Role of Solvent (THF) in H₂–Splitting Barrier
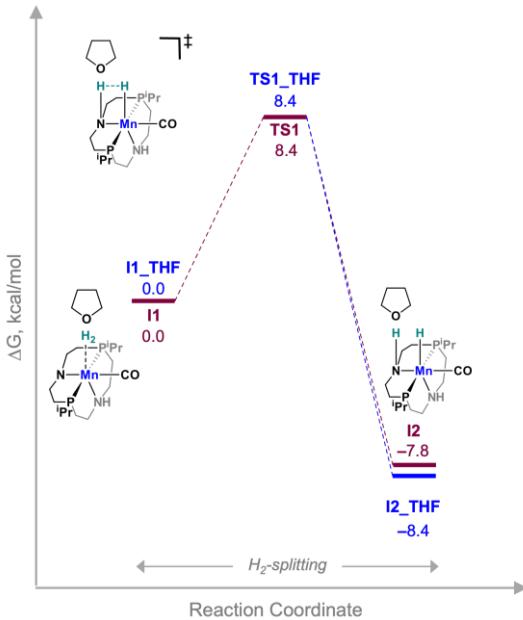

Figure S1. Role of explicit solvent (THF) on the H₂–splitting barrier of **2Mn**.

**Conformational Analysis of 2Mn and 3Fe**
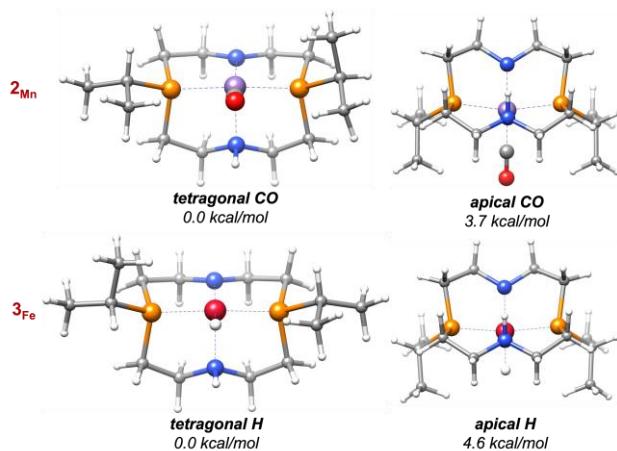
Figure S2. Different conformers of **2Mn** and **3Fe** along with their relative energies computed at the DFT–ωB97xD level of theory.

**Calculation of Hydricity (ΔG°$_{H-}$)**

For the calculation of thermodynamic hydricities of the metal–hydride intermediate (**I2**), we used a solvent–dependent protocol developed by Muckerman et. al. [44] Hydricity (ΔG°$_{H-}$) of a metal–hydride intermediate (MH) can be defined as the standard free energy change of the reaction,

$$MH \rightarrow M^+ + H^-$$
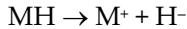
Therefore, mathematically, the hydricity of the metal–hydride intermediates (ΔG°$_{H-}$) can be expressed as:

$$\Delta G°_{H-} = G°(M^+) + G°(H^-) - G°(MH) \ldots\ldots\ldots (1)$$

To overcome the challenge of calculating the absolute free energy of a solvated hydride, G°(H$^-$), Muckerman et. al. proposed a protocol based on hydricity–half–reaction (HHR) as follows,

$$MH \rightarrow M^+$$
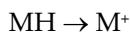
and by calculating its corresponding standard free energy change ΔG°$_{HHR}$(MH).

$$\Delta G°_{HHR}(MH) = G°(M^+) - G°(MH) = \Delta G°_{H-} - G°(H^-) \ldots\ldots\ldots (2)$$

Thus, the experimentally determined hydricity ΔG°$_{H-}$(expt.) changes linearly with the hydricity–half–reaction ΔG°$_{HHR}$(expt.) giving a unit slope and an intercept which is basically the absolute free energy of a solvated hydride(G°(H$^-$)). By using this protocol, it is, therefore, possible to calculate the HHR free energy change ΔG°$_{HHR}$(calc.) of a series of species whose hydricities are known experimentally.

In this work, to set up our linear fit equation, we choose already existing six different metal–hydride donor species whose hydricities were determined experimentally. Along with these six species, we have considered formate (HCOO$^-$) to match our theoretical ΔG°$_{H-}$(CO$_2$) value with its experimentally reported value.

Table S1. Experimental hydricities for the training set.

Species	ΔG°$_{H-}$(expt.) (kcal/mol)	References
HCOO$^-$	43	44
Ph$_3$CH	99	45
BNAH[a]	59	46
[Pt(dmpp)H]$^+$	50.7	47
[Ni(dmpp)H]$^+$	62.1	47
p–(Me$_2$NC$_6$H$_4$)$_3$CH	74	45
(SiP^{iPr}$_3$)Fe(H$_2$)(H)	54.3	48

[a]BNAH: 1–benzyl–1,4–dihydronicotinamide; [b]dmpp: bis(dimethylphosphino)propane

Now, the DFT–ωB97XD calculated values of ΔG°$_{HHR}$ in acetonitrile solvent are plotted against the experimental hydricities ΔG°$_{H-}$ in Figure S3.
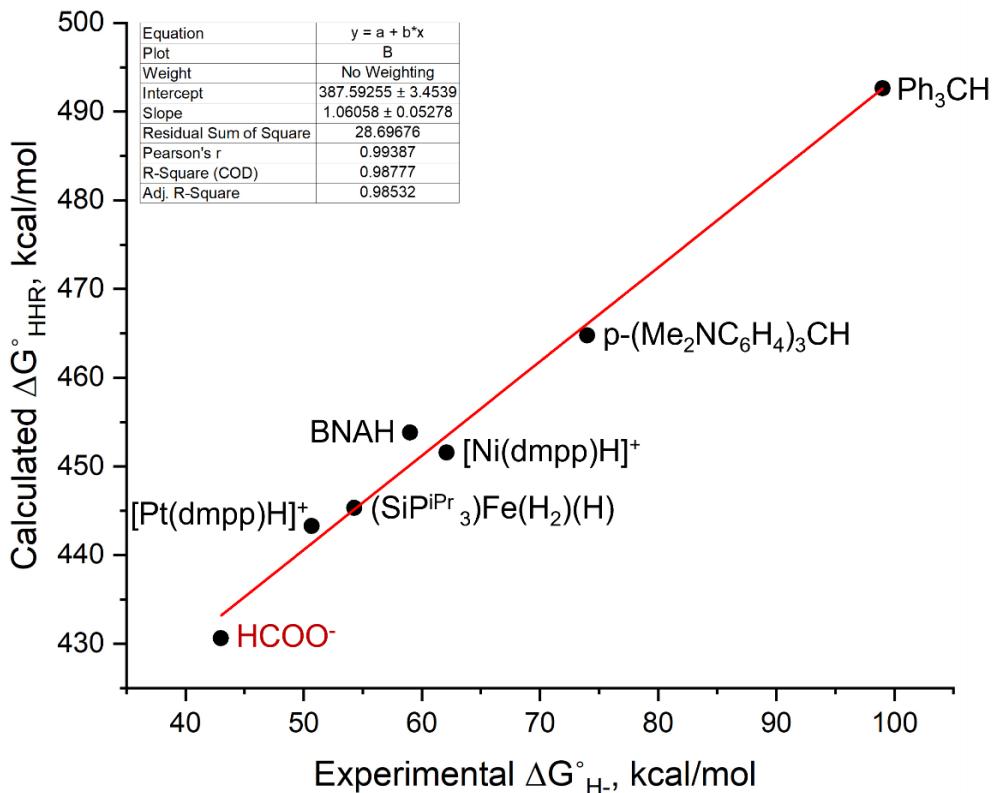
Figure S3. Correlation plot between calculated $\Delta G°_{HHR}$ and experimental $\Delta G°_{H-}$ of seven different species.

Figure S3 gives rise to the linear–fit equation, $\Delta G°_{HHR} = 387.6 + 1.06 \cdot \Delta G°_{H-}$ following which the hydricities of the species of our interest have been calculated, which are tabulated in Table S2.

Table S2. Calculated hydricities ($\Delta G°_{H-}$ in kcal/mol) for all the species involved

Species	Hydricity
1_{Mn}	55.2
2_{Mn}	47.1
3_{Fe}	48.7

Our calculation shows an uncertainty of about ±3.5 kcal/mol in $\Delta G°_{HHR}$ in calculating absolute hydricity values which are clearly seen in Figure S3. This indicates that the level of theory and the solvation model plays a crucial role in the calculation of $\Delta G°_{HHR}$ values significantly which was predicted earlier by Muckerman et.al. But, this absolute error in the calculated hydricity can be neglected as we are mainly focusing on the relative hydricity of the reported species as we are concerned about the reactivity of that complexes towards the CO_2 hydrogenation reaction.

Table S3. Calculated hydricity and overall barriers for H_2 splitting and hydride transfer step.

Species	Calculated Hydricity ($\Delta G_{H^-}^{\circ}$, kcal/mol)	Overall H_2–Splitting Barrier ($\Delta G^{\ddagger}$, kcal/mol)	Overall Hydride Transfer Barrier ($\Delta G^{\ddagger}$, kcal/mol)
1_{Mn}	55.2	14.6	11.5
2_{Mn}	47.1	10.0	7.4
3_{Fe}	48.7	9.9	8.1
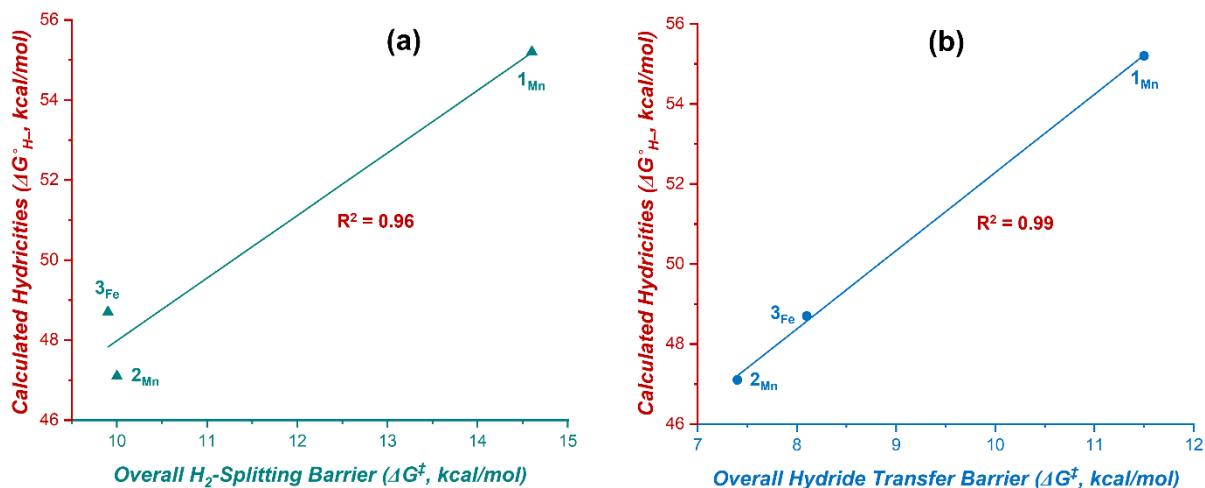
Figure S4. Correlation plot between the "overall" free energy barrier of the key steps of CO_2 hydrogenation and calculated hydricities of the metal–hydride intermediates obtained at the DFT– ωB97xD level. (**a**) H_2 splitting (**b**) hydride transfer.

Table S3 collects the free energy barriers for the two key steps of CO_2 hydrogenation, that is, H_2 splitting and hydride transfer calculated relative to the separated reactants for the three complexes 1_{Mn}, 2_{Mn}, and 3_{Fe}. These "overall" free energy barriers are marked in the reaction free energy profiles presented in Figures 1, 2, and 3 in the main text. Although very good correlations, R^2 = 0.96 for H_2–splitting (Figure S4a) and R^2 = 0.99 for hydride transfer (Figure S4b), were observed between the calculated hydricity and overall free energy barriers, the correlation for the H_2 splitting step yields a positive slope. This implies that the metal–hydride intermediate possessing a lower hydricity exhibits a lower H_2 splitting barrier and vice versa. At the same time, the hydride transfer step also shows a positive correlation (Figure S4b), suggesting a similar electronic requirement for both steps. This doesn't corroborate the established opposite electronic structure requirement of the two key steps of CO_2 hydrogenation. [30,36,37] Therefore, we considered the "intrinsic" free energy barriers, the barriers computed using the H_2 and CO_2 bound species, **I1** and **I3** as the reference to generate the correlation plots. This gives thermodynamic correlations that appropriately reflect the oppositive electronic requirements of the key reaction steps: negative correlation for the H_2 splitting step (Figure S5a) and positive correlation for the

hydride transfer step (Figure S5b). The unexpected correlation observed with the "overall" barrier might be due to the uncertainties (e.g., different spin states of the free catalyst, error in entropy contribution) associated with the barriers calculated from separated reactants.
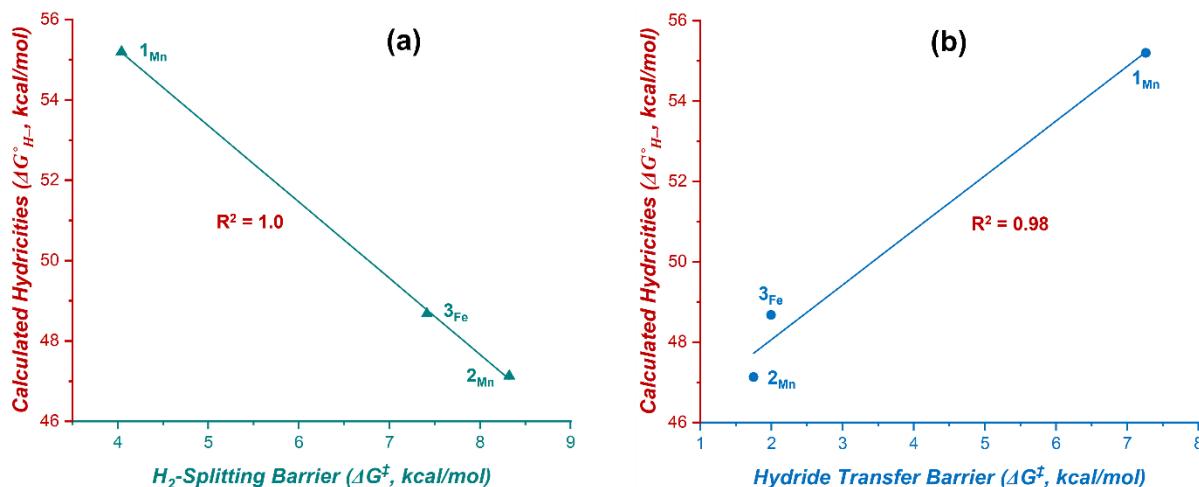

Figure S5. Correlation plot between the "intrinsic" free energy barrier of the key steps of CO_2 hydrogenation and calculated hydricities of the metal–hydride intermediates obtained at the DFT– ωB97xD level. (**a**) H_2 splitting (**b**) hydride transfer.

Table S4. Optimized Cartesian Coordinates for the Species Involved.

1_{Mn}

25	0.109297000	0.462231000	−0.483405000
7	0.082954000	−1.302687000	−1.437311000
6	0.118755000	1.675592000	0.822880000
8	0.116747000	2.455561000	1.681043000
6	3.009227000	−1.131960000	−1.333346000
1	3.625447000	−0.569127000	−2.042013000
1	3.645188000	−1.875121000	−0.842946000
6	−2.779769000	−0.810813000	−1.550247000
6	0.127851000	1.709443000	−1.723692000
8	0.137782000	2.462496000	−2.605747000
15	−2.150960000	0.307289000	−0.260521000
15	2.310680000	0.061861000	−0.142910000
6	2.220587000	−0.838198000	1.456385000
6	2.480608000	−0.180624000	2.663822000
6	1.714368000	−2.143054000	1.492649000
6	2.256209000	−0.821571000	3.878643000
1	2.853700000	0.838810000	2.657258000
6	1.497673000	−2.784288000	2.707781000
1	1.446225000	−2.647156000	0.570796000
6	1.769229000	−2.125869000	3.904463000
1	2.462363000	−0.298070000	4.806894000
1	1.101201000	−3.794699000	2.716767000
1	1.596986000	−2.624890000	4.853282000

6	3.591331000	1.331907000	0.132722000
6	4.884645000	0.975441000	0.534806000
6	3.288884000	2.676879000	−0.084898000
6	5.855974000	1.951086000	0.718893000
1	5.125997000	−0.069230000	0.711590000
6	4.264514000	3.654870000	0.098176000
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1	6.305114000	4.055254000	0.644114000
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6	−3.962491000	−0.921200000	1.523667000
6	−2.001648000	−1.592310000	3.379897000
1	−0.623120000	−0.598856000	2.074666000
6	−4.304697000	−1.629084000	2.669244000
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6	−3.321964000	−1.969634000	3.597781000
1	−1.226527000	−1.852902000	4.093237000
1	−5.337205000	−1.918687000	2.837716000
1	−3.588940000	−2.527794000	4.489854000
6	−3.169862000	1.827140000	−0.289714000
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6	−4.016929000	3.707286000	−1.559755000
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1	0.823060000	−1.759509000	−4.643858000
1	1.510116000	−0.228028000	−4.089470000

| 1 | −3.778785000 | −1.203853000 | −1.341739000 |
| 1 | −2.809899000 | −0.253581000 | −2.493292000 |

I1

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6	−2.866319000	−2.803671000	1.046859000
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TS1

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1	−2.382154000	1.778303000	1.871044000
1	−0.230251000	0.807100000	−1.276636000
1	−0.268057000	−0.115175000	−1.542058000
I2			
25	0.018949000	−0.166511000	0.294874000
7	−0.166800000	1.910271000	−0.721691000
6	0.028837000	−1.853885000	0.816619000
8	0.024245000	−2.973723000	1.122071000
6	2.371386000	1.035319000	−1.686316000
1	3.413141000	1.206968000	−1.970992000
1	1.845297000	0.675986000	−2.578607000
6	−2.658811000	1.706699000	0.834137000
6	0.304906000	0.519439000	1.913366000
8	0.494063000	0.975040000	2.969996000
15	−2.230026000	−0.023026000	0.374932000
15	2.136817000	−0.290541000	−0.428114000
6	2.716584000	−1.806960000	−1.305176000
6	4.072215000	−2.149885000	−1.360695000
6	1.790538000	−2.617353000	−1.968788000
6	4.490954000	−3.271552000	−2.069100000
1	4.808576000	−1.545798000	−0.840507000
6	2.210698000	−3.738565000	−2.678137000
1	0.738194000	−2.359261000	−1.921233000
6	3.561153000	−4.068902000	−2.730638000
1	5.546297000	−3.524926000	−2.099256000
1	1.477536000	−4.359618000	−3.183712000
1	3.888036000	−4.947074000	−3.279159000
6	3.502092000	−0.031158000	0.780237000
6	4.647178000	0.732167000	0.535059000
6	3.373094000	−0.659516000	2.023648000
6	5.631944000	0.874190000	1.509470000
1	4.783492000	1.226893000	−0.421289000
6	4.359979000	−0.529141000	2.994175000
1	2.486389000	−1.250404000	2.232993000
6	5.490612000	0.243070000	2.741274000
1	6.510733000	1.477623000	1.303348000
1	4.239955000	−1.023592000	3.952839000
1	6.257203000	0.354122000	3.501761000
6	−3.144914000	−0.317895000	−1.193836000
6	−2.805452000	−1.457944000	−1.932596000
6	−4.168106000	0.506159000	−1.669474000
6	−3.473024000	−1.765994000	−3.111283000
1	−2.000112000	−2.094097000	−1.579330000
6	−4.825529000	0.209810000	−2.863077000
1	−4.465200000	1.390339000	−1.115602000

6	−4.481034000	−0.927467000	−3.584457000
1	−3.199635000	−2.656770000	−3.668179000
1	−5.610264000	0.868222000	−3.222777000
1	−4.994458000	−1.160966000	−4.512009000
6	−3.197593000	−1.020033000	1.578402000
6	−2.618804000	−1.295865000	2.821530000
6	−4.492028000	−1.478157000	1.316594000
6	−3.324746000	−2.005101000	3.787529000
1	−1.609308000	−0.957608000	3.031909000
6	−5.194306000	−2.194308000	2.281455000
1	−4.953147000	−1.282405000	0.353588000
6	−4.613435000	−2.457584000	3.518655000
1	−2.861825000	−2.212899000	4.747044000
1	−6.196995000	−2.549271000	2.063765000
1	−5.161448000	−3.018903000	4.269128000
14	−1.521649000	2.886390000	−0.103757000
14	1.461686000	2.551802000	−1.043512000
6	−2.412095000	3.675032000	−1.558663000
1	−3.294953000	4.232109000	−1.226872000
1	−1.754274000	4.372921000	−2.087057000
1	−2.745484000	2.917468000	−2.275467000
6	−0.904104000	4.195578000	1.084064000
1	−0.310270000	4.970158000	0.589616000
1	−1.766000000	4.686266000	1.549269000
1	−0.303259000	3.749424000	1.882222000
6	1.386586000	3.896434000	−2.357748000
1	0.891363000	3.540458000	−3.267120000
1	0.833224000	4.769450000	−1.993819000
1	2.390916000	4.235348000	−2.633127000
6	2.263207000	3.228090000	0.507798000
1	3.343743000	3.305856000	0.348576000
1	1.892820000	4.225281000	0.757511000
1	2.108274000	2.574669000	1.370042000
1	−3.723708000	1.945235000	0.752150000
1	−2.394688000	1.774485000	1.896048000
1	−0.475671000	1.417752000	−1.561886000
1	−0.177372000	−0.672601000	−1.204995000

I3

25	−0.063854000	−0.292689000	0.425733000
7	0.115995000	−0.835985000	−1.808901000
6	−0.076825000	0.367391000	2.062488000
8	−0.071133000	0.837648000	3.124364000
6	−2.419757000	0.467758000	−1.776392000
1	−3.463335000	0.573257000	−2.085575000
1	−1.898040000	1.380270000	−2.086114000
6	2.602310000	−1.937665000	−0.682443000
6	−0.399230000	−1.973146000	0.913359000
8	−0.620811000	−3.072396000	1.230642000
15	2.179688000	−0.515535000	0.404412000
15	−2.179251000	0.365447000	0.046801000

6	−2.754693000	2.016180000	0.630916000
6	−4.118660000	2.317777000	0.722962000
6	−1.822062000	3.009133000	0.940084000
6	−4.538011000	3.586626000	1.106590000
1	−4.859969000	1.555178000	0.504611000
6	−2.243014000	4.280081000	1.322382000
1	−0.764764000	2.780848000	0.872164000
6	−3.600093000	4.572034000	1.406386000
1	−5.599381000	3.804765000	1.175847000
1	−1.504541000	5.039989000	1.557914000
1	−3.928228000	5.561875000	1.708882000
6	−3.546855000	−0.716272000	0.637640000
6	−4.676086000	−1.054796000	−0.112765000
6	−3.434758000	−1.219851000	1.938513000
6	−5.663465000	−1.881632000	0.417732000
1	−4.797450000	−0.679341000	−1.123752000
6	−4.424053000	−2.035797000	2.474565000
1	−2.559237000	−0.974339000	2.532351000
6	−5.540086000	−2.373090000	1.713050000
1	−6.529812000	−2.139957000	−0.183578000
1	−4.317537000	−2.416885000	3.485194000
1	−6.308578000	−3.018482000	2.126843000
6	3.146270000	0.891837000	−0.275990000
6	2.918742000	2.153306000	0.288445000
6	4.085920000	0.777447000	−1.302051000
6	3.614877000	3.268455000	−0.160977000
1	2.173773000	2.258127000	1.071669000
6	4.769551000	1.899653000	−1.769868000
1	4.293685000	−0.186355000	−1.753967000
6	4.537385000	3.145700000	−1.199756000
1	3.423130000	4.238168000	0.286841000
1	5.486468000	1.793923000	−2.578238000
1	5.071267000	4.019222000	−1.560719000
6	3.111482000	−0.894620000	1.943418000
6	2.465653000	−1.607686000	2.957704000
6	4.453726000	−0.539993000	2.112615000
6	3.149962000	−1.965480000	4.115276000
1	1.422021000	−1.880609000	2.842895000
6	5.135239000	−0.893411000	3.272687000
1	4.968466000	0.021385000	1.338792000
6	4.485017000	−1.607400000	4.275844000
1	2.634449000	−2.516500000	4.895467000
1	6.175639000	−0.607821000	3.394072000
1	5.016881000	−1.879428000	5.182344000
14	1.467561000	−1.928567000	−2.191727000
14	−1.503478000	−0.993872000	−2.528414000
6	2.349035000	−1.269896000	−3.714815000
1	3.270462000	−1.826627000	−3.916816000
1	1.707006000	−1.351926000	−4.597983000
1	2.610264000	−0.214152000	−3.590972000
6	0.859273000	−3.676560000	−2.480754000

1	0.264092000	–3.771856000	–3.393920000
1	1.724100000	–4.341786000	–2.579073000
1	0.261367000	–4.029551000	–1.635020000
6	–1.400995000	–0.820215000	–4.398396000
1	–0.873948000	0.098025000	–4.677453000
1	–0.863782000	–1.664947000	–4.843870000
1	–2.398139000	–0.789195000	–4.849996000
6	–2.319252000	–2.617414000	–2.075545000
1	–3.392818000	–2.548900000	–2.280207000
1	–1.924421000	–3.450916000	–2.661323000
1	–2.204101000	–2.854374000	–1.014773000
1	3.668930000	–2.022523000	–0.912929000
1	2.333193000	–2.815976000	–0.083579000
1	0.429619000	0.116539000	–2.009344000
1	0.184225000	1.194483000	–0.106924000
6	0.713756000	2.975297000	–1.968761000
8	0.560493000	3.887975000	–1.265922000
8	0.859940000	2.099083000	–2.729317000

TS2

25	–0.040449000	0.039392000	0.355024000
7	0.090435000	–1.612789000	–1.206611000
6	–0.043192000	1.468998000	1.398354000
8	–0.029858000	2.418112000	2.064598000
6	–2.529285000	–0.616897000	–1.759645000
1	–3.585884000	–0.745134000	–2.011397000
1	–2.079793000	–0.001233000	–2.547607000
6	2.604038000	–1.978665000	0.285920000
6	–0.347889000	–1.119548000	1.669763000
8	–0.543448000	–1.893951000	2.514725000
15	2.220556000	–0.198873000	0.522434000
15	–2.237618000	0.307172000	–0.199419000
6	–2.929931000	1.973722000	–0.546092000
6	–4.310670000	2.153543000	–0.697185000
6	–2.081655000	3.071065000	–0.698513000
6	–4.829179000	3.405586000	–1.002275000
1	–4.986282000	1.313493000	–0.563111000
6	–2.603161000	4.326236000	–1.004678000
1	–1.011471000	2.945217000	–0.595119000
6	–3.974226000	4.495916000	–1.156907000
1	–5.901429000	3.532783000	–1.115249000
1	–1.929870000	5.168864000	–1.124336000
1	–4.379845000	5.474939000	–1.393165000
6	–3.480388000	–0.339956000	0.990319000
6	–4.559290000	–1.155089000	0.641356000
6	–3.332070000	0.037719000	2.330006000
6	–5.463163000	–1.591651000	1.607297000
1	–4.704555000	–1.463799000	–0.388645000
6	–4.238038000	–0.388393000	3.293354000
1	–2.496437000	0.668295000	2.620170000
6	–5.304911000	–1.208958000	2.934697000

1	−6.291846000	−2.230975000	1.318847000
1	−4.105932000	−0.085741000	4.327183000
1	−6.008404000	−1.549548000	3.687862000
6	3.260002000	0.686429000	−0.699629000
6	3.109768000	2.076023000	−0.772698000
6	4.193164000	0.064800000	−1.531979000
6	3.874793000	2.824914000	−1.657423000
1	2.370934000	2.569176000	−0.147981000
6	4.951986000	0.814324000	−2.428968000
1	4.336552000	−1.009578000	−1.494199000
6	4.795629000	2.194480000	−2.491572000
1	3.737041000	3.899797000	−1.708666000
1	5.665743000	0.315480000	−3.077162000
1	5.385266000	2.778258000	−3.191343000
6	3.093718000	0.198835000	2.092071000
6	2.387265000	0.195615000	3.297613000
6	4.469943000	0.452171000	2.114712000
6	3.043043000	0.435697000	4.501965000
1	1.319643000	0.008583000	3.300332000
6	5.123694000	0.694224000	3.317672000
1	5.032599000	0.470019000	1.186143000
6	4.411125000	0.686322000	4.514412000
1	2.479364000	0.433460000	5.429473000
1	6.190864000	0.893431000	3.319948000
1	4.921248000	0.879794000	5.452978000
14	1.499834000	−2.694712000	−1.067787000
14	−1.523249000	−2.206560000	−1.670977000
6	2.357382000	−2.728368000	−2.736661000
1	3.315767000	−3.256388000	−2.689089000
1	1.729999000	−3.237798000	−3.475692000
1	2.542279000	−1.713429000	−3.102164000
6	1.008674000	−4.426179000	−0.541916000
1	0.403382000	−4.942525000	−1.293149000
1	1.917452000	−5.018220000	−0.387038000
1	0.455825000	−4.413479000	0.402265000
6	−1.445884000	−3.015660000	−3.365637000
1	−0.997445000	−2.335423000	−4.097033000
1	−0.845171000	−3.931620000	−3.343895000
1	−2.445246000	−3.285594000	−3.722793000
6	−2.225269000	−3.402125000	−0.411358000
1	−3.296838000	−3.531953000	−0.595692000
1	−1.759272000	−4.387592000	−0.484628000
1	−2.110978000	−3.041027000	0.613819000
1	3.671505000	−2.185193000	0.159999000
1	2.297481000	−2.446635000	1.229288000
1	0.336738000	−0.928269000	−1.934182000
1	0.194513000	1.041016000	−0.945031000
6	0.525528000	1.528242000	−2.551794000
8	0.556999000	2.703388000	−2.455026000
8	0.581948000	0.493244000	−3.144204000

I4

25	0.033848000	−0.177323000	0.229371000
7	−0.109861000	1.926027000	−0.445024000
6	0.077956000	−1.930759000	0.552255000
8	0.106508000	−3.066024000	0.767181000
6	2.539512000	1.339328000	−1.369801000
1	3.591422000	1.590167000	−1.533843000
1	2.099126000	1.102290000	−2.346426000
6	−2.595133000	1.648222000	1.107180000
6	0.352698000	0.282794000	1.911595000
8	0.541787000	0.642221000	2.997278000
15	−2.244131000	−0.065400000	0.569869000
15	2.280644000	−0.160244000	−0.353498000
6	3.012730000	−1.538606000	−1.317538000
6	4.398897000	−1.738540000	−1.339370000
6	2.189280000	−2.378787000	−2.070867000
6	4.949995000	−2.759001000	−2.104358000
1	5.050876000	−1.102435000	−0.748218000
6	2.746939000	−3.397869000	−2.839528000
1	1.114829000	−2.236245000	−2.095328000
6	4.123332000	−3.591773000	−2.856217000
1	6.025496000	−2.906590000	−2.111105000
1	2.094892000	−4.036297000	−3.426449000
1	4.554415000	−4.389831000	−3.452891000
6	3.451766000	−0.041629000	1.051716000
6	4.483434000	0.895541000	1.129940000
6	3.313968000	−0.979334000	2.082016000
6	5.349672000	0.907145000	2.220897000
1	4.620140000	1.627572000	0.341297000
6	4.182293000	−0.974340000	3.166187000
1	2.520021000	−1.719405000	2.033842000
6	5.200555000	−0.026523000	3.240494000
1	6.142473000	1.646959000	2.270131000
1	4.060389000	−1.707727000	3.956704000
1	5.875138000	−0.017119000	4.090669000
6	−3.304235000	−0.364514000	−0.888071000
6	−3.110343000	−1.560095000	−1.587558000
6	−4.302316000	0.516206000	−1.313187000
6	−3.896407000	−1.866953000	−2.690710000
1	−2.320104000	−2.241834000	−1.288864000
6	−5.086310000	0.210206000	−2.421963000
1	−4.473347000	1.450994000	−0.790596000
6	−4.884952000	−0.981685000	−3.110663000
1	−3.716697000	−2.786979000	−3.235838000
1	−5.851358000	0.907460000	−2.748597000
1	−5.490782000	−1.215975000	−3.980168000
6	−3.049051000	−1.106136000	1.851725000
6	−2.297339000	−1.624528000	2.909305000
6	−4.426499000	−1.351557000	1.815473000
6	−2.909812000	−2.367950000	3.914362000
1	−1.227935000	−1.454593000	2.953410000

6	−5.036919000	−2.095472000	2.818768000
1	−5.023062000	−0.969054000	0.992805000
6	−4.279578000	−2.605004000	3.870823000
1	−2.311525000	−2.766923000	4.727193000
1	−6.105431000	−2.281866000	2.776051000
1	−4.756281000	−3.189754000	4.651321000
14	−1.539489000	2.847300000	0.093936000
14	1.474488000	2.717310000	−0.642410000
6	−2.429673000	3.458752000	−1.436576000
1	−3.415719000	3.871212000	−1.198035000
1	−1.844166000	4.246717000	−1.922067000
1	−2.551888000	2.647662000	−2.160883000
6	−1.104486000	4.280431000	1.225164000
1	−0.515947000	5.053892000	0.722439000
1	−2.033667000	4.747789000	1.569953000
1	−0.554173000	3.944623000	2.109281000
6	1.332474000	4.118331000	−1.883003000
1	0.873615000	3.751126000	−2.806716000
1	0.715302000	4.937891000	−1.499254000
1	2.315064000	4.532971000	−2.131018000
6	2.162589000	3.338314000	0.987538000
1	3.222671000	3.585120000	0.867267000
1	1.652618000	4.246219000	1.318143000
1	2.087279000	2.592121000	1.782934000
1	−3.662156000	1.890147000	1.128859000
1	−2.235420000	1.694790000	2.142274000
1	−0.344524000	1.639406000	−1.435209000
1	−0.263734000	−0.506408000	−1.503783000
6	−0.479613000	−0.278053000	−2.682597000
8	−0.553510000	−1.308564000	−3.322368000
8	−0.555445000	0.936864000	−2.925328000

TS3

25	0.019176000	−0.122152000	0.272225000
7	−0.108002000	1.862505000	−0.523570000
6	0.051411000	−1.857213000	0.683781000
8	0.073221000	−2.979281000	0.967569000
6	2.573808000	1.288112000	−1.376529000
1	3.630589000	1.547670000	−1.485597000
1	2.201508000	1.009980000	−2.369858000
6	−2.669844000	1.742422000	0.906980000
6	0.347503000	0.398447000	1.930634000
8	0.542415000	0.811758000	2.993680000
15	−2.256959000	−0.002258000	0.585415000
15	2.273575000	−0.168568000	−0.317956000
6	2.972050000	−1.596996000	−1.234709000
6	4.356162000	−1.806061000	−1.276170000
6	2.132823000	−2.459953000	−1.943189000
6	4.887845000	−2.855880000	−2.014665000
1	5.020882000	−1.151236000	−0.720266000
6	2.668575000	−3.508720000	−2.686628000

1	1.058538000	–2.319197000	–1.942422000
6	4.043608000	–3.709710000	–2.722150000
1	5.962222000	–3.009616000	–2.036456000
1	2.003161000	–4.164829000	–3.237872000
1	4.459529000	–4.530010000	–3.298860000
6	3.425769000	–0.047270000	1.100496000
6	4.431301000	0.914621000	1.204955000
6	3.292203000	–0.999107000	2.118915000
6	5.280138000	0.933481000	2.309706000
1	4.557413000	1.663016000	0.430602000
6	4.143332000	–0.985524000	3.216211000
1	2.516750000	–1.757026000	2.051300000
6	5.138263000	–0.015160000	3.316005000
1	6.052598000	1.692702000	2.380353000
1	4.026376000	–1.729887000	3.997175000
1	5.799338000	0.000575000	4.176626000
6	–3.218028000	–0.504905000	–0.886059000
6	–3.051139000	–1.816523000	–1.347441000
6	–4.080202000	0.350998000	–1.573267000
6	–3.730482000	–2.259907000	–2.473589000
1	–2.374787000	–2.491083000	–0.829241000
6	–4.754551000	–0.092609000	–2.708662000
1	–4.226407000	1.371702000	–1.237953000
6	–4.580604000	–1.395915000	–3.159949000
1	–3.580127000	–3.274027000	–2.827756000
1	–5.412773000	0.586353000	–3.241303000
1	–5.099958000	–1.737489000	–4.049446000
6	–3.087186000	–0.941282000	1.924039000
6	–2.355173000	–1.424588000	3.010595000
6	–4.472693000	–1.139296000	1.895238000
6	–2.995770000	–2.089858000	4.052915000
1	–1.280505000	–1.288377000	3.048209000
6	–5.111010000	–1.803969000	2.935294000
1	–5.051991000	–0.781442000	1.048830000
6	–4.372722000	–2.280470000	4.016825000
1	–2.414079000	–2.463231000	4.889578000
1	–6.185408000	–1.954497000	2.900217000
1	–4.871240000	–2.803269000	4.827077000
14	–1.504440000	2.843156000	–0.115685000
14	1.436938000	2.664919000	–0.736232000
6	–2.355392000	3.458065000	–1.677657000
1	–3.325285000	3.915559000	–1.452116000
1	–1.736028000	4.218775000	–2.164921000
1	–2.506272000	2.651493000	–2.400454000
6	–1.140657000	4.335793000	0.975171000
1	–0.521280000	5.085725000	0.473021000
1	–2.086084000	4.820696000	1.244250000
1	–0.639241000	4.042175000	1.902819000
6	1.334844000	4.007914000	–2.051938000
1	0.893669000	3.609024000	–2.971148000
1	0.719417000	4.851798000	–1.721386000

1	2.328098000	4.401357000	−2.293126000
6	2.166087000	3.401016000	0.834977000
1	3.204332000	3.704294000	0.658756000
1	1.616593000	4.291976000	1.148977000
1	2.162739000	2.691328000	1.666868000
1	−3.736299000	1.965246000	0.803772000
1	−2.408053000	1.900350000	1.960481000
1	−0.375676000	1.419239000	−1.829493000
1	−0.321296000	−0.630539000	−1.580616000
6	−0.480801000	−0.322679000	−2.672990000
8	−0.557110000	−1.209796000	−3.486547000
8	−0.536696000	0.953153000	−2.838101000

I5

25	−0.052302000	−0.456563000	−0.223250000
7	0.125643000	1.330248000	−1.255954000
6	−0.091089000	−1.769457000	0.980736000
8	−0.118266000	−2.636139000	1.750402000
6	−2.483904000	1.868281000	−0.170550000
1	−3.532623000	2.156413000	−0.280569000
1	−2.056662000	2.467409000	0.640678000
6	2.734809000	0.183342000	−1.966552000
6	−0.472008000	−1.547307000	−1.541769000
8	−0.734226000	−2.202195000	−2.460078000
15	2.214234000	−0.632495000	−0.430077000
15	−2.234043000	0.131525000	0.330402000
6	−2.690526000	0.053014000	2.105118000
6	−3.990807000	−0.226856000	2.533804000
6	−1.698415000	0.318139000	3.055241000
6	−4.293693000	−0.240989000	3.891980000
1	−4.767746000	−0.442196000	1.806421000
6	−2.005517000	0.307525000	4.411898000
1	−0.687345000	0.545563000	2.729478000
6	−3.302382000	0.025563000	4.832497000
1	−5.305768000	−0.463440000	4.215507000
1	−1.228279000	0.512912000	5.141492000
1	−3.539903000	0.010219000	5.891689000
6	−3.537528000	−0.869125000	−0.471724000
6	−4.577215000	−0.326262000	−1.227859000
6	−3.474757000	−2.258589000	−0.305517000
6	−5.532721000	−1.154794000	−1.812487000
1	−4.645599000	0.745310000	−1.378164000
6	−4.433237000	−3.083402000	−0.879874000
1	−2.670921000	−2.696151000	0.279810000
6	−5.463827000	−2.532466000	−1.638814000
1	−6.330835000	−0.718729000	−2.404895000
1	−4.371121000	−4.157980000	−0.741561000
1	−6.208448000	−3.176922000	−2.095196000
6	2.952228000	0.323620000	0.944371000
6	2.712466000	−0.120321000	2.251855000
6	3.657736000	1.511827000	0.751829000

6	3.161202000	0.616807000	3.339599000
1	2.167413000	−1.044970000	2.419660000
6	4.101915000	2.254641000	1.844126000
1	3.850199000	1.882739000	−0.248411000
6	3.851727000	1.811584000	3.137849000
1	2.968100000	0.261619000	4.347037000
1	4.631290000	3.186945000	1.677760000
1	4.193814000	2.393275000	3.988094000
6	3.107888000	−2.225782000	−0.355216000
6	2.440169000	−3.408714000	−0.679693000
6	4.466039000	−2.275537000	−0.021972000
6	3.120596000	−4.623685000	−0.676637000
1	1.385403000	−3.383663000	−0.932765000
6	5.143173000	−3.489208000	−0.016323000
1	4.990852000	−1.362128000	0.243860000
6	4.470711000	−4.665031000	−0.344447000
1	2.591618000	−5.537349000	−0.927962000
1	6.195821000	−3.519116000	0.246930000
1	4.999832000	−5.612871000	−0.336847000
14	1.485211000	1.583556000	−2.322840000
14	−1.376090000	2.106240000	−1.695551000
6	2.314445000	3.259005000	−2.088023000
1	3.348663000	3.241096000	−2.451486000
1	1.783388000	4.027481000	−2.659112000
1	2.306304000	3.581479000	−1.043039000
6	1.070119000	1.414018000	−4.156253000
1	0.449305000	2.240003000	−4.518482000
1	1.995110000	1.420289000	−4.744496000
1	0.543513000	0.476211000	−4.361904000
6	−1.155468000	3.952966000	−1.990669000
1	−0.550849000	4.395429000	−1.191331000
1	−0.648862000	4.151728000	−2.941436000
1	−2.122128000	4.467209000	−2.020899000
6	−2.255848000	1.334183000	−3.173266000
1	−3.265164000	1.749642000	−3.275680000
1	−1.723824000	1.529448000	−4.107947000
1	−2.349940000	0.249457000	−3.063176000
1	3.788818000	0.477805000	−1.972265000
1	2.602404000	−0.573130000	−2.749234000
1	0.950004000	3.363159000	2.786434000
6	0.905358000	3.328306000	1.686584000
8	1.259636000	4.240322000	0.977312000
8	0.411049000	2.171385000	1.281176000
1	0.406289000	2.056783000	0.267968000

2Mn

15	2.246182000	−0.212203000	−0.031371000
7	−0.039297000	−0.487593000	1.831989000
6	1.123710000	−1.326400000	2.199135000
6	−1.293015000	−1.231653000	2.083496000
6	−2.515456000	−0.513104000	1.518360000

6	2.442706000	−0.704719000	1.745543000
1	3.272167000	−1.397693000	1.922631000
1	−2.719630000	0.397378000	2.094077000
15	−2.126009000	0.002412000	−0.221674000
1	2.639905000	0.204303000	2.323397000
1	−3.397635000	−1.156843000	1.596572000
1	1.136415000	−1.523819000	3.281030000
1	0.983832000	−2.286946000	1.694552000
1	−1.182799000	−2.198016000	1.582563000
1	−1.418966000	−1.431941000	3.157696000
6	3.714174000	0.859665000	−0.412612000
1	4.612564000	0.228726000	−0.381207000
6	−3.486093000	1.187437000	−0.658247000
1	−3.310025000	1.393793000	−1.722474000
6	3.549493000	1.434214000	−1.825856000
1	3.453377000	0.654543000	−2.586821000
1	2.656164000	2.064653000	−1.876914000
1	4.418455000	2.047733000	−2.086291000
6	3.862963000	1.998045000	0.603406000
1	4.128626000	1.634714000	1.600063000
1	4.657972000	2.679583000	0.282898000
1	2.937601000	2.578456000	0.678474000
6	−3.337048000	2.506665000	0.107068000
1	−3.510797000	2.365484000	1.180107000
1	−2.343809000	2.942027000	−0.021241000
1	−4.078652000	3.230891000	−0.246381000
6	−4.892069000	0.601692000	−0.498123000
1	−5.644823000	1.322514000	−0.835236000
1	−5.025809000	−0.315460000	−1.078836000
1	−5.106150000	0.373085000	0.551892000
1	−0.034031000	0.347061000	2.413408000
6	−2.439432000	−1.466145000	−1.290174000
1	−3.333009000	−2.037901000	−1.018415000
1	−2.589143000	−1.064523000	−2.299383000
6	−1.176393000	−2.330714000	−1.253915000
1	−1.130804000	−2.938703000	−2.174585000
6	2.510918000	−1.741523000	−1.026010000
1	3.302029000	−2.389457000	−0.632992000
1	2.818369000	−1.406188000	−2.021801000
6	1.161939000	−2.462044000	−1.119221000
1	1.146202000	−3.076261000	−2.036741000
7	0.034589000	−1.540757000	−1.087793000
25	0.083325000	0.195848000	−0.215560000
1	−1.282191000	−3.071957000	−0.431509000
1	1.094614000	−3.196973000	−0.287409000
6	0.200142000	1.947341000	−0.015962000
8	0.304748000	3.115540000	0.051608000

I1

15	2.225758000	−0.206629000	−0.026512000
7	−0.055263000	−0.362730000	1.800200000

6	1.142711000	−1.053058000	2.326597000
6	−1.262719000	−1.168354000	2.064174000
6	−2.505802000	−0.521785000	1.460870000
6	2.424988000	−0.417527000	1.800520000
1	3.296669000	−1.021159000	2.075074000
1	−2.771163000	0.383345000	2.020632000
15	−2.116480000	−0.017322000	−0.279783000
1	2.553099000	0.578419000	2.237635000
1	−3.356618000	−1.207668000	1.521834000
1	1.132776000	−1.063359000	3.425849000
1	1.084687000	−2.091502000	1.992189000
1	−1.090882000	−2.142282000	1.601103000
1	−1.396762000	−1.328912000	3.144331000
6	3.731011000	0.736725000	−0.565790000
1	4.597361000	0.074054000	−0.437750000
6	−3.493474000	1.137686000	−0.742666000
1	−3.338641000	1.299427000	−1.818171000
6	3.594710000	1.098956000	−2.049384000
1	3.427599000	0.221707000	−2.681296000
1	2.753744000	1.784362000	−2.197296000
1	4.504567000	1.595668000	−2.402117000
6	3.938634000	2.001924000	0.274301000
1	4.207506000	1.771929000	1.308882000
1	4.751321000	2.601557000	−0.149030000
1	3.035969000	2.621926000	0.283600000
6	−3.341591000	2.488327000	−0.035442000
1	−3.479671000	2.387756000	1.047298000
1	−2.358479000	2.931132000	−0.207653000
1	−4.103065000	3.188920000	−0.394095000
6	−4.892786000	0.551672000	−0.532009000
1	−5.655089000	1.253061000	−0.887837000
1	−5.031651000	−0.390866000	−1.068523000
1	−5.087280000	0.369639000	0.530733000
1	−0.149351000	0.518093000	2.302266000
6	−2.401150000	−1.523954000	−1.294839000
1	−3.358602000	−2.014210000	−1.089416000
1	−2.402855000	−1.187206000	−2.338091000
6	−1.210567000	−2.453228000	−1.042023000
1	−1.150997000	−3.185715000	−1.871630000
6	2.451281000	−1.889835000	−0.739709000
1	3.255800000	−2.449344000	−0.248819000
1	2.736544000	−1.739456000	−1.786235000
6	1.100680000	−2.615573000	−0.683570000
1	1.113946000	−3.421816000	−1.443675000
7	0.009736000	−1.707871000	−0.898868000
25	0.085416000	0.295752000	−0.292048000
1	−1.454837000	−3.082252000	−0.147822000
1	1.033374000	−3.170426000	0.287502000
6	0.184909000	1.994586000	0.181339000
8	0.264498000	3.111147000	0.523115000
1	0.591035000	0.593445000	−1.855358000

| 1 | −0.226916000 | 0.692852000 | −1.886953000 |

TS1

15	2.232922000	−0.194931000	−0.022285000
7	−0.040987000	−0.457870000	1.828778000
6	1.124213000	−1.267220000	2.242208000
6	−1.296770000	−1.178020000	2.121157000
6	−2.513115000	−0.467140000	1.532409000
6	2.437211000	−0.651216000	1.763391000
1	3.272214000	−1.335427000	1.949054000
1	−2.714270000	0.457679000	2.086192000
15	−2.115709000	0.009040000	−0.216578000
1	2.634136000	0.271644000	2.319367000
1	−3.399811000	−1.103495000	1.620697000
1	1.137280000	−1.409981000	3.332954000
1	0.995554000	−2.253929000	1.788926000
1	−1.199913000	−2.167431000	1.665604000
1	−1.421084000	−1.328992000	3.203870000
6	3.726452000	0.825049000	−0.440431000
1	4.612585000	0.180747000	−0.362641000
6	−3.491894000	1.152460000	−0.707635000
1	−3.310777000	1.317988000	−1.778053000
6	3.593188000	1.330758000	−1.882738000
1	3.515054000	0.514850000	−2.606840000
1	2.699659000	1.954032000	−1.985511000
1	4.468480000	1.931188000	−2.152477000
6	3.879638000	2.008992000	0.521573000
1	4.119019000	1.689812000	1.539827000
1	4.694219000	2.658405000	0.184063000
1	2.964889000	2.609801000	0.552210000
6	−3.358993000	2.502285000	0.005547000
1	−3.534176000	2.401205000	1.082916000
1	−2.369649000	2.942007000	−0.136369000
1	−4.106739000	3.204457000	−0.378053000
6	−4.893269000	0.561176000	−0.529635000
1	−5.650306000	1.264076000	−0.893845000
1	−5.020195000	−0.376514000	−1.077931000
1	−5.108546000	0.368714000	0.527325000
1	0.170134000	0.511656000	−1.899627000
1	−0.035466000	0.408465000	2.362421000
6	−2.427322000	−1.511125000	−1.224765000
1	−3.348180000	−2.038052000	−0.954270000
1	−2.536252000	−1.155822000	−2.256506000
6	−1.207414000	−2.433120000	−1.116283000
1	−1.207165000	−3.128876000	−1.975290000
6	2.491701000	−1.770917000	−0.958064000
1	3.322046000	−2.370788000	−0.569866000
1	2.747841000	−1.473667000	−1.980327000
6	1.176431000	−2.559660000	−0.970423000
1	1.194542000	−3.270492000	−1.816687000
7	0.027114000	−1.685086000	−1.040633000

1	0.123608000	−0.468790000	−1.759941000
25	0.084701000	0.270249000	−0.231316000
1	−1.331026000	−3.082929000	−0.224169000
1	1.131301000	−3.198943000	−0.063508000
6	0.184810000	1.999237000	0.079827000
8	0.270397000	3.157625000	0.236061000

I2

15	2.207701000	−0.167849000	−0.016699000
7	−0.048948000	−0.502113000	1.817860000
6	1.124814000	−1.266688000	2.279497000
6	−1.317781000	−1.172444000	2.155838000
6	−2.518830000	−0.458366000	1.531331000
6	2.429679000	−0.646872000	1.773607000
1	3.271236000	−1.325640000	1.952390000
1	−2.719458000	0.472588000	2.075101000
15	−2.089256000	0.023521000	−0.221208000
1	2.629024000	0.275718000	2.329130000
1	−3.413763000	−1.084433000	1.615383000
1	1.138121000	−1.353554000	3.376599000
1	1.017590000	−2.282925000	1.886487000
1	−1.250912000	−2.192980000	1.764194000
1	−1.444168000	−1.261253000	3.245627000
6	3.723971000	0.827625000	−0.417358000
1	4.609273000	0.196120000	−0.260232000
6	−3.481734000	1.138979000	−0.731858000
1	−3.304101000	1.277664000	−1.806473000
6	3.659530000	1.263085000	−1.886921000
1	3.687152000	0.413674000	−2.575778000
1	2.734369000	1.815720000	−2.076596000
1	4.512837000	1.907364000	−2.124561000
6	3.816110000	2.059934000	0.491163000
1	3.979530000	1.794774000	1.539691000
1	4.657945000	2.687434000	0.179809000
1	2.904673000	2.662167000	0.425046000
6	−3.341759000	2.506976000	−0.055489000
1	−3.499230000	2.432976000	1.027015000
1	−2.354924000	2.942224000	−0.224956000
1	−4.097477000	3.197210000	−0.445484000
6	−4.881904000	0.553747000	−0.528934000
1	−5.640569000	1.245744000	−0.910467000
1	−5.014478000	−0.400148000	−1.047991000
1	−5.092618000	0.393742000	0.534317000
1	0.169994000	0.769854000	−1.776313000
1	−0.036652000	0.410097000	2.266465000
6	−2.430749000	−1.524102000	−1.201679000
1	−3.342898000	−2.048669000	−0.898194000
1	−2.568027000	−1.196869000	−2.239143000
6	−1.226782000	−2.462743000	−1.107264000
1	−1.264433000	−3.218599000	−1.906762000
6	2.504827000	−1.766372000	−0.928996000

1	3.327248000	–2.357928000	–0.511883000
1	2.784339000	–1.493239000	–1.951715000
6	1.211325000	–2.583296000	–0.957020000
1	1.261514000	–3.355433000	–1.740145000
7	0.038416000	–1.716571000	–1.139340000
1	0.117040000	–1.206114000	–2.019801000
25	0.083662000	0.297684000	–0.230126000
1	–1.256549000	–3.012720000	–0.159343000
1	1.079181000	–3.113646000	–0.006942000
6	0.170588000	2.008093000	0.110155000
8	0.247108000	3.174669000	0.235151000

I3

15	2.034317000	–0.708557000	–0.016098000
7	–0.455472000	–2.223572000	0.264994000
6	0.632356000	–3.085831000	–0.233562000
6	–1.768639000	–2.611595000	–0.281389000
6	–2.864846000	–1.622907000	0.123848000
6	2.001154000	–2.561616000	0.204656000
1	2.802255000	–3.085275000	–0.329074000
1	–3.125904000	–1.772354000	1.178464000
15	–2.197416000	0.114729000	–0.024446000
1	2.135701000	–2.758107000	1.273607000
1	–3.770770000	–1.804093000	–0.464573000
1	0.495272000	–4.128244000	0.091535000
1	0.564795000	–3.087583000	–1.326100000
1	–1.667051000	–2.624684000	–1.371586000
1	–2.039691000	–3.634360000	0.021681000
6	3.623751000	–0.191645000	0.796258000
1	4.455749000	–0.687269000	0.277453000
6	–3.482869000	1.162403000	0.807853000
1	–3.161515000	2.184269000	0.566505000
6	3.781062000	1.328607000	0.673737000
1	3.831783000	1.660028000	–0.368253000
1	2.937534000	1.834808000	1.152676000
1	4.704646000	1.652158000	1.165285000
6	3.636210000	–0.599271000	2.274860000
1	3.662654000	–1.684385000	2.408415000
1	4.525975000	–0.190021000	2.764954000
1	2.756000000	–0.208089000	2.794816000
6	–3.401988000	0.995225000	2.329039000
1	–3.700807000	–0.014557000	2.634269000
1	–2.392134000	1.176620000	2.702308000
1	–4.084950000	1.696584000	2.820118000
6	–4.910518000	0.954441000	0.295331000
1	–5.595941000	1.650986000	0.790219000
1	–4.994325000	1.118866000	–0.783010000
1	–5.263940000	–0.059655000	0.512594000
1	0.221515000	1.528634000	0.217288000
1	–0.491939000	–2.307118000	1.277511000
6	–2.434016000	0.529693000	–1.824168000

1	–3.393659000	0.197717000	–2.234288000
1	–2.408453000	1.624154000	–1.886836000
6	–1.280013000	–0.064104000	–2.632168000
1	–1.227147000	0.400773000	–3.628219000
6	2.405152000	–0.497544000	–1.829224000
1	3.146238000	–1.211077000	–2.205960000
1	2.821646000	0.507277000	–1.950151000
6	1.102762000	–0.596146000	–2.625235000
1	1.237371000	–0.172976000	–3.631980000
7	–0.001771000	0.070426000	–1.916677000
1	0.225721000	1.060182000	–1.832079000
25	–0.035842000	–0.060143000	0.287833000
1	–1.453187000	–1.133670000	–2.797184000
1	0.818770000	–1.645562000	–2.762317000
6	0.042260000	0.197923000	2.013844000
8	0.127883000	0.469093000	3.154171000
6	1.362842000	3.399644000	–0.788557000
8	1.371954000	2.897316000	–1.847972000
8	1.413044000	4.005514000	0.201961000

TS2

15	–2.098983000	–0.598113000	–0.021529000
7	0.319330000	–2.144993000	–0.618882000
6	–0.794817000	–3.032895000	–0.234918000
6	1.625688000	–2.677333000	–0.187407000
6	2.757461000	–1.680416000	–0.447606000
6	–2.148593000	–2.389152000	–0.539800000
1	–2.959297000	–2.960181000	–0.073715000
1	2.987164000	–1.652464000	–1.519503000
15	2.177807000	0.029095000	0.022951000
1	–2.317509000	–2.403232000	–1.621711000
1	3.666894000	–1.999827000	0.072424000
1	–0.711931000	–4.011517000	–0.731089000
1	–0.701109000	–3.218026000	0.839616000
1	1.548370000	–2.877074000	0.886160000
1	1.840906000	–3.641534000	–0.672024000
6	–3.672872000	0.113977000	–0.704094000
1	–4.517960000	–0.409813000	–0.236744000
6	3.490909000	1.155396000	–0.645846000
1	3.218745000	2.130643000	–0.220912000
6	–3.743608000	1.605810000	–0.356206000
1	–3.720186000	1.787577000	0.722600000
1	–2.903191000	2.141830000	–0.806610000
1	–4.673947000	2.036166000	–0.741538000
6	–3.743874000	–0.071342000	–2.224950000
1	–3.842427000	–1.121487000	–2.513965000
1	–4.616402000	0.458051000	–2.621844000
1	–2.853306000	0.340138000	–2.710653000
6	3.375978000	1.262337000	–2.170229000
1	3.625104000	0.311393000	–2.655676000
1	2.368872000	1.547453000	–2.480717000

1	4.079861000	2.011799000	−2.547154000
6	4.916832000	0.803626000	−0.213211000
1	5.622723000	1.548891000	−0.595258000
1	5.026639000	0.772345000	0.874756000
1	5.222148000	−0.169428000	−0.613724000
1	−0.172356000	1.579703000	0.076457000
1	0.327817000	−2.066425000	−1.632450000
6	2.458336000	0.111677000	1.860319000
1	3.407280000	−0.327916000	2.184917000
1	2.483192000	1.178218000	2.113931000
6	1.288453000	−0.562732000	2.576532000
1	1.276317000	−0.283120000	3.640500000
6	−2.425421000	−0.661470000	1.808808000
1	−3.203772000	−1.380718000	2.086226000
1	−2.774055000	0.334798000	2.098785000
6	−1.117493000	−0.963835000	2.540758000
1	−1.211471000	−0.716940000	3.608625000
7	0.007359000	−0.234196000	1.930002000
1	−0.170478000	0.762943000	2.059028000
25	0.000281000	0.002156000	−0.260904000
1	1.406965000	−1.651575000	2.541904000
1	−0.887902000	−2.033678000	2.485787000
6	−0.092229000	0.528672000	−1.927900000
8	−0.182709000	0.966723000	−3.012830000
6	−0.903504000	3.083647000	1.076756000
8	−0.948957000	2.596718000	2.155553000
8	−0.990256000	3.856923000	0.202396000

I4

15	−2.323225000	−0.219258000	0.035244000
7	−0.186024000	−1.567462000	−1.484154000
6	−1.358468000	−2.446321000	−1.297486000
6	1.069086000	−2.347995000	−1.577001000
6	2.305651000	−1.453753000	−1.483281000
6	−2.643818000	−1.632049000	−1.130336000
1	−3.468060000	−2.278756000	−0.811599000
1	2.423955000	−0.871101000	−2.404480000
15	2.058269000	−0.237054000	−0.106039000
1	−2.923500000	−1.199115000	−2.096644000
1	3.203704000	−2.068484000	−1.364445000
1	−1.458899000	−3.152354000	−2.134615000
1	−1.167520000	−3.041448000	−0.400290000
1	1.068125000	−3.057931000	−0.745211000
1	1.086736000	−2.944216000	−2.500077000
6	−3.751187000	0.944980000	−0.169112000
1	−4.663295000	0.434064000	0.166696000
6	3.474265000	0.943023000	−0.203475000
1	3.407986000	1.482678000	0.749294000
6	−3.503473000	2.176768000	0.712844000
1	−3.410711000	1.924349000	1.772730000
1	−2.583753000	2.687568000	0.410672000

1	–4.335847000	2.880537000	0.612518000
6	–3.919504000	1.366754000	–1.633566000
1	–4.237458000	0.538885000	–2.273594000
1	–4.684971000	2.145767000	–1.706848000
1	–2.987807000	1.778344000	–2.034810000
6	3.228358000	1.966917000	–1.315357000
1	3.128527000	1.491619000	–2.298690000
1	2.325930000	2.542810000	–1.102513000
1	4.072863000	2.661520000	–1.370606000
6	4.838989000	0.260893000	–0.321603000
1	5.636909000	1.008285000	–0.264941000
1	5.010919000	–0.467102000	0.477604000
1	4.943659000	–0.255952000	–1.282327000
1	–0.315452000	1.543282000	0.950485000
1	–0.306218000	–1.080478000	–2.369210000
6	2.362599000	–1.187053000	1.454826000
1	3.206982000	–1.880648000	1.390044000
1	2.593252000	–0.427030000	2.208896000
6	1.085002000	–1.919611000	1.868696000
1	1.159169000	–2.227347000	2.921764000
6	–2.568664000	–0.936884000	1.724571000
1	–3.481362000	–1.535780000	1.813357000
1	–2.657191000	–0.087307000	2.409636000
6	–1.330676000	–1.754013000	2.093206000
1	–1.309379000	–1.943671000	3.175561000
7	–0.100662000	–1.069230000	1.661535000
1	0.044918000	–0.223262000	2.267310000
25	–0.144271000	0.143393000	–0.145293000
1	0.955455000	–2.837692000	1.282887000
1	–1.371478000	–2.736088000	1.607126000
6	–0.187379000	1.305885000	–1.480557000
8	–0.243460000	2.062552000	–2.364929000
6	0.576716000	1.912172000	1.669505000
8	0.631090000	1.273859000	2.745792000
8	1.189462000	2.877897000	1.234844000

3_{Fe}

15	–2.169893000	0.176485000	0.116763000
7	–0.106702000	–0.904678000	–1.450353000
6	–1.301302000	–1.699437000	–1.662769000
6	1.049174000	–1.689163000	–1.839886000
6	2.359954000	–0.909281000	–1.664851000
6	–2.579797000	–0.926549000	–1.306995000
1	–3.428875000	–1.594236000	–1.125614000
1	2.501976000	–0.229257000	–2.513364000
15	2.156134000	0.180131000	–0.187899000
1	–2.847160000	–0.260146000	–2.135241000
1	3.229302000	–1.573856000	–1.616270000
1	–1.375201000	–2.046230000	–2.709271000
1	–1.277912000	–2.633741000	–1.056207000
1	1.120047000	–2.628064000	–1.244215000
1	0.973803000	–2.027750000	–2.888990000

6	−3.520869000	1.435700000	0.206750000
1	−3.345511000	1.936114000	1.168044000
6	3.526121000	1.420478000	−0.304431000
1	3.324932000	1.928179000	−1.257344000
6	−3.325133000	2.473511000	−0.903191000
1	−2.315832000	2.892930000	−0.867359000
1	−3.476138000	2.029880000	−1.893820000
1	−4.048359000	3.288688000	−0.794607000
6	−4.930462000	0.839762000	0.198284000
1	−5.077453000	0.119546000	1.009417000
1	−5.680852000	1.629323000	0.314089000
1	−5.134275000	0.328111000	−0.748514000
6	4.924044000	0.799143000	−0.363174000
1	5.159442000	0.272282000	0.568346000
1	5.023724000	0.088442000	−1.188970000
1	5.682495000	1.577736000	−0.498737000
6	3.403498000	2.458208000	0.815747000
1	4.101642000	3.284575000	0.645198000
1	2.385623000	2.852904000	0.872219000
1	3.651242000	2.019603000	1.789532000
26	−0.009988000	0.401499000	−0.028644000
6	2.569668000	−0.844211000	1.301351000
1	2.842534000	−0.153904000	2.107873000
1	3.415799000	−1.520610000	1.144192000
6	1.323538000	−1.639431000	1.686833000
1	1.158187000	−2.431710000	0.949900000
1	1.454080000	−2.122611000	2.666084000
6	−2.379330000	−0.824939000	1.660816000
1	−3.244593000	−1.495206000	1.638717000
1	−2.527871000	−0.116194000	2.484286000
6	−1.096660000	−1.627302000	1.873981000
1	−1.046611000	−2.430067000	1.131497000
1	−1.087278000	−2.097740000	2.867856000
7	0.109626000	−0.797809000	1.673196000
1	0.030121000	1.742604000	0.831520000
1	0.169905000	−0.099337000	2.410854000

I1

15	2.169757000	0.168967000	−0.133016000
7	0.103324000	−0.911357000	1.483503000
6	1.290394000	−1.701295000	1.649605000
6	−1.055121000	−1.685985000	1.828583000
6	−2.341939000	−0.860189000	1.684616000
6	2.553335000	−0.887074000	1.330391000
1	3.434559000	−1.522840000	1.191656000
1	−2.420899000	−0.154586000	2.520434000
15	−2.161446000	0.178657000	0.171954000
1	2.758199000	−0.196055000	2.156471000
1	−3.239108000	−1.488853000	1.682491000
1	1.383191000	−2.091409000	2.682446000
1	1.301023000	−2.622672000	1.012543000

1	–1.167615000	–2.612981000	1.209859000
1	–1.001798000	–2.065463000	2.868225000
6	3.556889000	1.386106000	–0.278034000
1	3.404602000	1.841997000	–1.265098000
6	–3.548675000	1.403543000	0.240870000
1	–3.353521000	1.953409000	1.171721000
6	3.392153000	2.485084000	0.776961000
1	2.412553000	2.963114000	0.694866000
1	3.491301000	2.081421000	1.790904000
1	4.163384000	3.252340000	0.651620000
6	4.949376000	0.752355000	–0.227424000
1	5.078698000	–0.018709000	–0.993211000
1	5.721353000	1.512849000	–0.387309000
1	5.136019000	0.293059000	0.749042000
6	–4.939576000	0.770005000	0.328516000
1	–5.170298000	0.201609000	–0.579326000
1	–5.030181000	0.094323000	1.183879000
1	–5.706137000	1.545552000	0.432173000
6	–3.442223000	2.393907000	–0.923463000
1	–4.154846000	3.214825000	–0.790713000
1	–2.432016000	2.804549000	–1.000013000
1	–3.679490000	1.908022000	–1.876991000
26	0.004195000	0.490342000	–0.012819000
6	–2.568318000	–0.924967000	–1.257431000
1	–2.833880000	–0.279916000	–2.102920000
1	–3.418478000	–1.586167000	–1.062390000
6	–1.324415000	–1.745619000	–1.590662000
1	–1.178190000	–2.516598000	–0.829617000
1	–1.442223000	–2.254810000	–2.558477000
6	2.371820000	–0.918652000	–1.615773000
1	3.241659000	–1.580420000	–1.554367000
1	2.513430000	–0.257977000	–2.479420000
6	1.094642000	–1.739749000	–1.777546000
1	1.062706000	–2.520850000	–1.013448000
1	1.072132000	–2.236695000	–2.758452000
7	–0.109499000	–0.909041000	–1.584765000
1	–0.055173000	1.628194000	–1.105358000
1	–0.169566000	–0.232088000	–2.342449000
1	0.032656000	1.945420000	0.771818000
1	0.125413000	1.413136000	1.372189000

TS1

15	2.145503000	0.182310000	–0.154557000
7	0.110214000	–0.873325000	1.643780000
6	1.330537000	–1.700964000	1.667380000
6	–1.095699000	–1.698383000	1.845073000
6	–2.374085000	–0.883532000	1.649207000
6	2.570459000	–0.885863000	1.300464000
1	3.422771000	–1.549638000	1.123055000
1	–2.524052000	–0.203516000	2.496407000
15	–2.152970000	0.176823000	0.145704000

1	2.838161000	−0.215902000	2.125775000
1	−3.243040000	−1.547700000	1.598530000
1	1.459929000	−2.187307000	2.645717000
1	1.183680000	−2.494086000	0.927775000
1	−1.055261000	−2.496832000	1.097770000
1	−1.086475000	−2.177913000	2.835163000
6	3.516406000	1.420214000	−0.261275000
1	3.310977000	1.939158000	−1.207065000
6	−3.515452000	1.420768000	0.260937000
1	−3.344562000	1.896601000	1.235529000
6	3.388312000	2.442980000	0.872238000
1	2.370189000	2.836876000	0.927041000
1	3.628978000	1.990438000	1.841481000
1	4.088371000	3.270753000	0.717093000
6	4.916418000	0.804845000	−0.326726000
1	5.020914000	0.106320000	−1.162278000
1	5.671863000	1.588329000	−0.450395000
1	5.152888000	0.266127000	0.597686000
6	−4.921739000	0.817380000	0.236040000
1	−5.125342000	0.335662000	−0.726364000
1	−5.064183000	0.071110000	1.024082000
1	−5.675531000	1.599326000	0.378104000
6	−3.324919000	2.489494000	−0.820353000
1	−4.054281000	3.296023000	−0.689846000
1	−2.317417000	2.910706000	−0.774567000
1	−3.473582000	2.071268000	−1.822465000
26	−0.006374000	0.443806000	−0.005695000
1	0.040569000	1.677143000	0.962549000
1	0.164454000	−0.165145000	2.373011000
6	−2.568087000	−0.895088000	−1.309518000
1	−2.803683000	−0.205600000	−2.128878000
1	−3.441520000	−1.536955000	−1.154054000
6	−1.322847000	−1.719481000	−1.674780000
1	−1.299685000	−2.627998000	−1.035643000
1	−1.438065000	−2.098237000	−2.706730000
6	2.354794000	−0.885157000	−1.655889000
1	3.242624000	−1.525642000	−1.628090000
1	2.472885000	−0.187836000	−2.494329000
6	1.074463000	−1.713641000	−1.848505000
1	1.144897000	−2.625501000	−1.217761000
1	1.045426000	−2.086456000	−2.888672000
7	−0.108424000	−0.953351000	−1.519843000
1	−0.098357000	1.400055000	−1.349247000
1	−0.120708000	0.455733000	−1.662850000

I2

15	2.117866000	0.204926000	−0.146975000
7	0.111558000	−0.941342000	1.606848000
6	1.351844000	−1.726601000	1.685951000
6	−1.101917000	−1.734970000	1.848839000
6	−2.366684000	−0.895457000	1.633857000

6	2.571246000	−0.880036000	1.303115000
1	3.440240000	−1.523154000	1.127425000
1	−2.514870000	−0.224006000	2.488316000
15	−2.117878000	0.204894000	0.146964000
1	2.824520000	−0.204474000	2.128672000
1	−3.245918000	−1.545705000	1.571320000
1	1.486466000	−2.166597000	2.686061000
1	1.247079000	−2.563800000	0.986297000
1	−1.085915000	−2.570518000	1.139547000
1	−1.099642000	−2.177251000	2.857018000
6	3.506779000	1.421607000	−0.270291000
1	3.323774000	1.906942000	−1.238087000
6	−3.506732000	1.421637000	0.270256000
1	−3.323693000	1.906987000	1.238037000
6	3.348181000	2.485269000	0.820985000
1	2.332373000	2.888239000	0.819931000
1	3.543467000	2.063969000	1.814343000
1	4.063877000	3.299597000	0.664308000
6	4.906696000	0.803616000	−0.276536000
1	5.030356000	0.066039000	−1.075808000
1	5.666121000	1.579887000	−0.420732000
1	5.123255000	0.308870000	0.676816000
6	−4.906670000	0.803690000	0.276535000
1	−5.123254000	0.308923000	−0.676800000
1	−5.030344000	0.066140000	1.075830000
1	−5.666070000	1.579989000	0.420717000
6	−3.348111000	2.485265000	−0.821047000
1	−4.063788000	3.299612000	−0.664385000
1	−2.332293000	2.888206000	−0.820005000
1	−3.543411000	2.063945000	−1.814394000
26	−0.000021000	0.470707000	−0.000008000
1	0.066646000	1.582008000	1.104390000
1	0.152804000	−0.163301000	2.263744000
6	−2.571261000	−0.880094000	−1.303103000
1	−2.824524000	−0.204546000	−2.128675000
1	−3.440256000	−1.523207000	−1.127407000
6	−1.351850000	−1.726668000	−1.685911000
1	−1.247094000	−2.563854000	−0.986239000
1	−1.486465000	−2.166683000	−2.686013000
6	2.366669000	−0.895482000	−1.633831000
1	3.245914000	−1.545713000	−1.571275000
1	2.514841000	−0.224059000	−2.488315000
6	1.101919000	−1.735028000	−1.848786000
1	1.085934000	−2.570558000	−1.139473000
1	1.099651000	−2.177336000	−2.856954000
7	−0.111563000	−0.941409000	−1.606814000
1	−0.066852000	1.581869000	−1.104543000
1	−0.152807000	−0.163370000	−2.263712000

I3

15	−2.209883000	0.033524000	−0.070042000

7	−0.403396000	−2.188730000	−0.512189000
6	−1.687173000	−2.686015000	0.004111000
6	0.741871000	−3.034832000	−0.147223000
6	2.062033000	−2.408856000	−0.610478000
6	−2.827935000	−1.710552000	−0.308779000
1	−3.713531000	−1.957600000	0.286350000
1	2.179414000	−2.550621000	−1.691607000
15	1.992805000	−0.564809000	−0.335397000
1	−3.107776000	−1.797809000	−1.365242000
1	2.907721000	−2.903484000	−0.120720000
1	−1.917591000	−3.687363000	−0.390739000
1	−1.577550000	−2.794260000	1.089249000
1	0.737749000	−3.130171000	0.944572000
1	0.635038000	−4.052645000	−0.552700000
6	−3.511132000	1.102694000	−0.835436000
1	−3.229109000	2.110488000	−0.502699000
6	3.443384000	0.065342000	−1.297865000
1	3.236184000	−0.281139000	−2.318896000
6	−3.371393000	1.060652000	−2.360593000
1	−2.336985000	1.251092000	−2.657190000
1	−3.661206000	0.080157000	−2.756796000
1	−4.026429000	1.807182000	−2.822512000
6	−4.940246000	0.805862000	−0.375990000
1	−5.046577000	0.866543000	0.711714000
1	−5.640084000	1.522906000	−0.818744000
1	−5.255430000	−0.194883000	−0.691727000
6	4.799287000	−0.483904000	−0.848702000
1	5.044104000	−0.147181000	0.164654000
1	4.826084000	−1.578095000	−0.857135000
1	5.594454000	−0.127109000	−1.512305000
6	3.417656000	1.596656000	−1.313396000
1	4.197047000	1.984950000	−1.977749000
1	2.445102000	1.961993000	−1.651708000
1	3.609933000	2.003897000	−0.312954000
26	−0.096331000	−0.073682000	−0.394371000
1	−0.188742000	−0.081096000	−1.959620000
1	−0.453267000	−2.094850000	−1.526005000
6	2.485461000	−0.350353000	1.449984000
1	2.825836000	0.685784000	1.558128000
1	3.303917000	−1.004102000	1.769795000
6	1.250014000	−0.571577000	2.329143000
1	1.039314000	−1.643655000	2.415223000
1	1.433753000	−0.201117000	3.348945000
6	−2.400884000	0.342832000	1.758920000
1	−3.320590000	−0.064937000	2.192151000
1	−2.433774000	1.432232000	1.882516000
6	−1.174757000	−0.221910000	2.484582000
1	−1.261422000	−1.311290000	2.566702000
1	−1.120812000	0.169293000	3.511927000
7	0.060515000	0.061596000	1.737907000
1	0.084271000	1.477108000	−0.454687000

1	0.213014000	1.068406000	1.713715000
6	0.998185000	3.449272000	0.472684000
8	0.895635000	4.048071000	−0.518790000
8	1.158447000	2.979985000	1.535732000

TS2

15	−2.024309000	−0.314304000	−0.094206000
7	0.162081000	−2.135166000	−0.645681000
6	−1.029681000	−2.892435000	−0.234075000
6	1.426132000	−2.792323000	−0.280780000
6	2.632108000	−1.922854000	−0.656157000
6	−2.311406000	−2.104386000	−0.522841000
1	−3.161334000	−2.554898000	0.000364000
1	2.807864000	−1.981255000	−1.737155000
15	2.230154000	−0.139093000	−0.291359000
1	−2.531021000	−2.134502000	−1.596448000
1	3.535016000	−2.290697000	−0.157315000
1	−1.064834000	−3.879034000	−0.720415000
1	−0.940941000	−3.076030000	0.842632000
1	1.404142000	−2.952668000	0.803063000
1	1.509358000	−3.786626000	−0.745390000
6	−3.488998000	0.578185000	−0.787837000
1	−3.416627000	1.574863000	−0.333271000
6	3.533530000	0.806088000	−1.200689000
1	3.387009000	0.492630000	−2.242709000
6	−3.308235000	0.749716000	−2.299365000
1	−2.331567000	1.185760000	−2.522006000
1	−3.375537000	−0.213912000	−2.818140000
1	−4.094140000	1.396918000	−2.702851000
6	−4.843405000	−0.035973000	−0.427905000
1	−4.977277000	−0.137619000	0.653796000
1	−5.657983000	0.590777000	−0.806403000
1	−4.958426000	−1.027956000	−0.878515000
6	4.968823000	0.485127000	−0.777843000
1	5.151740000	0.790875000	0.258157000
1	5.195590000	−0.582586000	−0.860668000
1	5.682249000	1.026380000	−1.408585000
6	3.225540000	2.304902000	−1.117706000
1	3.903249000	2.867665000	−1.768504000
1	2.192408000	2.502613000	−1.414056000
1	3.362931000	2.681199000	−0.097088000
26	0.091320000	−0.018296000	−0.366779000
1	0.018429000	0.078496000	−1.927429000
1	0.134757000	−1.978624000	−1.652598000
6	2.651615000	0.074453000	1.510729000
1	2.781604000	1.150779000	1.673584000
1	3.579406000	−0.420529000	1.816828000
6	1.473189000	−0.432703000	2.348326000
1	1.476498000	−1.528442000	2.366994000
1	1.570483000	−0.098703000	3.392169000
6	−2.282173000	−0.233709000	1.750508000

1	−3.101643000	−0.861800000	2.116057000
1	−2.535675000	0.807513000	1.980985000
6	−0.971285000	−0.605312000	2.453225000
1	−0.832944000	−1.692256000	2.436194000
1	−1.007523000	−0.306213000	3.511481000
7	0.187983000	−0.007860000	1.769473000
1	0.097733000	1.550716000	−0.330262000
1	0.113390000	1.007096000	1.841348000
6	−0.935985000	3.097104000	0.489792000
8	−1.357215000	3.554992000	−0.500373000
8	−0.676214000	2.897834000	1.624755000

I4

15	−2.096788000	−0.210197000	−0.062377000
7	0.068001000	−1.981305000	−0.860784000
6	−1.138726000	−2.755051000	−0.506979000
6	1.308540000	−2.722381000	−0.565906000
6	2.547143000	−1.873273000	−0.864882000
6	−2.409348000	−1.923382000	−0.694027000
1	−3.260701000	−2.416746000	−0.214863000
1	2.711091000	−1.820097000	−1.947605000
15	2.234938000	−0.135591000	−0.295981000
1	−2.641150000	−1.825396000	−1.760754000
1	3.437420000	−2.327999000	−0.418981000
1	−1.190456000	−3.683626000	−1.092989000
1	−1.036587000	−3.047771000	0.542653000
1	1.280419000	−2.983139000	0.496752000
1	1.343531000	−3.667758000	−1.125846000
6	−3.499374000	0.829892000	−0.647102000
1	−3.371416000	1.756853000	−0.075228000
6	3.536641000	0.878655000	−1.122683000
1	3.402052000	0.648780000	−2.187756000
6	−3.288866000	1.183905000	−2.122154000
1	−2.327046000	1.684791000	−2.249604000
1	−3.314908000	0.293785000	−2.762624000
1	−4.084997000	1.856494000	−2.457454000
6	−4.876969000	0.225848000	−0.368298000
1	−5.019857000	−0.009374000	0.691318000
1	−5.661281000	0.932115000	−0.659110000
1	−5.033945000	−0.692499000	−0.945649000
6	4.966194000	0.521439000	−0.708555000
1	5.141490000	0.759279000	0.345980000
1	5.188107000	−0.539977000	−0.859151000
1	5.686115000	1.098611000	−1.297828000
6	3.225886000	2.366468000	−0.921046000
1	3.945737000	2.978588000	−1.473740000
1	2.219576000	2.609348000	−1.271474000
1	3.293722000	2.651431000	0.134684000
26	0.063979000	0.043283000	−0.336491000
1	−0.021654000	0.351442000	−1.855618000
1	0.038583000	−1.766099000	−1.856467000

6	2.648410000	−0.119352000	1.512803000
1	2.777957000	0.934658000	1.784990000
1	3.575913000	−0.645483000	1.760628000
6	1.463809000	−0.699665000	2.293918000
1	1.461906000	−1.793593000	2.213977000
1	1.567151000	−0.462969000	3.362619000
6	−2.283234000	−0.302880000	1.781184000
1	−3.137202000	−0.901895000	2.113618000
1	−2.441177000	0.732041000	2.104733000
6	−0.979929000	−0.820325000	2.402138000
1	−0.898463000	−1.906767000	2.275149000
1	−0.983300000	−0.627722000	3.484721000
7	0.189680000	−0.195014000	1.763229000
1	0.212324000	1.772167000	−0.159561000
1	0.125103000	0.834315000	1.945639000
6	−0.522436000	2.491613000	0.466735000
8	−1.248294000	3.163746000	−0.251410000
8	−0.340454000	2.440110000	1.702784000