | -3.098954873 |
| C3   | 0.780453823  | -4.459680630 | -4.141436532 |
| C4   | -0.882838436 | -4.159232039 | -2.679715907 |
| C5   | -0.738405014 | -4.879925639 | 0.880212487  |
| C6   | 0.790551498  | -5.031096074 | 0.767378478  |
| C7   | -2.392398754 | -0.287626839 | 2.422446422  |
| C8   | -1.350979386 | 1.438144203  | 2.645144734  |
| Fe9  | 0.600310715  | 5.120868865  | 0.089814515  |
| Fe10 | -1.205393437 | 2.654726059  | 1.010100450  |
| Fe11 | 1.667085280  | 2.764237987  | 0.926432913  |
| Fe12 | 0.420625283  | 2.882572486  | -1.489648484 |
| Fe13 | 0.372825120  | 0.261026463  | -1.360860503 |
| Fe14 | -1.257553396 | 0.163774438  | 1.024169387  |
| Fe15 | 1.697668366  | 0.212240544  | 0.830544135  |
| H16  | 3.262546251  | 7.189111047  | 0.169795869  |
| H17  | 2.705532816  | 8.786053429  | 0.763179845  |

|     |              |              |              |
|-----|--------------|--------------|--------------|
| H18 | 2.576107683  | 7.343954085  | 1.812669883  |
| H19 | 2.150288076  | -3.192449540 | -2.928514179 |
| H20 | 1.285143718  | -4.821486498 | -5.027360725 |
| H21 | -1.859232917 | -4.222138344 | -2.215172992 |
| H22 | -1.161551084 | -5.351967291 | -4.432717380 |
| H23 | -1.214635667 | -5.646237857 | 0.234414226  |
| H24 | -1.045101611 | -5.105019856 | 1.918564487  |
| H25 | -3.938620472 | 0.518083045  | 1.740922136  |
| H26 | -2.224521581 | 1.773165733  | 3.211617139  |
| H27 | -0.472679507 | 1.318786866  | 3.294565016  |
| H28 | -2.073235557 | -0.942482509 | 3.243294787  |
| H29 | -2.242394432 | 3.536484279  | 1.672022774  |
| N30 | 0.149339392  | -3.484975098 | -2.201559723 |
| N31 | -0.550521129 | -4.775218315 | -3.864283764 |
| N32 | 0.427388447  | 1.457540718  | 0.162155759  |
| O33 | 1.353201545  | -6.113556766 | 1.006354452  |
| O34 | 1.382740217  | -3.919223972 | 0.397078764  |
| O35 | -1.160484708 | -3.588489617 | 0.511258671  |
| O36 | -3.729798678 | -0.074678758 | 2.525492932  |
| S37 | 0.798054266  | 7.410701719  | 0.097474118  |
| S38 | -1.254251411 | 4.278246837  | -0.890901285 |
| S39 | 0.364662984  | 4.092767496  | 2.176595652  |
| S40 | 0.414077748  | 1.466845027  | -3.208361879 |
| S41 | 2.342470280  | 4.048543842  | -0.897545351 |
| S42 | -1.500573287 | -1.015748472 | -0.959987585 |
| S43 | -2.918148310 | 1.573353115  | 0.133780984  |
| S44 | 0.441157227  | -1.203014953 | 2.033593676  |
| S45 | 2.088295289  | -1.173766302 | -0.890952583 |
| S46 | 3.238541298  | 1.405864264  | 1.772811020  |
| V47 | 0.164714280  | -2.292732478 | 0.034203206  |

### **KK. v26ch22h6chohtd.car\_3**

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 2.510074982  | 7.705014045  | 0.779884829  |
| C2   | 1.189462188  | -3.661358743 | -3.098954873 |
| C3   | 0.780453823  | -4.459680630 | -4.141436532 |
| C4   | -0.882838436 | -4.159232039 | -2.679715907 |
| C5   | -0.738405014 | -4.879925639 | 0.880212487  |
| C6   | 0.790551498  | -5.031096074 | 0.767378478  |
| C7   | -2.392398754 | -0.287626839 | 2.422446422  |
| C8   | -1.350979386 | 1.438144203  | 2.645144734  |
| Fe9  | 0.600310715  | 5.120868865  | 0.089814515  |
| Fe10 | -1.205393437 | 2.654726059  | 1.010100450  |
| Fe11 | 1.667085280  | 2.764237987  | 0.926432913  |
| Fe12 | 0.420625283  | 2.882572486  | -1.489648484 |
| Fe13 | 0.372825120  | 0.261026463  | -1.360860503 |
| Fe14 | -1.257553396 | 0.163774438  | 1.024169387  |
| Fe15 | 1.697668366  | 0.212240544  | 0.830544135  |
| H16  | 3.262546251  | 7.189111047  | 0.169795869  |
| H17  | 2.705532816  | 8.786053429  | 0.763179845  |
| H18  | 2.576107683  | 7.343954085  | 1.812669883  |
| H19  | 2.150288076  | -3.192449540 | -2.928514179 |
| H20  | 1.285143718  | -4.821486498 | -5.027360725 |
| H21  | -1.859232917 | -4.222138344 | -2.215172992 |
| H22  | -1.161551084 | -5.351967291 | -4.432717380 |
| H23  | -1.214635667 | -5.646237857 | 0.234414226  |
| H24  | -1.045101611 | -5.105019856 | 1.918564487  |
| H25  | -3.938620472 | 0.518083045  | 1.740922136  |
| H26  | -2.224521581 | 1.773165733  | 3.211617139  |
| H27  | -0.472679507 | 1.318786866  | 3.294565016  |
| H28  | -2.073235557 | -0.942482509 | 3.243294787  |
| H29  | -2.242394432 | 3.536484279  | 1.672022774  |
| N30  | 0.149339392  | -3.484975098 | -2.201559723 |
| N31  | -0.550521129 | -4.775218315 | -3.864283764 |
| N32  | 0.427388447  | 1.457540718  | 0.162155759  |
| O33  | 1.353201545  | -6.113556766 | 1.006354452  |
| O34  | 1.382740217  | -3.919223972 | 0.397078764  |
| O35  | -1.160484708 | -3.588489617 | 0.511258671  |
| O36  | -3.729798678 | -0.074678758 | 2.525492932  |
| S37  | 0.798054266  | 7.410701719  | 0.097474118  |
| S38  | -1.254251411 | 4.278246837  | -0.890901285 |
| S39  | 0.364662984  | 4.092767496  | 2.176595652  |
| S40  | 0.414077748  | 1.466845027  | -3.208361879 |

|     |              |              |              |
|-----|--------------|--------------|--------------|
| S41 | 2.342470280  | 4.048543842  | -0.897545351 |
| S42 | -1.500573287 | -1.015748472 | -0.959987585 |
| S43 | -2.918148310 | 1.573353115  | 0.133780984  |
| S44 | 0.441157227  | -1.203014953 | 2.033593676  |
| S45 | 2.088295289  | -1.173766302 | -0.890952583 |
| S46 | 3.238541298  | 1.405864264  | 1.772811020  |
| V47 | 0.164714280  | -2.292732478 | 0.034203206  |

### LL. v2hx2ch26hotg.car\_2

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 2.288843495  | 7.731934102  | -0.045299524 |
| C2   | 0.931125115  | -3.857441039 | -3.071909668 |
| C3   | 0.468465407  | -4.756546928 | -4.006481398 |
| C4   | -1.028828101 | -4.484375697 | -2.371084160 |
| C5   | -0.552418948 | -4.998064664 | 1.150395837  |
| C6   | 0.975426400  | -5.027980942 | 0.953360596  |
| C7   | -1.565226257 | 0.050473948  | 3.030447181  |
| C8   | -1.728482257 | 2.793710029  | 3.075958520  |
| Fe9  | 0.411411210  | 5.032925141  | -0.302694091 |
| Fe10 | -1.423055465 | 2.875078997  | 1.311592915  |
| Fe11 | 1.506583264  | 2.700343751  | 0.732010954  |
| Fe12 | 0.119652653  | 2.633251341  | -1.522445297 |
| Fe13 | 0.039246219  | 0.079150184  | -1.373540223 |
| Fe14 | -1.258040857 | 0.124883553  | 1.025054052  |
| Fe15 | 1.492078314  | 0.118282521  | 0.757767755  |
| H16  | 2.986182516  | 7.185130630  | -0.689517308 |
| H17  | 2.439477444  | 8.813045828  | -0.178018486 |
| H18  | 2.481439330  | 7.468814384  | 1.001665185  |
| H19  | 1.868224805  | -3.316978593 | -3.046119695 |
| H20  | 0.894861615  | -5.140357112 | -4.924458053 |
| H21  | -1.921634728 | -4.598851788 | -1.769020868 |
| H22  | -1.414268113 | -5.807071343 | -4.000777641 |
| H23  | -0.984900714 | -5.903451644 | 0.681536061  |
| H24  | -0.766434559 | -5.061182030 | 2.233652981  |
| H25  | -2.696905184 | 2.470679717  | 3.477162169  |
| H26  | -1.040077265 | 3.172681071  | 3.847980174  |
| H27  | -0.733909379 | 0.568270398  | 3.581240444  |
| H28  | -2.662936190 | 3.703332730  | 1.539244468  |
| N29  | -0.008163902 | -3.698277679 | -2.068177468 |
| N30  | -0.787974255 | -5.152310305 | -3.547147485 |
| N31  | 0.107088635  | 1.285544717  | 0.140290094  |
| O32  | 1.653079764  | -6.013723774 | 1.291007849  |
| O33  | 1.433558041  | -3.925309636 | 0.409185953  |
| O34  | -1.122130278 | -3.825054483 | 0.613307277  |
| O35  | -2.494875026 | -0.464148159 | 3.622748562  |
| S36  | 0.527553887  | 7.319497858  | -0.508969359 |
| S37  | -1.521120300 | 4.078637423  | -1.019322374 |
| S38  | 0.413560815  | 4.302365380  | 1.887081204  |
| S39  | 0.049743141  | 1.199565670  | -3.228176457 |
| S40  | 2.088326077  | 3.815707764  | -1.236498353 |
| S41  | -1.729270707 | -1.214538736 | -0.823880221 |
| S42  | -3.054527521 | 1.411050993  | 0.718097351  |
| S43  | 0.373122891  | -1.369419031 | 2.039799677  |
| S44  | 1.817085535  | -1.226045866 | -1.010514483 |
| S45  | 3.073869559  | 1.329959644  | 1.591172052  |
| V46  | 0.055162099  | -2.423198052 | 0.032305590  |

### LL-TS-MM. v2hx2ch26choth\_1\_4591.11

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 2.226667614  | 7.750794941  | 0.091875940  |
| C2   | 0.963065368  | -3.811306077 | -3.102534559 |
| C3   | 0.497335735  | -4.679381346 | -4.063661038 |
| C4   | -0.989067224 | -4.474525556 | -2.408360895 |
| C5   | -0.521388272 | -5.034673949 | 1.080124716  |
| C6   | 1.008999478  | -5.025575726 | 0.896987788  |
| C7   | -1.421657957 | 0.420796614  | 3.035472277  |
| C8   | -1.654499016 | 2.435478597  | 3.043217749  |
| Fe9  | 0.348907631  | 5.046725168  | -0.176027734 |
| Fe10 | -1.441559033 | 2.740368565  | 1.215414821  |
| Fe11 | 1.387985439  | 2.671310265  | 0.840615616  |
| Fe12 | 0.046563467  | 2.653636466  | -1.437734439 |
| Fe13 | 0.021532969  | 0.102131583  | -1.435996261 |

|      |              |              |              |
|------|--------------|--------------|--------------|
| Fe14 | -1.375922206 | 0.190814771  | 0.946783477  |
| Fe15 | 1.427385448  | 0.094144981  | 0.769405368  |
| H16  | 2.899897011  | 7.208803872  | -0.581107483 |
| H17  | 2.365748583  | 8.832848007  | -0.042031172 |
| H18  | 2.461973259  | 7.485060997  | 1.129251190  |
| H19  | 1.894982358  | -3.262570339 | -3.062566276 |
| H20  | 0.918754508  | -5.026988629 | -4.997082145 |
| H21  | -1.873859132 | -4.611203514 | -1.799099569 |
| H22  | -1.381266266 | -5.740018412 | -4.078374585 |
| H23  | -0.920961557 | -5.953070786 | 0.607459879  |
| H24  | -0.741003605 | -5.109001919 | 2.163905206  |
| H25  | -2.633507185 | 2.365468999  | 3.527556529  |
| H26  | -0.843122226 | 2.682631325  | 3.748118498  |
| H27  | -0.425720641 | 0.511860646  | 3.513659637  |
| H28  | -2.585501576 | 3.626980035  | 1.585997830  |
| N29  | 0.029619249  | -3.692830849 | -2.089446272 |
| N30  | -0.752749034 | -5.100328373 | -3.607233547 |
| N31  | 0.027092649  | 1.286858711  | 0.170475594  |
| O32  | 1.712277240  | -6.001112510 | 1.208195741  |
| O33  | 1.449012216  | -3.896486690 | 0.388535429  |
| O34  | -1.118154527 | -3.878624697 | 0.535637156  |
| O35  | -2.382758757 | -0.095055085 | 3.624379473  |
| S36  | 0.449972679  | 7.341027766  | -0.304829062 |
| S37  | -1.600474216 | 4.086943493  | -0.884179831 |
| S38  | 0.309178079  | 4.261360980  | 1.990484869  |
| S39  | 0.025136938  | 1.323851504  | -3.229133278 |
| S40  | 2.016009752  | 3.840697740  | -1.108103561 |
| S41  | -1.732360111 | -1.226672356 | -0.920389247 |
| S42  | -3.120370188 | 1.391355739  | 0.512956117  |
| S43  | 0.252294477  | -1.402665572 | 1.969991105  |
| S44  | 1.802289463  | -1.190749777 | -1.015324802 |
| S45  | 2.919830903  | 1.298305220  | 1.757947125  |
| V46  | 0.053390217  | -2.437414821 | -0.011233373 |

### MM. v2hx2ch26chote.car\_1

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 2.280806499  | 7.736981390  | -0.020787169 |
| C2   | 0.946208837  | -3.865942848 | -3.034943314 |
| C3   | 0.474768875  | -4.743738941 | -3.984815322 |
| C4   | -1.011114493 | -4.505320076 | -2.335309335 |
| C5   | -0.560137710 | -5.012293351 | 1.160179834  |
| C6   | 0.973806692  | -5.011176162 | 0.982539987  |
| C7   | -1.442596493 | 0.770529429  | 3.183824982  |
| C8   | -1.638306272 | 2.217744574  | 2.981016972  |
| Fe9  | 0.380515250  | 5.042949623  | -0.249374843 |
| Fe10 | -1.436282357 | 2.789394717  | 1.120740106  |
| Fe11 | 1.408799832  | 2.689100045  | 0.831034870  |
| Fe12 | 0.056914969  | 2.618416583  | -1.461448312 |
| Fe13 | 0.029269577  | 0.077143999  | -1.448052186 |
| Fe14 | -1.345584029 | 0.134283535  | 0.868759617  |
| Fe15 | 1.394402723  | 0.108571350  | 0.778470016  |
| H16  | 2.947725817  | 7.178410284  | -0.687654486 |
| H17  | 2.424966287  | 8.814428540  | -0.175658388 |
| H18  | 2.516791100  | 7.486492629  | 1.020719869  |
| H19  | 1.880984745  | -3.323008402 | -3.001374843 |
| H20  | 0.894837402  | -5.105542022 | -4.913927450 |
| H21  | -1.898947170 | -4.626574265 | -1.727382419 |
| H22  | -1.411555464 | -5.791015288 | -3.988607665 |
| H23  | -0.961712118 | -5.935635649 | 0.699752268  |
| H24  | -0.785608800 | -5.069231532 | 2.242864113  |
| H25  | -2.609791916 | 2.485394371  | 3.461992850  |
| H26  | -0.786363698 | 2.721038777  | 3.692373438  |
| H27  | -0.370038586 | 0.491861267  | 3.440344445  |
| H28  | -2.554590054 | 3.682288970  | 1.516398399  |
| N29  | 0.011706135  | -3.726929896 | -2.023827046 |
| N30  | -0.778015873 | -5.148703008 | -3.525446884 |
| N31  | 0.036059421  | 1.311477340  | 0.099857652  |
| O32  | 1.668715723  | -5.990378637 | 1.304864386  |
| O33  | 1.416782804  | -3.889288756 | 0.467031342  |
| O34  | -1.147244777 | -3.862634200 | 0.594490179  |
| O35  | -2.364021586 | -0.040459231 | 3.602971172  |
| S36  | 0.499380072  | 7.333438360  | -0.408055865 |
| S37  | -1.583747161 | 4.097419544  | -0.947048552 |

|     |              |              |              |
|-----|--------------|--------------|--------------|
| S38 | 0.308425835  | 4.281230245  | 1.927031717  |
| S39 | 0.030861204  | 1.275605809  | -3.244427478 |
| S40 | 2.036866600  | 3.796365942  | -1.148028194 |
| S41 | -1.741613883 | -1.238717047 | -0.923319739 |
| S42 | -3.090224784 | 1.457486747  | 0.482412815  |
| S43 | 0.183547803  | -1.366345722 | 1.992318506  |
| S44 | 1.790183952  | -1.219403903 | -0.987494430 |
| S45 | 2.899504180  | 1.305183036  | 1.763890326  |
| V46 | 0.024664905  | -2.430898231 | 0.021104175  |

### NN. v2hchoh6hchohtg\_car\_2

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 2.058483512  | 7.798709530  | 0.120992555  |
| C2   | 1.359431407  | -3.811914847 | -3.180321590 |
| C3   | 0.999228974  | -4.699978606 | -4.165328984 |
| C4   | -0.658484945 | -4.465263375 | -2.684321361 |
| C5   | -0.403985762 | -5.018546796 | 0.926649542  |
| C6   | 1.129106149  | -5.088972249 | 0.762801917  |
| C7   | -2.159942513 | 2.628864815  | 2.994652746  |
| C8   | -0.846239536 | -0.003408658 | 2.626323644  |
| Fe9  | 0.240691194  | 5.031129704  | -0.191279055 |
| Fe10 | -1.569524587 | 2.817013925  | 1.244168363  |
| Fe11 | 1.533524487  | 2.820809289  | 0.804824334  |
| Fe12 | 0.236164000  | 2.592475229  | -1.446581113 |
| Fe13 | 0.298182043  | -0.009870407 | -1.604440633 |
| Fe14 | -1.134062134 | 0.141809641  | 0.716606039  |
| Fe15 | 1.775377201  | 0.125848712  | 0.565275475  |
| H16  | 2.790771691  | 7.265783011  | -0.496805990 |
| H17  | 2.167506678  | 8.881564283  | -0.035014502 |
| H18  | 2.246061273  | 7.568346421  | 1.176804915  |
| H19  | 2.277512236  | -3.253277453 | -3.052342660 |
| H20  | 1.526262068  | -5.076246772 | -5.032310367 |
| H21  | -1.609933153 | -4.583596582 | -2.182268651 |
| H22  | -0.861388402 | -5.773738326 | -4.355405329 |
| H23  | -0.845211350 | -5.924098989 | 0.464600852  |
| H24  | -0.636430244 | -5.070103304 | 2.009003426  |
| H25  | -2.480965681 | -0.917970353 | 3.050219405  |
| H26  | -3.628048419 | 1.606634739  | 2.514240057  |
| H27  | -2.765499580 | 3.700129559  | 1.371902948  |
| H28  | -1.727411361 | 3.140973597  | 3.875696134  |
| H29  | -0.095282923 | 0.571949478  | 3.181047054  |
| N30  | 0.323287917  | -3.678362670 | -2.272129977 |
| N31  | -0.294353988 | -5.111721104 | -3.839029537 |
| N32  | 0.290894840  | 1.138128789  | 0.007208772  |
| O33  | 1.774641288  | -6.093914730 | 1.104636524  |
| O34  | 1.640734287  | -3.995472686 | 0.239055193  |
| O35  | -0.945491720 | -3.853239159 | 0.352459007  |
| O36  | -3.319811968 | 2.061629171  | 3.367695561  |
| O37  | -1.711715407 | -0.556902891 | 3.537436250  |
| S38  | 0.314512209  | 7.324285750  | -0.360300514 |
| S39  | -1.542288632 | 3.917928517  | -1.034957497 |
| S40  | 0.153045553  | 4.179010956  | 2.008600248  |
| S41  | 0.243734559  | 1.382629660  | -3.320933279 |
| S42  | 2.051625618  | 4.036536940  | -1.089903135 |
| S43  | -1.514961428 | -1.305137605 | -1.086544569 |
| S44  | -3.039590327 | 1.219508604  | 0.444003642  |
| S45  | 0.680672546  | -1.373227831 | 1.837992189  |
| S46  | 2.195071775  | -1.248866952 | -1.165898825 |
| S47  | 3.160233259  | 1.466614488  | 1.544244331  |
| V48  | 0.323881633  | -2.504488608 | -0.253030467 |

### NN-TS-OO. v2hchoh6hchohtq\_orig

|     |        |        |        |
|-----|--------|--------|--------|
| C1  | 2.619  | 7.666  | -0.079 |
| C2  | 1.108  | -3.938 | -3.071 |
| C3  | 0.693  | -4.839 | -4.024 |
| C4  | -0.945 | -4.448 | -2.556 |
| C5  | -0.769 | -4.955 | 1.047  |
| C6  | 0.760  | -5.115 | 0.904  |
| C7  | -1.793 | 2.444  | 2.852  |
| C8  | -0.968 | 0.530  | 2.687  |
| Fe9 | 0.623  | 4.993  | -0.307 |



|      |        |        |        |
|------|--------|--------|--------|
| Fe10 | -1.352 | 2.852  | 1.038  |
| Fe11 | 1.599  | 2.621  | 0.734  |
| Fe12 | 0.318  | 2.611  | -1.593 |
| Fe13 | 0.252  | 0.044  | -1.552 |
| Fe14 | -1.133 | 0.157  | 0.794  |
| Fe15 | 1.626  | 0.032  | 0.620  |
| H16  | 3.331  | 7.075  | -0.667 |
| H17  | 2.792  | 8.735  | -0.264 |
| H18  | 2.769  | 7.457  | 0.986  |
| H19  | 2.062  | -3.437 | -2.958 |
| H20  | 1.194  | -5.274 | -4.878 |
| H21  | -1.898 | -4.492 | -2.046 |
| H22  | -1.229 | -5.802 | -4.175 |
| H23  | -1.257 | -5.851 | 0.618  |
| H24  | -1.019 | -4.941 | 2.127  |
| H25  | -2.268 | -0.797 | 3.123  |
| H26  | -3.531 | 1.881  | 2.458  |
| H27  | -2.413 | 3.902  | 1.265  |
| H28  | -1.201 | 2.807  | 3.706  |
| H29  | -0.023 | 0.856  | 3.129  |
| N30  | 0.082  | -3.707 | -2.173 |
| N31  | -0.621 | -5.158 | -3.685 |
| N32  | 0.291  | 1.261  | 0.016  |
| O33  | 1.339  | -6.136 | 1.315  |
| O34  | 1.325  | -4.086 | 0.323  |
| O35  | -1.235 | -3.778 | 0.423  |
| O36  | -3.066 | 2.233  | 3.278  |
| O37  | -1.644 | -0.220 | 3.610  |
| S38  | 0.861  | 7.269  | -0.578 |
| S39  | -1.307 | 4.093  | -1.136 |
| S40  | 0.432  | 4.197  | 1.878  |
| S41  | 0.273  | 1.248  | -3.357 |
| S42  | 2.297  | 3.756  | -1.177 |
| S43  | -1.589 | -1.179 | -1.112 |
| S44  | -2.989 | 1.402  | 0.355  |
| S45  | 0.453  | -1.483 | 1.810  |
| S46  | 1.962  | -1.334 | -1.123 |
| S47  | 3.151  | 1.237  | 1.578  |
| V48  | 0.081  | -2.486 | -0.165 |

## OO. v2hchoh6hchohtj\_2\_4790.51

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 2.311754082  | 7.759681475  | 0.093450867  |
| C2   | 1.284560926  | -3.829397257 | -3.142987071 |
| C3   | 0.913535587  | -4.727627576 | -4.115915954 |
| C4   | -0.747997929 | -4.432160577 | -2.652101729 |
| C5   | -0.571589782 | -5.005519486 | 0.942487907  |
| C6   | 0.962330616  | -5.093574541 | 0.807128868  |
| C7   | -1.854096039 | 2.038820517  | 3.033002155  |
| C8   | -1.185909620 | 0.732608907  | 2.834027502  |
| Fe9  | 0.434607615  | 5.031549687  | -0.208195606 |
| Fe10 | -1.450237066 | 2.770936640  | 0.971234330  |
| Fe11 | 1.533294536  | 2.694483012  | 0.771730222  |
| Fe12 | 0.248710044  | 2.664473067  | -1.539488085 |
| Fe13 | 0.242736559  | 0.077529024  | -1.553142692 |
| Fe14 | -1.088253739 | 0.082022368  | 0.804713445  |
| Fe15 | 1.596531205  | 0.078965076  | 0.646836190  |
| H16  | 3.051013694  | 7.209781137  | -0.500491862 |
| H17  | 2.443535543  | 8.838785351  | -0.068114819 |
| H18  | 2.463081984  | 7.535012765  | 1.156117542  |
| H19  | 2.217669049  | -3.295507942 | -3.015233242 |
| H20  | 1.435010519  | -5.126029467 | -4.976185858 |
| H21  | -1.701665675 | -4.527773215 | -2.148834081 |
| H22  | -0.967649723 | -5.767697971 | -4.297818520 |
| H23  | -1.018812031 | -5.911214747 | 0.489065794  |
| H24  | -0.829920707 | -5.025897423 | 2.019199437  |
| H25  | -2.206108918 | -0.925563472 | 3.018283612  |
| H26  | -3.620903132 | 1.606161331  | 2.534209884  |
| H27  | -2.545171244 | 3.744350605  | 1.346610159  |
| H28  | -1.299743470 | 2.748487558  | 3.659014958  |
| H29  | -0.109838905 | 0.858587473  | 3.018728552  |
| N30  | 0.244818236  | -3.657637217 | -2.247644409 |
| N31  | -0.389764738 | -5.107617314 | -3.791675896 |

|     |              |              |              |
|-----|--------------|--------------|--------------|
| N32 | 0.236816534  | 1.236744187  | 0.001624245  |
| O33 | 1.585717889  | -6.098498456 | 1.190811448  |
| O34 | 1.481854885  | -4.020985803 | 0.258526958  |
| O35 | -1.080943965 | -3.834174210 | 0.341891976  |
| O36 | -3.221025250 | 2.036460816  | 3.335477781  |
| O37 | -1.759167121 | -0.334850675 | 3.648858099  |
| S38 | 0.575549205  | 7.312893646  | -0.429394476 |
| S39 | -1.431786367 | 4.103657903  | -1.102670609 |
| S40 | 0.243337548  | 4.141622467  | 1.947206246  |
| S41 | 0.247108754  | 1.319609094  | -3.329960541 |
| S42 | 2.175646516  | 3.891891618  | -1.108388964 |
| S43 | -1.546039821 | -1.228600311 | -1.106476407 |
| S44 | -2.986992444 | 1.286798381  | 0.330538398  |
| S45 | 0.412003701  | -1.449752006 | 1.828612571  |
| S46 | 2.006213831  | -1.235583625 | -1.113893947 |
| S47 | 3.097154363  | 1.297594827  | 1.608456758  |
| V48 | 0.169017096  | -2.463832327 | -0.189258528 |

### PP. bhhohcchoh.car\_6

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 2.432430987  | 7.574930216  | 0.177788667  |
| C2   | 1.181257746  | -4.020298963 | -3.190712773 |
| C3   | 0.749685716  | -4.844297335 | -4.205531149 |
| C4   | -0.872359384 | -4.518420547 | -2.705492038 |
| C5   | -0.492777378 | -5.052560109 | 0.981542914  |
| C6   | 1.028862476  | -5.157719263 | 0.782925937  |
| C7   | -2.098058259 | 2.390150570  | 2.979760633  |
| C8   | -1.294578252 | 1.188213675  | 2.843795918  |
| Fe9  | 0.556345343  | 4.895177730  | -0.002661425 |
| Fe10 | -1.210724739 | 2.617134213  | 1.120221282  |
| Fe11 | 1.819832186  | 2.584122997  | 0.764220762  |
| Fe12 | 0.323568892  | 2.580434019  | -1.442957030 |
| Fe13 | 0.257086362  | 0.022012405  | -1.476196263 |
| Fe14 | -1.058665356 | 0.105147843  | 0.907449686  |
| Fe15 | 1.814724837  | 0.046114594  | 0.605070601  |
| H16  | 3.057998791  | 6.993279754  | -0.508285452 |
| H17  | 2.588484060  | 8.647752020  | -0.003473387 |
| H18  | 2.713866592  | 7.339336186  | 1.210796551  |
| H19  | 2.145526424  | -3.546694033 | -3.056882609 |
| H20  | 1.233787834  | -5.223749579 | -5.096139093 |
| H21  | -1.836291573 | -4.579726820 | -2.215655165 |
| H22  | -1.192351972 | -5.750107369 | -4.427291322 |
| H23  | -0.981512399 | -5.840643421 | 0.377126464  |
| H24  | -0.730438877 | -5.277008497 | 2.038009921  |
| H25  | -2.992152723 | 0.275861704  | 2.790682900  |
| H26  | -3.716842352 | 1.923285292  | 2.060586125  |
| H27  | -2.255080188 | 3.598519087  | 1.528900970  |
| H28  | -1.776245578 | 3.150427667  | 3.689954882  |
| H29  | -0.356276472 | 1.069293117  | 3.385130891  |
| N30  | 0.166328394  | -3.827840052 | -2.269854406 |
| N31  | -0.570611973 | -5.161314041 | -3.885656205 |
| N32  | 0.345570057  | 1.242264622  | 0.028047005  |
| O33  | 1.644027598  | -6.214375336 | 0.997085566  |
| O34  | 1.559821425  | -4.023357346 | 0.372988973  |
| O35  | -0.967377437 | -3.779076257 | 0.630288091  |
| O36  | -3.500030761 | 2.168386550  | 3.023041215  |
| O37  | -2.058044090 | -0.036410019 | 2.814245227  |
| S38  | 0.629126781  | 7.182503487  | -0.097854786 |
| S39  | -1.343347028 | 3.976631661  | -0.840982949 |
| S40  | 0.550214264  | 3.918475991  | 2.110333406  |
| S41  | 0.252684080  | 1.260156894  | -3.257812867 |
| S42  | 2.237306951  | 3.869042357  | -1.116099074 |
| S43  | -1.457610757 | -1.286229856 | -0.904558380 |
| S44  | -2.889753770 | 1.360714128  | 0.183222730  |
| S45  | 0.599349037  | -1.266906815 | 1.980150769  |
| S46  | 2.003482576  | -1.343599983 | -1.149621541 |
| S47  | 3.466069216  | 1.216667732  | 1.402486785  |
| V48  | 0.293693767  | -2.445674807 | 0.067877134  |

### QQ. bhhohcchoh.car\_10

|    |             |             |             |
|----|-------------|-------------|-------------|
| C1 | 2.600918850 | 7.620377070 | 0.151858862 |
|----|-------------|-------------|-------------|

|      |              |              |              |
|------|--------------|--------------|--------------|
| C2   | 1.190346627  | -4.107881441 | -3.160666873 |
| C3   | 0.677024880  | -4.883949227 | -4.175528790 |
| C4   | -0.895523281 | -4.444123787 | -2.651295706 |
| C5   | -0.288700114 | -5.246955725 | 0.911056147  |
| C6   | 1.235084732  | -5.245045319 | 0.670274658  |
| C7   | -2.536664038 | 2.658324768  | 3.305200868  |
| C8   | -1.416587309 | 1.801904386  | 2.680226632  |
| Fe9  | 0.677038877  | 4.935027561  | -0.182968619 |
| Fe10 | -1.054734190 | 2.318908458  | 0.725178062  |
| Fe11 | 1.801853653  | 2.590866085  | 0.658682156  |
| Fe12 | 0.423916635  | 2.630503829  | -1.652435578 |
| Fe13 | 0.286626700  | -0.005473698 | -1.510182353 |
| Fe14 | -1.342246740 | -0.266378761 | 0.875569085  |
| Fe15 | 1.600733734  | 0.023380509  | 0.753534317  |
| H16  | 3.263426442  | 7.104653082  | -0.552207410 |
| H17  | 2.744354315  | 8.706795571  | 0.062106177  |
| H18  | 2.849826669  | 7.311103698  | 1.174285741  |
| H19  | 2.193210942  | -3.722338184 | -3.029622626 |
| H20  | 1.112713050  | -5.288548599 | -5.080017075 |
| H21  | -1.850564826 | -4.429116056 | -2.142143830 |
| H22  | -1.343352804 | -5.611978023 | -4.379732039 |
| H23  | -0.728075234 | -6.111820360 | 0.377850612  |
| H24  | -0.469949580 | -5.408400628 | 1.991697184  |
| H25  | -2.835952751 | 0.443118657  | 2.794523542  |
| H26  | -3.809116749 | 2.063870507  | 1.921864472  |
| H27  | -2.402453625 | 3.716690004  | 3.037292052  |
| H28  | -2.523787633 | 2.576376193  | 4.404105199  |
| H29  | -0.491669671 | 1.859626781  | 3.259212690  |
| N30  | 0.204244925  | -3.843557444 | -2.226629900 |
| N31  | -0.660568793 | -5.095090222 | -3.837885350 |
| N32  | 0.444138105  | 1.341261715  | 0.039537286  |
| O33  | 1.924187661  | -6.260228271 | 0.867698208  |
| O34  | 1.675001065  | -4.081210110 | 0.249066175  |
| O35  | -0.884179078 | -4.040164347 | 0.487599421  |
| O36  | -3.848592068 | 2.174627816  | 2.917761880  |
| O37  | -1.850488169 | 0.374830825  | 2.802684734  |
| S38  | 0.814328623  | 7.233874857  | -0.231402060 |
| S39  | -1.247266872 | 4.019281786  | -1.061864200 |
| S40  | 0.547720757  | 3.971392360  | 1.896937155  |
| S41  | 0.294830092  | 1.229241823  | -3.358165221 |
| S42  | 2.374999397  | 3.816581079  | -1.214950254 |
| S43  | -1.513039188 | -1.426118243 | -1.065083764 |
| S44  | -2.891607722 | 1.250459043  | 0.050553792  |
| S45  | 0.359436319  | -1.482371525 | 1.930465111  |
| S46  | 2.073834488  | -1.324454090 | -0.990520803 |
| S47  | 3.253274959  | 1.160708476  | 1.562692079  |
| V48  | 0.262047936  | -2.608582875 | -0.056211850 |

**Fig 15. Formation of methane: reactant. v2h6ch33bhtia\_1\_4418.25**

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 1.817939456  | 7.902699325  | 0.761032507  |
| C2   | 1.005786278  | -3.732751444 | -2.985727957 |
| C3   | 0.490114144  | -4.495335038 | -4.005883143 |
| C4   | -1.103776061 | -4.019061450 | -2.513910332 |
| C5   | -0.315236505 | -5.124854586 | 1.062778773  |
| C6   | 1.202183847  | -5.159602985 | 0.786345485  |
| C7   | -1.781975010 | 0.645514626  | 3.064776494  |
| Fe8  | 0.116525818  | 5.216267056  | 0.027689478  |
| Fe9  | -1.730467564 | 3.393521185  | 0.743199943  |
| Fe10 | 1.163131542  | 2.857623564  | 0.959480786  |
| Fe11 | 0.029612348  | 2.844685301  | -1.436193363 |
| Fe12 | 0.017422936  | 0.193905697  | -1.157054096 |
| Fe13 | -1.579504747 | 0.663099302  | 1.044002779  |
| Fe14 | 1.505596500  | 0.275439437  | 0.915816846  |
| H15  | 2.625965221  | 7.436931317  | 0.184995178  |
| H16  | 1.958403378  | 8.993455492  | 0.769023276  |
| H17  | 1.847254088  | 7.527415376  | 1.791213490  |
| H18  | 2.012985914  | -3.369327002 | -2.836415296 |
| H19  | 0.934631672  | -4.919522334 | -4.896586629 |
| H20  | -2.064659521 | -3.985159828 | -2.017666443 |
| H21  | -1.540734151 | -5.182481052 | -4.243298334 |
| H22  | -0.793168972 | -5.973781920 | 0.540106227  |
| H23  | -0.489446365 | -5.276243361 | 2.143517281  |

|     |              |              |              |
|-----|--------------|--------------|--------------|
| H24 | -0.769368207 | 0.611223022  | 3.495984121  |
| H25 | -2.359229190 | -0.235020402 | 3.390918911  |
| H26 | -2.754097624 | 4.362027868  | 1.227424180  |
| H27 | -2.281848085 | 1.548241008  | 3.446394261  |
| H28 | -0.168482429 | -1.129285540 | 2.740544250  |
| N29 | 0.005296270  | -3.444319651 | -2.069807756 |
| N30 | -0.859001776 | -4.672367213 | -3.693972231 |
| N31 | 0.010550979  | 1.386394470  | 0.316204792  |
| O32 | 1.860321605  | -6.189524952 | 1.021677597  |
| O33 | 1.646543824  | -4.033628081 | 0.292723983  |
| O34 | -0.885781094 | -3.903704511 | 0.647864728  |
| S35 | 0.168295993  | 7.514411000  | -0.021331795 |
| S36 | -1.639753495 | 4.431327484  | -1.200165175 |
| S37 | -0.215055248 | 4.316828593  | 2.136190289  |
| S38 | 0.038566307  | 1.303220632  | -3.056086690 |
| S39 | 1.905249282  | 4.118548653  | -0.857572436 |
| S40 | -1.737186990 | -1.126121588 | -0.315572897 |
| S41 | -3.281524073 | 1.902663086  | 0.746392068  |
| S42 | 0.973027341  | -1.588659832 | 2.181151705  |
| S43 | 1.890261755  | -1.060095629 | -0.905443807 |
| S44 | 2.903162466  | 1.686896877  | 1.776756846  |
| V45 | 0.221468144  | -2.511491972 | -0.001517894 |

**Fig 15. Formation of methane: TS v2h6ch33bhth\_1\_4401.60**

|      |               |              |              |
|------|---------------|--------------|--------------|
| C1   | 1.888559243   | 7.871776988  | 0.708847747  |
| C2   | 0.948752117   | -3.789985756 | -3.007225519 |
| C3   | 0.423178265   | -4.560580713 | -4.018708203 |
| C4   | -1.146009177  | -4.097859585 | -2.497711697 |
| C5   | -0.430164159  | -4.995681019 | 1.058344973  |
| C6   | 1.092812923   | -4.997839282 | 0.8040111046 |
| C7   | -1.577913544  | 0.597152291  | 3.354401833  |
| Fe8  | 0.133512591   | 5.179112345  | 0.023354032  |
| Fe9  | -1.566913428  | 3.074400278  | 0.672555800  |
| Fe10 | 1.244834790   | 2.817395621  | 0.926059124  |
| Fe11 | 0.079551771   | 2.912832919  | -1.524396408 |
| Fe12 | 0.067622846   | 0.244482814  | -1.279971834 |
| Fe13 | -1.300888664  | 0.321336349  | 1.193815026  |
| Fe14 | 1.530322254   | 0.277237035  | 0.861584365  |
| H15  | 2.679141857   | 7.407469957  | 0.108478756  |
| H16  | 2.017407291   | 8.963071043  | 0.701649342  |
| H17  | 1.961170950   | 7.507419411  | 1.740541185  |
| H18  | 1.956863161   | -3.417550281 | -2.880486306 |
| H19  | 0.853220887   | -4.975660016 | -4.921427510 |
| H20  | -2.098542145  | -4.071758850 | -1.986483310 |
| H21  | -1.606478557  | -5.264268214 | -4.219300573 |
| H22  | -0.877743177  | -5.851052161 | 0.517425659  |
| H23  | -0.607805409  | -5.163866965 | 2.137206146  |
| H24  | -0.7114037966 | 0.708866972  | 4.025180370  |
| H25  | -2.287303552  | -0.130542582 | 3.775027282  |
| H26  | -2.651404352  | 3.977300134  | 1.220520295  |
| H27  | -2.065934341  | 1.571015938  | 3.278729428  |
| H28  | -0.529933848  | -0.518498294 | 2.673960248  |
| N29  | -0.037279186  | -3.509493646 | -2.073349100 |
| N30  | -0.917246883  | -4.753128855 | -3.680220500 |
| N31  | 0.103370376   | 1.418603307  | 0.311726058  |
| O32  | 1.777666279   | -6.012326094 | 1.021363821  |
| O33  | 1.533067810   | -3.851231690 | 0.347659868  |
| O34  | -1.029527179  | -3.784309305 | 0.650004132  |
| S35  | 0.212236045   | 7.477781060  | -0.010155665 |
| S36  | -1.629304058  | 4.386987195  | -1.191085993 |
| S37  | -0.123589256  | 4.219822993  | 2.114553310  |
| S38  | 0.080654409   | 1.415966266  | -3.155335756 |
| S39  | 1.946201934   | 4.129743612  | -0.874637737 |
| S40  | -1.750443009  | -1.086856411 | -0.685412016 |
| S41  | -3.123289939  | 1.542374038  | 0.762850728  |
| S42  | 0.600680361   | -1.344069086 | 2.148940170  |
| S43  | 1.901843646   | -1.085760717 | -0.917329868 |
| S44  | 2.942520357   | 1.627957387  | 1.780665800  |
| V45  | 0.096559666   | -2.387786431 | 0.003781453  |

**Fig 15. Formation of methane: product. v2h6ch33bhth3delch4.car\_3**

|      |              |              |              |
|------|--------------|--------------|--------------|
| C1   | 1.540970265  | 7.920538702  | 0.773449351  |
| C2   | 0.976370634  | -3.991124742 | -2.308261196 |
| C3   | 0.456343969  | -4.788539472 | -3.304329479 |
| C4   | -1.134604421 | -4.208820761 | -1.847688897 |
| C5   | -0.809511920 | -4.663510427 | 1.733298916  |
| C6   | 0.732087399  | -4.682791464 | 1.688853723  |
| Fe7  | -0.169034080 | 5.190828659  | 0.055471884  |
| Fe8  | -1.739251230 | 3.141437684  | 0.985191296  |
| Fe9  | 1.108664716  | 2.925280637  | 1.169299224  |
| Fe10 | 0.003215230  | 2.797105055  | -1.273952207 |
| Fe11 | 0.149352465  | 0.221249097  | -1.097421579 |
| Fe12 | -1.390266374 | 0.431483105  | 1.058026346  |
| Fe13 | 1.235264468  | 0.365848790  | 1.293645432  |
| H14  | 2.378007210  | 7.411885607  | 0.281177811  |
| H15  | 1.686556060  | 9.008203322  | 0.708144145  |
| H16  | 1.511354322  | 7.624147982  | 1.828871574  |
| H17  | 1.991936151  | -3.640457672 | -2.167101167 |
| H18  | 0.898001625  | -5.254597667 | -4.177373214 |
| H19  | -2.099556299 | -4.125582061 | -1.365959247 |
| H20  | -1.591422114 | -5.419225631 | -3.545197510 |
| H21  | -1.179993702 | -5.560998226 | 1.199536591  |
| H22  | -1.117727591 | -4.770689355 | 2.793397453  |
| H23  | -2.909878408 | 4.011237194  | 1.371583610  |
| N24  | -0.022000270 | -3.639621388 | -1.416545314 |
| N25  | -0.898706951 | -4.923472613 | -2.997122381 |
| N26  | -0.013103326 | 1.511049961  | 0.312005372  |
| O27  | 1.395477563  | -5.681814445 | 2.009377338  |
| O28  | 1.232725596  | -3.533148275 | 1.285642801  |
| O29  | -1.327339937 | -3.479274622 | 1.180376004  |
| S30  | -0.063360377 | 7.482610338  | -0.076683245 |
| S31  | -1.847259104 | 4.155762714  | -1.067497072 |
| S32  | -0.323265192 | 4.340294976  | 2.215513725  |
| S33  | 0.230274551  | 1.319563953  | -2.962076495 |
| S34  | 1.752750193  | 4.134999209  | -0.668424172 |
| S35  | -1.703717523 | -0.964750355 | -0.656466143 |
| S36  | -3.034306088 | 1.572688592  | 1.840557800  |
| S37  | -0.260375062 | -0.823757191 | 2.554076782  |
| S38  | 1.829456592  | -1.087017705 | -0.369928309 |
| S39  | 2.585460482  | 1.781550324  | 2.326485599  |
| V40  | -0.059589520 | -2.108571829 | 0.638044853  |