

## Supporting Information

(Total of 66 pages)

### Can the bis(imino)pyridine Iron, (PDI)FeL<sup>1</sup>L<sup>2</sup>, Complexes Catalyze the C-H Bond Functionalization?

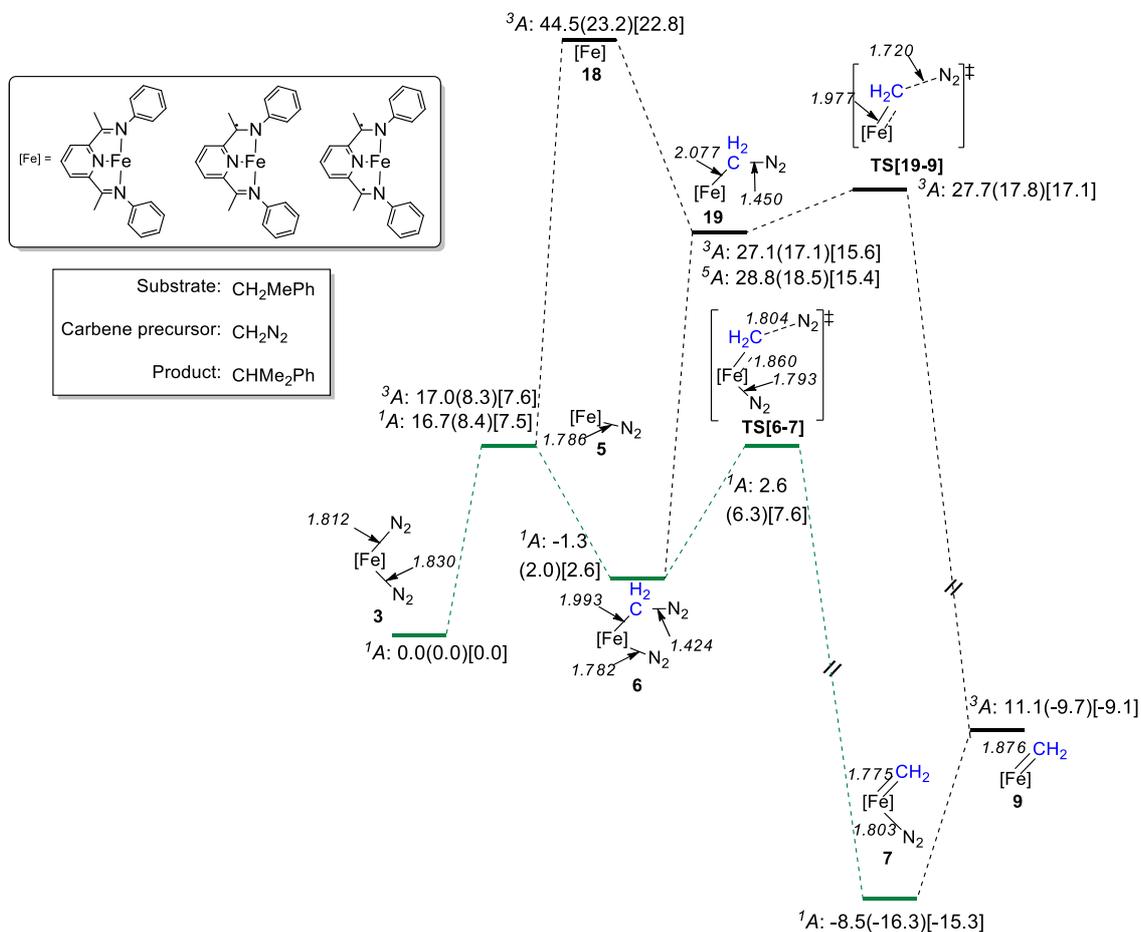
Adrián Varela-Álvarez and Djamaladdin G. Musaev

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2. **Scheme S2.** Complete reaction profile for the C-H functionalization reaction (1) and several competing reaction (including diazo coupling) catalyzed by **4**. In these reactions the CH<sub>2</sub>N<sub>2</sub> employed as a carbene precursor.
3. **Scheme S3.** Key steps of the reaction (1). Here we present energies { $\Delta H(\Delta G)[\Delta G_{\text{sol}}]$  in kcal/mol} and schematic structures of the reactants, intermediates and products of the reactions (1b) and (1c) utilizing the model complex **3** and the donor-acceptor(D/A) CPh(COH)N<sub>2</sub> carbene precursor.
4. **Scheme S4.** Complete reaction profile for the C-H functionalization reaction (1) and several competing reaction (including diazo coupling) catalyzed by **4**. In these reactions the donor-acceptor CPh(COH)N<sub>2</sub> employed as a carbene precursor.
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9. **Table S4.** Absolute energies of the structures involved in the C-H functionalization reaction (1) and related competing processes catalyzed by **4**. In these reactions the donor-acceptor CPh(COH)N<sub>2</sub> employed as a carbene precursor.
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**Scheme S1.** Complete reaction profile for the C-H functionalization reaction (1) and the competing homocoupling reaction catalyzed by complex **3**. In these reactions the  $\text{CH}_2\text{N}_2$  employed as a carbene precursor. All energy values (presented as  $\Delta\text{H}(\Delta\text{G})[\Delta\text{G}_{\text{sol}}]$ ) are given in kcal/mol and all distances (in blue) are given in Å.

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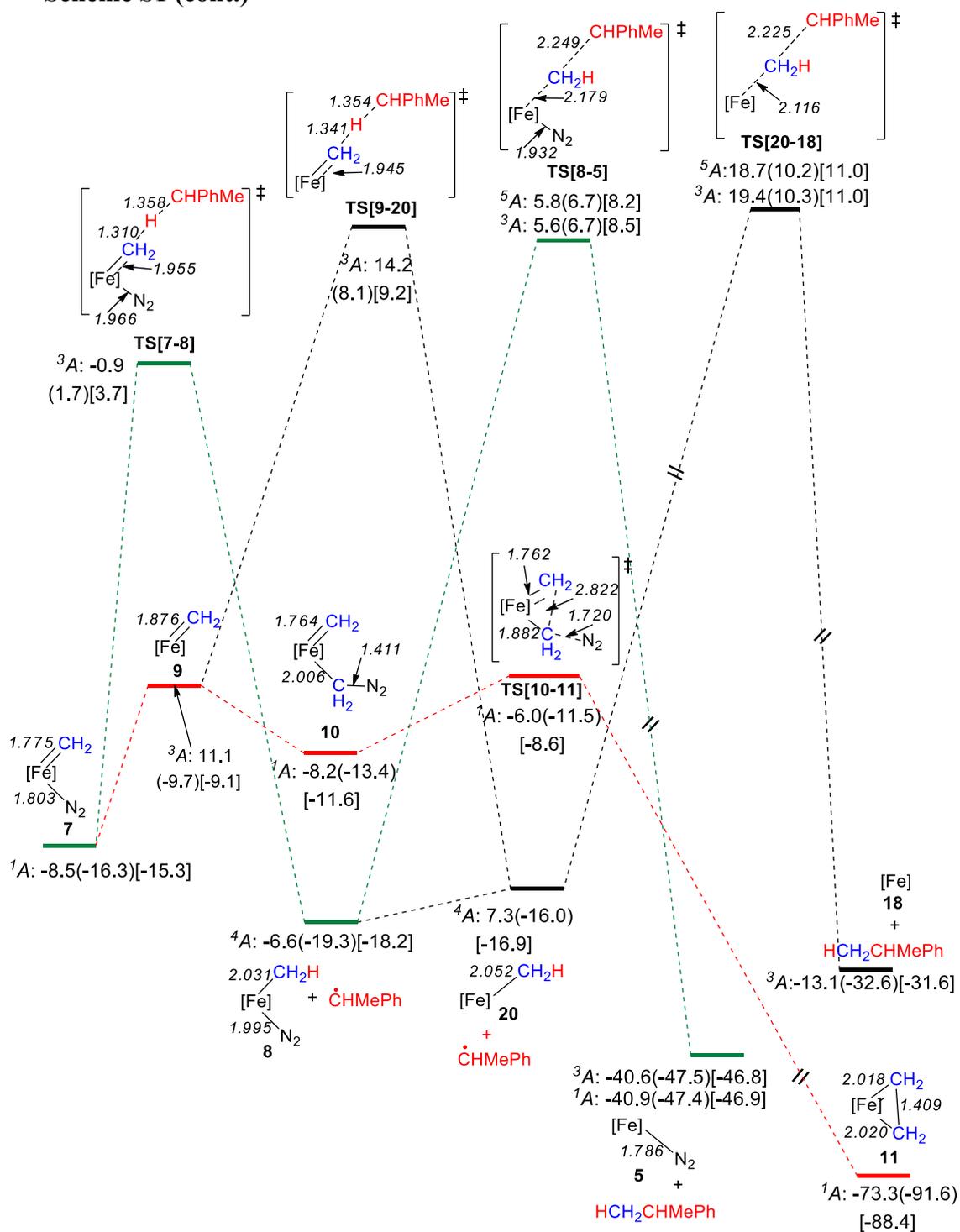


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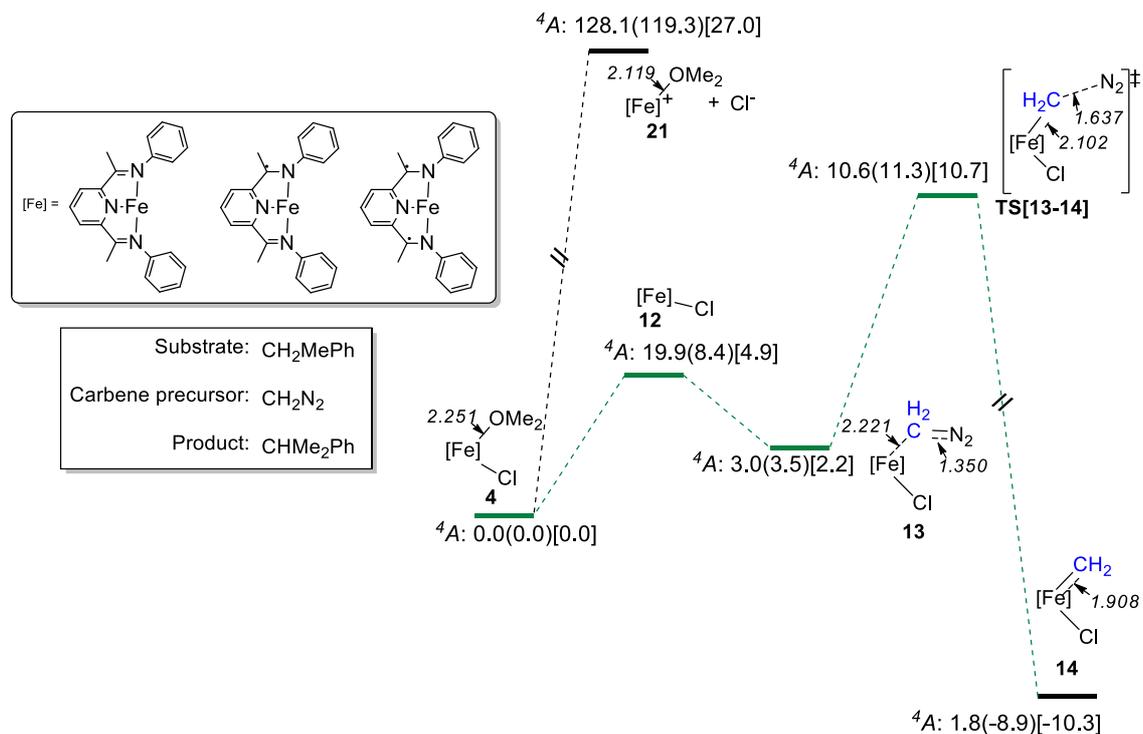
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Scheme S1 (cont.)



5 **Scheme S2.** Complete reaction profile for the C-H functionalization reaction (1) and several competing reaction (including diazo coupling) catalyzed by **4**. In these reactions the  $\text{CH}_2\text{N}_2$  employed as a carbene precursor. All energy values (presented as  $\Delta\text{H}(\Delta\text{G})[\Delta\text{G}_{\text{sol}}]$ ) are given in kcal/mol and all distances (in blue) are given in Å.

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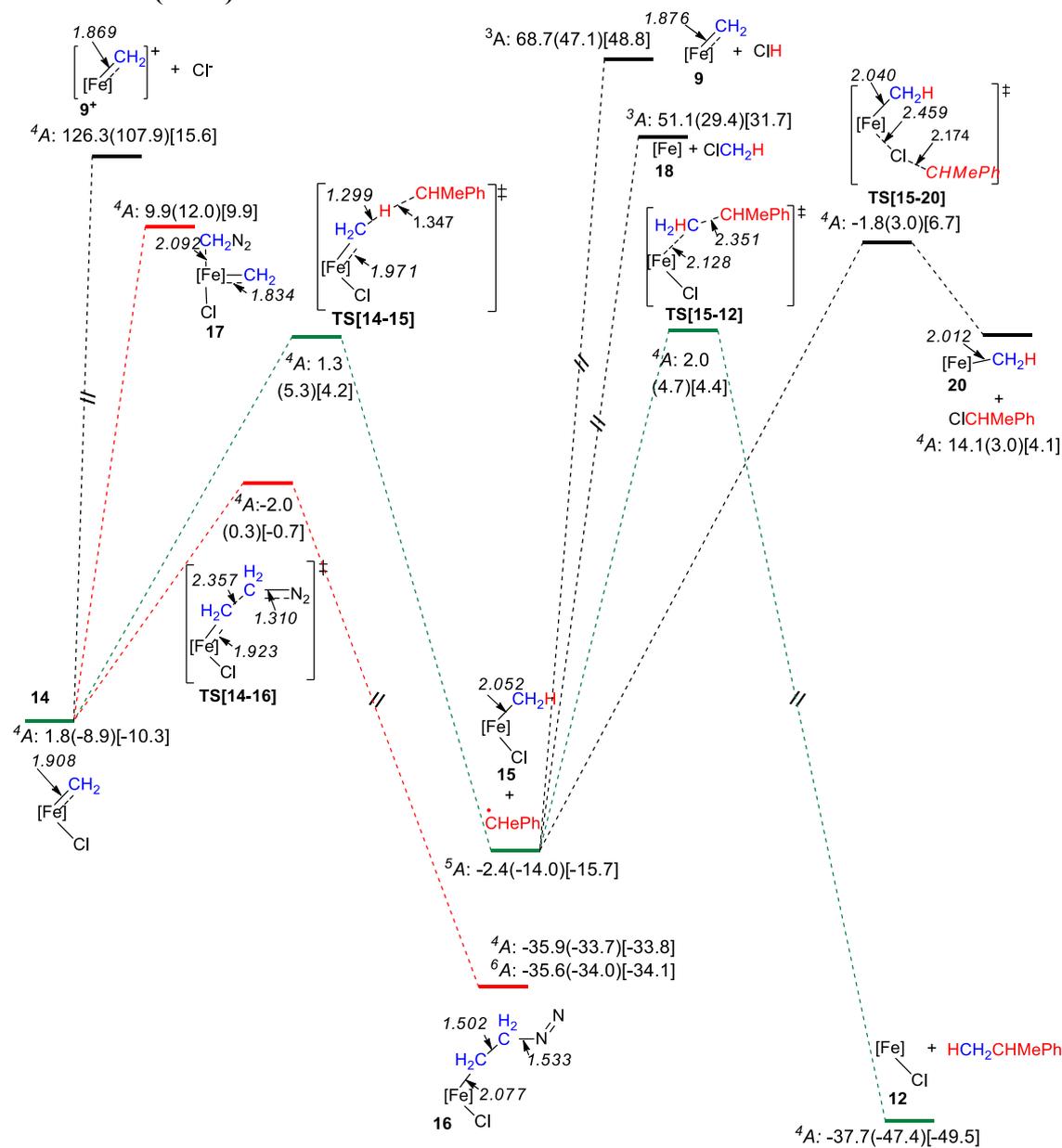
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Scheme S2 (cont.).



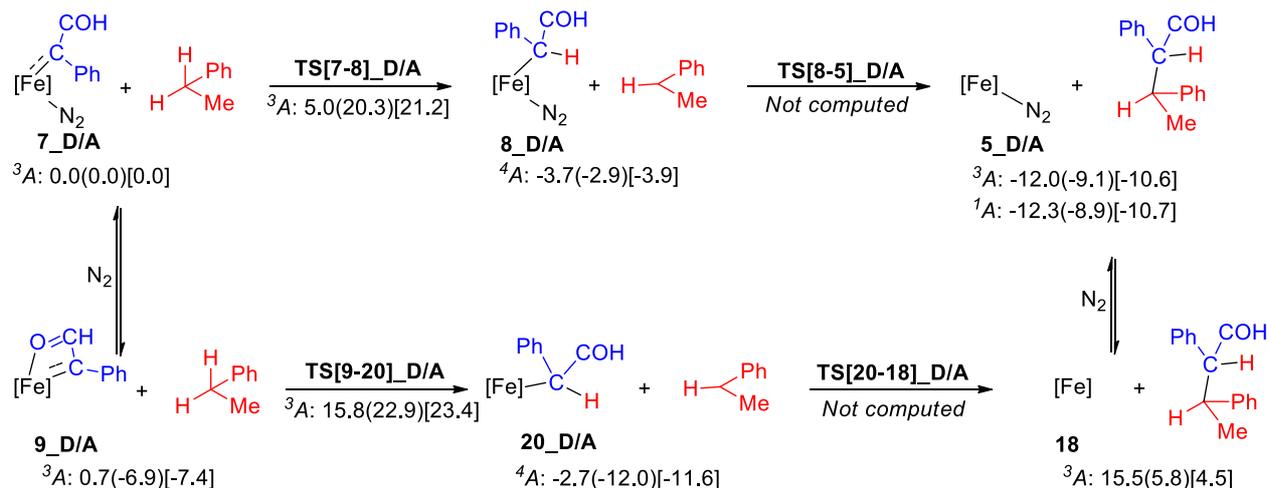
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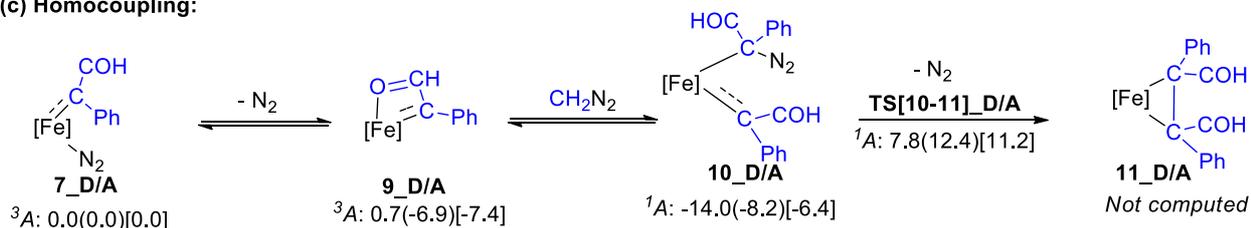
5 **Scheme S3.** Key steps of the reaction (1). Here we present energies  $\{\Delta H(\Delta G)[\Delta G_{\text{sol}}]$  in kcal/mol} and schematic structures of the reactants, intermediates and products of the reactions (1b) and (1c) utilizing the model complex **3** and the donor-acceptor(D/A) CPh(COH)N<sub>2</sub> carbene precursor.

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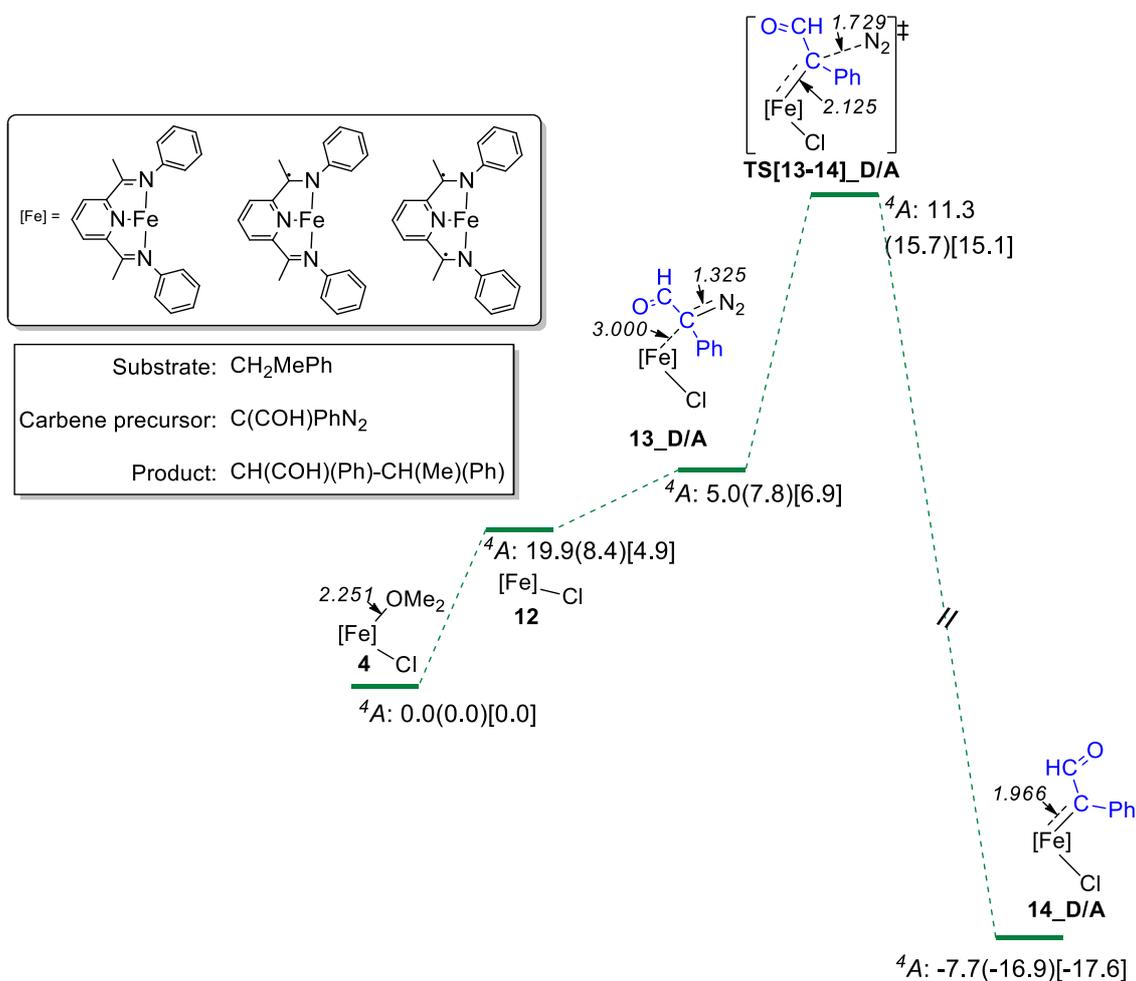
(b) C-H Functionalization:



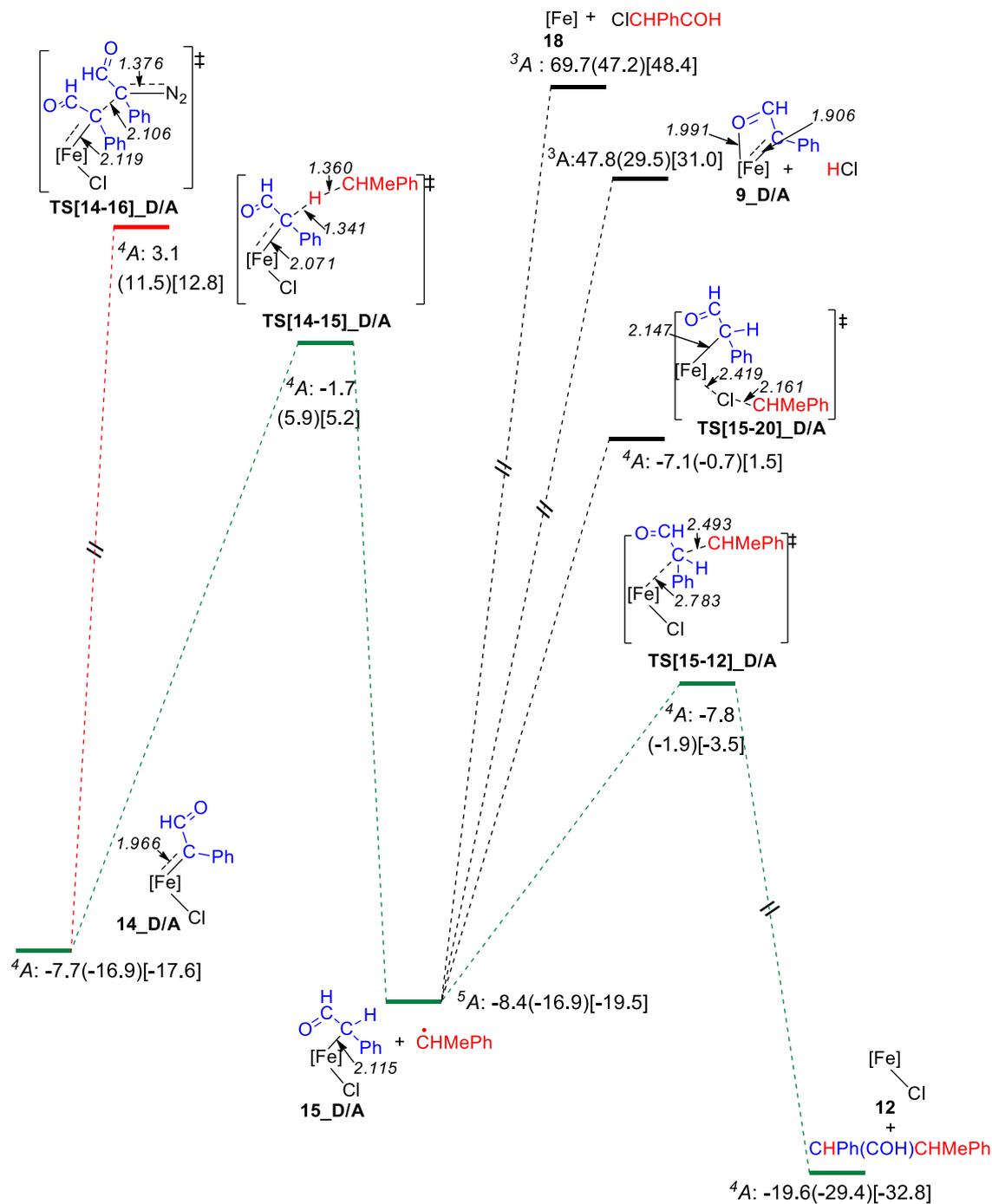
(c) Homocoupling:



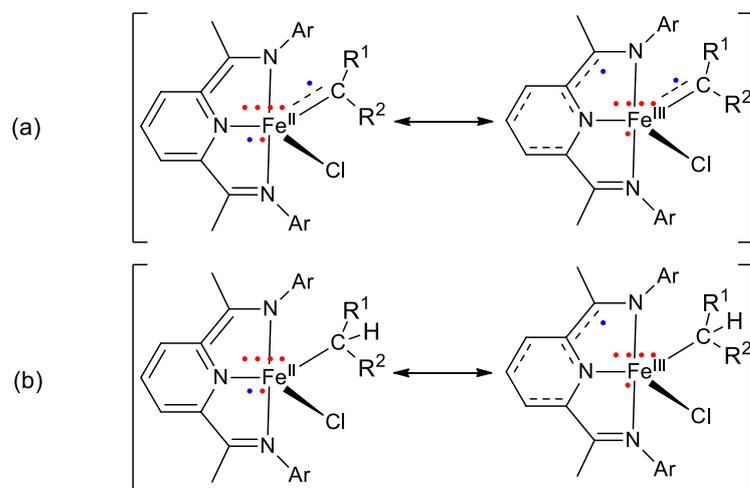
**Scheme S4.** Complete reaction profile for the C-H functionalization reaction (1) and several competing reaction (including diazo coupling) catalyzed by **4**. In these reactions the donor-acceptor CPh(COH)N<sub>2</sub> employed as a carbene precursor. All energy values (presented as  $\Delta H(\Delta G)[\Delta G_{sol}]$ ) are given in kcal/mol and all distances (in blue) are given in Å.



Scheme S4 (cont.)



**Chart S1.** Main resonance structures contributing to the carbenoids (**14** and **14\_D/A**) and alkyl complexes (**15** and **15\_D/A**) presented in this paper.



**Table S1.** Absolute energies of the structures involved in the C-H functionalization reaction (1) and related competing processes catalyzed by **3**. In these reactions the CH<sub>2</sub>N<sub>2</sub> employed as a carbene precursor. Thermodynamic parameters were computed at 298.15 K and 1 atm. All values are given in a.u., but entropy values are given in cal·mol<sup>-1</sup>·K<sup>-1</sup>.

STRUCTURE	M <sub>s</sub>	E	H	S	G	E <sub>solv</sub>
<b>3</b>	7	-1318.390723	-1317.999428	204.4	-1318.096529	-1318.399735
	5	-1318.425268	-1318.032485	190.8	-1318.123131	-1318.434783
	3	-1318.425668	-1318.032261	184.5	-1318.119930	-1318.433316
	1	-1318.462056	-1318.066522	178.8	-1318.151465	-1318.470469
CH <sub>2</sub> N <sub>2</sub>	1	-148.729695	-148.693343	58.2	-148.720996	-148.732231
N <sub>2</sub>	1	-109.512732	-109.503907	45.8	-109.525669	-109.513089
CH <sub>2</sub> MePh (BnH)	1	-310.842513	-310.677147	84.6	-310.717355	-310.844513
<b>5</b>	7	-1208.865221	-1208.483879	178.8	-1208.568825	-1208.879207
	5	-1208.899931	-1208.518065	170.7	-1208.599152	-1208.911984
	3	-1208.916856	-1208.535515	162.2	-1208.612601	-1208.925998
	1	-1208.918780	-1208.536023	160.7	-1208.612374	-1208.928300
<b>6</b>	7	-1357.631509	-1357.211476	201.8	-1357.307335	-1357.642830
	5	-1357.657687	-1357.236764	195.4	-1357.329588	-1357.669609
	3	-1357.658813	-1357.238314	193.7	-1357.330369	-1357.668735
	1	-1357.680663	-1357.257973	180.2	-1357.343605	-1357.690249
TS[6-7]	7	-1357.620829	-1357.203565	203.1	-1357.300080	-1357.629716
	5	-1357.645611	-1357.227235	198.4	-1357.321505	-1357.656024
	3	-1357.655049	-1357.236384	195.2	-1357.329145	-1357.663855
	1	-1357.672729	-1357.251821	178.8	-1357.336780	-1357.681187
<b>7</b>	7	-1248.120288	-1247.713809	193.9	-1247.805929	-1248.127533
	5	-1248.141192	-1247.733714	188.4	-1247.823227	-1248.150270
	3	-1248.163676	-1247.755375	183.1	-1247.842385	-1248.172393
	1	-1248.176737	-1247.765637	171.4	-1247.847065	-1248.185414
<b>18</b>	7	-1099.336691	-1098.965367	159.6	-1099.041176	-1099.351858
	5	-1099.352921	-1098.981226	152.2	-1099.053533	-1099.367647
	3	-1099.358936	-1098.987849	158.6	-1099.063200	-1099.367255
	1	-1099.344532	-1098.973109	147.4	-1099.043131	-1099.344933
<b>19</b>	7	-1248.099457	-1247.689557	185.1	-1247.777486	-1248.114816
	5	-1248.116918	-1247.706084	180.2	-1247.791721	-1248.132027
	3	-1248.118861	-1247.708905	178.8	-1247.793848	-1248.131446
	1	-1248.107501	-1247.697047	174.7	-1247.780044	-1248.120585
TS[19-9]	7	-1248.090778	-1247.683371	186.0	-1247.771751	-1248.105363
	5	-1248.106843	-1247.698823	182.5	-1247.785548	-1248.119961
	3	-1248.116108	-1247.707842	178.9	-1247.792823	-1248.127366
	1	-1248.104210	-1247.694754	167.6	-1247.774400	-1248.113635

**Table S1 (cont.).**

STRUCTURE	M <sub>s</sub>	E	H	S	G	E <sub>solv</sub>
<b>9</b>	7	-1138.597600	-1138.200337	172.1	-1138.282117	-1138.611942
	5	-1138.616928	-1138.219719	172.7	-1138.301787	-1138.623938
	3	-1138.628013	-1138.230424	169.4	-1138.310910	-1138.636949
	1	-1138.627784	-1138.229615	165.5	-1138.308249	-1138.636189
<b>10</b>	7	-1287.348905	-1286.913986	194.9	-1287.006584	-1287.361118
	5	-1287.371627	-1286.936701	191.5	-1287.027696	-1287.380876
	3	-1287.381708	-1286.946536	189.6	-1287.036629	-1287.391142
	1	-1287.392619	-1286.954586	175.2	-1287.037843	-1287.402171
<b>TS[10-11]</b>	7	-1287.348854	-1286.914728	189.7	-1287.004863	-1287.358782
	5	-1287.365190	-1286.931122	190.3	-1287.021551	-1287.375545
	3	-1287.372635	-1286.938908	187.8	-1287.028131	-1287.380004
	1	-1287.387685	-1286.951012	176.2	-1287.034725	-1287.395546
<b>11</b>	7	-1177.949069	-1177.522087	170.6	-1177.603136	-1177.958688
	5	-1177.974395	-1177.546074	177.6	-1177.630437	-1177.982986
	3	-1177.981599	-1177.554741	167.2	-1177.634161	-1177.988752
	1	-1177.983828	-1177.554465	173.1	-1177.636701	-1177.990788
<b>TS[7-8]</b>	7	-1558.964388	-1558.395964	228.2	-1558.504373	-1558.972275
	5	-1558.986670	-1558.417123	224.0	-1558.523559	-1558.995449
	3	-1559.000582	-1558.430686	221.0	-1558.535713	-1559.009655
	1	-1558.999202	-1558.426185	211.6	-1558.526724	-1559.010043
<b>8</b>	6	-1248.793197	-1248.373236	188.7	-1248.462893	-1248.800543
	4	-1248.814478	-1248.393284	185.2	-1248.481258	-1248.822824
	2	-1248.812792	-1248.390457	176.4	-1248.474287	-1248.820056
<b>TS[8-5]</b>	7	-1558.963619	-1558.391763	222.1	-1558.497270	-1558.972488
	5	-1558.994089	-1558.419970	227.0	-1558.527810	-1559.003919
	3	-1558.994366	-1558.420334	226.2	-1558.527799	-1559.003756
	1	-1558.997044	-1558.421767	217.9	-1558.525300	-1559.006663
<b>TS[9-20]</b>	7	-1449.434746	-1448.876234	213.2	-1448.977524	-1449.447247
	5	-1449.457722	-1448.898816	204.8	-1448.996144	-1449.467234
	3	-1449.461921	-1448.902661	204.8	-1448.999948	-1449.472032
	1	-1449.449135	-1448.888902	200.8	-1448.984332	-1449.458949
<b>20</b>	6	-1139.267788	-1138.857583	175.6	-1138.941039	-1139.277083
	4	-1139.277374	-1138.867215	174.9	-1138.950337	-1139.288442
	2	-1139.275077	-1138.864089	166.8	-1138.943355	-1139.284617
<b>TS[20-18]</b>	7	-1449.445480	-1448.882981	212.2	-1448.983817	-1449.455711
	5	-1449.459147	-1448.895502	212.7	-1448.996582	-1449.469713
	3	-1449.457515	-1448.894444	214.6	-1448.996416	-1449.468262
	1	-	-	-	-	-
rad. Bn	2	-310.197604	-310.046418	87.4	-310.087946	-310.199839
CH3Bn	1	-350.153156	-349.958381	91.0	-350.001612	-350.155134

**Table S2.** Absolute energies of the structures involved in the C-H functionalization reaction (1) and related competing processes catalyzed by **3**. In these reactions the donor-acceptor CPh(COH)N<sub>2</sub> employed as a carbene precursor. Thermodynamic parameters were computed at 298.15 K and 1 atm. All values are given in a.u., but entropy values are given in cal·mol<sup>-1</sup>·K<sup>-1</sup>.

STRUCTURE	M <sub>s</sub>	E	H	S	G	E <sub>solv</sub>
C(COH)PhN <sub>2</sub>	1	-493.090975	-492.956070	95.5	-493.001441	-493.096135
<b>7_D/A</b>	3	-1592.538571	-1592.031613	215.7	-1592.134102	-1592.549936
	1	-1592.534037	-1592.024739	198.3	-1592.118980	-1592.551264
<b>TS[7-8]_D/A</b>	3	-1903.369067	-1902.700717	249.2	-1902.819116	-1903.381035
	1	-1903.364244	-1902.693303	231.4	-1902.803270	-1903.377312
<b>8_D/A</b>	4	-1593.188195	-1592.668233	210.2	-1592.768102	-1593.200968
<b>9_D/A</b>	3	-1483.024197	-1482.526525	195.6	-1482.619451	-1483.035972
	1	-1483.008472	-1482.510735	193.8	-1482.602800	-1483.019303
<b>TS[9-20]_D/A</b>	3	-1793.838192	-1793.179712	230.6	-1793.289299	-1793.850424
	1	-1793.822619	-1793.163648	224.9	-1793.270522	-1793.834871
<b>20_D/A</b>	4	-1483.671855	-1483.162757	198.1	-1483.256895	-1483.682035
<b>10_D/A</b>	3	-1976.139797	-1975.506035	246.2	-1975.623009	-1976.153001
	1	-1976.101537	-1975.467663	234.5	-1975.579102	-1976.145230
<b>TS[10-11]_D/A</b>	3	-1976.101103	-1975.471302	250.0	-1975.590073	-1976.119282
	1	-1976.084566	-1975.452320	228.8	-1975.561031	-1976.100725

**Table S3.** Absolute energies of the structures involved in the C-H functionalization reaction (1) and related competing processes catalyzed by **4**. In these reactions the CH<sub>2</sub>N<sub>2</sub> employed as a carbene precursor. Thermodynamic parameters were computed at 298.15 K and 1 atm. All values are given in a.u., but entropy values are given in cal·mol<sup>-1</sup>·K<sup>-1</sup>.

STRUCTURE	M <sub>s</sub>	E	H	S	G	E <sub>solv</sub>
<b>4</b>	6	-1714.654094	-1714.191209	196.1	-1714.284361	-1714.669768
	4	-1714.66493	-1714.201543	195.0	-1714.294179	-1714.679850
	2	-1714.649013	-1714.185362	191.9	-1714.276496	-1714.664108
OMe <sub>2</sub>	1	-155.0008937	-154.915941	62.9	-154.945835	-155.003052
<b>12</b>	6	-1559.619465	-1559.242981	168.1	-1559.322843	-1559.635102
	4	-1559.630257	-1559.253848	170.8	-1559.334989	-1559.648522
	2	-1559.620513	-1559.245341	163.3	-1559.322949	-1559.637675
<b>13</b>	6	-1708.375102	-1707.961116	192.0	-1708.05234	-1708.392239
	4	-1708.388468	-1707.974171	188.6	-1708.063762	-1708.405894
	2	-1708.378422	-1707.963507	182.3	-1708.050106	-1708.395948
<b>TS[13-14]</b>	6	-1708.358897	-1707.976872	192.6	-1708.038959	-1708.376527
	4	-1708.37439	-1707.9621	188.0	-1708.051409	-1708.390625
	2	-1708.365206	-1707.952167	180.1	-1708.037751	-1708.381781

**Table S3 (Cont.).**

STRUCTURE	M <sub>s</sub>	E	H	S	G	E <sub>solv</sub>
<b>4</b>	6	-1714.654094	-1714.191209	196.1	-1714.284361	-1714.669768
	4	-1714.66493	-1714.201543	195.0	-1714.294179	-1714.679850
	2	-1714.649013	-1714.185362	191.9	-1714.276496	-1714.664108
OMe <sub>2</sub>	1	-155.0008937	-154.915941	62.9	-154.945835	-155.003052
<b>12</b>	6	-1559.619465	-1559.242981	168.1	-1559.322843	-1559.635102
	4	-1559.630257	-1559.253848	170.8	-1559.334989	-1559.648522
	2	-1559.620513	-1559.245341	163.3	-1559.322949	-1559.637675
<b>13</b>	6	-1708.375102	-1707.961116	192.0	-1708.05234	-1708.392239
	4	-1708.388468	-1707.974171	188.6	-1708.063762	-1708.405894
	2	-1708.378422	-1707.963507	182.3	-1708.050106	-1708.395948
<b>TS[13-14]</b>	6	-1708.358897	-1707.976872	192.6	-1708.038959	-1708.376527
	4	-1708.37439	-1707.9621	188.0	-1708.051409	-1708.390625
	2	-1708.365206	-1707.952167	180.1	-1708.037751	-1708.381781
<b>14</b>	6	-1598.852919	-1598.451901	179.9	-1598.53739	-1598.871965
	4	-1598.87339	-1598.472109	180.4	-1598.557799	-1598.890662
	2	-1598.862208	-1598.45996	172.2	-1598.541783	-1598.878905
<b>TS[14-15]</b>	6	-1909.701896	-1909.138908	216.4	-1909.241724	-1909.719535
	4	-1909.713576	-1909.15011	215.6	-1909.252555	-1909.732340
	2	-1909.699278	-1909.135154	211.6	-1909.235674	-1909.717271
<b>15</b>	5	-1599.524091	-1599.109537	180.8	-1599.195455	-1599.541464
	3	-1599.509991	-1599.095204	181.2	-1599.18131	-1599.525856
	1	-1599.516111	-1599.099742	168.6	-1599.179868	-1599.532281
<b>TS[15-12]</b>	6	-1909.710463	-1909.143091	223.2	-1909.249155	-1909.728064
	4	-1909.716346	-1909.149003	219.9	-1909.253475	-1909.733781
	2	-1909.706137	-1909.137824	215.7	-1909.240314	-1909.724244
CH <sub>3</sub> Cl	1	-500.0783537	-500.03651	55.9	-500.063071	-500.081089
HCl	1	-460.7760867	-460.765855	44.6	-460.787034	-460.779278
<b>TS[14-16]</b>	6	-1747.593413	-1747.155212	197.7	-1747.249127	-1747.609825
	4	-1747.61111	-1747.171551	195.0	-1747.26418	-1747.630252
	2	-1747.599905	-1747.159541	188.4	-1747.249069	-1747.619370
<b>16</b>	6	-1747.668494	-1747.225129	197.1	-1747.318771	-1747.686218
	4	-1747.669115	-1747.22563	195.2	-1747.318368	-1747.686810
	2	-1747.657356	-1747.21324	189.5	-1747.303297	-1747.661050
<b>17</b>	6	-	-	-	-	-
	4	-1747.592791	-1747.15257	195.7	-1747.24555	-1747.613542
	2	-	-	-	-	-

**Table S3 (cont.).**

STRUCTURE	M <sub>s</sub>	E	H	S	G	E <sub>solv</sub>
TS[15-20]	6	-1909.710073	-1909.142183	213.9	-1909.243814	-1909.720434
	4	-1909.722367	-1909.155063	213.1	-1909.256321	-1909.733329
	2	-1909.716469	-1909.147765	204.5	-1909.244952	-1909.725322
ClCHMePh	1	-770.419712	-770.262533	91.1	-770.305835	-770.423884
Cl <sup>-</sup>	1	-460.2313633	-460.229003	36.6	-460.246386	-460.336769
21 <sup>+</sup>	6	-1254.219441	-1253.758543	185.9	-1253.846867	-1254.276142
	4	-1254.229765	-1253.768389	187.9	-1253.857684	-1254.286404
	2	-1254.232111	-1253.771679	176.1	-1253.855338	-1254.284877
9 <sup>+</sup>	6	-1138.42177	-1138.022446	169.3	-1138.102905	-1138.481984
	4	-1138.444286	-1138.044696	169.8	-1138.125364	-1138.500896
	2	-1138.432495	-1138.03229	163.3	-1138.109885	-1138.488067

**Table S4.** Absolute energies of the structures involved in the C-H functionalization reaction (1) and related competing processes catalyzed by **4**. In these reactions the donor-acceptor CPh(COH)N<sub>2</sub> employed as a carbene precursor. Thermodynamic parameters were computed at 298.15 K and 1 atm. All values are given in a.u., but entropy values are given in cal·mol<sup>-1</sup>·K<sup>-1</sup>.

STRUCTURE	M <sub>s</sub>	E	H	S	G	E <sub>solv</sub>
13_D/A	4	-2052.746808	-2052.233731	217.9	-2052.337284	-2052.766209
TS[13-14]_D/A	4	-2052.733845	-2052.223679	212.9	-2052.324843	-2052.752722
14_D/A	6	-1943.241750	-1942.740652	211.0	-1942.840895	-1943.266580
	4	-1943.250408	-1942.750014	212.8	-1942.851109	-1943.269061
	2	-1943.239426	-1942.738827	210.3	-1942.838753	-1943.258937
TS[14-15]_D/A	6	-2254.068687	-2253.406891	245.9	-2253.523706	-2254.089991
	4	-2254.079710	-2253.417555	241.0	-2253.532047	-2254.100382
	2	-2254.060914	-2253.398335	235.1	-2253.510016	-2254.081328
15_D/A	5	-1943.894833	-1943.381840	207.7	-1943.480519	-1943.916254
TS[14-12]_D/A	4	-2254.093600	-2253.427276	246.8	-2253.544554	-2254.115689
CH(COH)PhCl	1	-844.407972	-844.269627	95.7	-844.315114	-844.415084
TS[14-16]_D/A	6	-2436.315021	-2435.679959	249.9	-2435.798710	-2436.324393
	4	-2436.324173	-2435.688871	249.2	-2435.807263	-2436.344843
	2	-2436.303980	-2435.668078	245.6	-2435.784786	-2436.336994
TS[15-20]_D/A	4	-2254.091692	-2253.426193	244.9	-2253.542546	-2254.107796

**Table S5.** Calculated cartesian coordinates (in Å) of all reported structures.

**3 (<sup>1</sup>A):**

1	6	0	-3.861228	-0.793879	-1.016664
2	6	0	-2.903664	-0.746471	0.004044
3	6	0	-2.847301	-1.787763	0.937116
4	6	0	-3.744231	-2.845927	0.856716
5	6	0	-4.699057	-2.888488	-0.157362
6	6	0	-4.750592	-1.859926	-1.094665
7	7	0	-1.945714	0.293379	0.054536
8	6	0	-2.325955	1.574954	0.056096
9	6	0	-3.737968	2.048396	0.156366
10	6	0	-1.226192	2.475248	-0.020198
11	7	0	-0.026893	1.794107	-0.097793
12	6	0	1.163578	2.488135	-0.196979
13	6	0	1.163372	3.879492	-0.228911
14	6	0	-0.044879	4.573826	-0.152629
15	6	0	-1.243243	3.867241	-0.045583
16	26	0	-0.006643	-0.029634	0.078261
17	7	0	1.896599	0.312896	-0.236606
18	6	0	2.878505	-0.711257	-0.216314
19	6	0	3.019199	-1.560651	-1.316856
20	6	0	3.954945	-2.589229	-1.284604
21	6	0	4.749481	-2.784114	-0.157137
22	6	0	4.604995	-1.941208	0.942597
23	6	0	3.676614	-0.906045	0.915705
24	6	0	2.269236	1.592618	-0.263819
25	6	0	3.686296	2.043996	-0.369709
26	1	0	2.103912	4.416803	-0.309743
27	1	0	-0.052281	5.658207	-0.178205
28	1	0	-2.191672	4.394316	0.007477
29	1	0	-4.377389	1.301577	0.631046
30	1	0	-3.790468	2.968050	0.745588
31	1	0	-4.176272	2.271628	-0.823798
32	1	0	4.275750	1.352718	-0.977451
33	1	0	3.747537	3.036390	-0.822344
34	1	0	4.176551	2.100417	0.609406
35	1	0	-2.094646	-1.755026	1.718620
36	1	0	-3.692757	-3.645455	1.590273
37	1	0	-5.392378	-3.721788	-0.221434
38	1	0	-5.480893	-1.889773	-1.898564
39	1	0	-3.879151	-0.003211	-1.761961
40	1	0	2.389443	-1.402438	-2.187338
41	1	0	4.060120	-3.243572	-2.145331
42	1	0	5.474627	-3.592163	-0.133508
43	1	0	5.215148	-2.091028	1.828948
44	1	0	3.544488	-0.251660	1.773864
45	7	0	0.204540	-0.609205	1.782183
46	7	0	-0.097353	-1.663116	-0.742579
47	7	0	0.377718	-0.886919	2.867425
48	7	0	-0.177243	-2.656457	-1.279105

**4 (<sup>4</sup>A):**

1	6	0	-2.936808	-1.730707	0.864379
2	6	0	-3.121167	-0.594940	0.065440
3	6	0	-4.240016	-0.526445	-0.775963
4	6	0	-5.162998	-1.565705	-0.799217
5	6	0	-4.989405	-2.680102	0.017805
6	6	0	-3.872186	-2.756410	0.847707
7	7	0	-2.120591	0.393913	0.072472
8	6	0	-2.402729	1.679636	0.163205
9	6	0	-3.757725	2.255559	0.426031
10	26	0	-0.078573	-0.127551	-0.402178

11	7	0	-0.084015	1.888984	-0.195364
12	6	0	-1.254088	2.551788	0.044437
13	6	0	-1.281667	3.941447	0.165606
14	6	0	-0.090776	4.662295	0.055683
15	6	0	1.104413	3.981436	-0.150345
16	6	0	1.091041	2.586710	-0.262827
17	6	0	2.255085	1.754057	-0.404754
18	6	0	3.609865	2.370818	-0.557445
19	7	0	2.001501	0.451238	-0.426671
20	6	0	3.030376	-0.499496	-0.338243
21	6	0	3.013492	-1.621272	-1.179883
22	6	0	3.960406	-2.626365	-1.023123
23	6	0	4.932493	-2.542350	-0.027116
24	6	0	4.954714	-1.431688	0.814203
25	6	0	4.016947	-0.416808	0.660409
26	17	0	-0.405286	-1.986733	-1.648583
27	1	0	-2.221435	4.454299	0.343225
28	1	0	-0.096269	5.743807	0.147397
29	1	0	2.045698	4.519719	-0.204595
30	1	0	4.334313	1.649367	-0.938072
31	1	0	3.569268	3.215153	-1.252449
32	1	0	4.003868	2.761319	0.389068
33	1	0	-4.443115	1.499987	0.812615
34	1	0	-3.694356	3.069112	1.154763
35	1	0	-4.211518	2.676832	-0.478957
36	1	0	2.238648	-1.696142	-1.936570
37	1	0	3.932403	-3.487877	-1.684545
38	1	0	5.664366	-3.335488	0.094249
39	1	0	5.702818	-1.355157	1.598916
40	1	0	4.020789	0.440625	1.329949
41	1	0	-2.047330	-1.784645	1.485636
42	1	0	-3.721413	-3.629231	1.477038
43	1	0	-5.712069	-3.490532	-0.003347
44	1	0	-6.018585	-1.506415	-1.466404
45	1	0	-4.357026	0.328460	-1.436439
46	8	0	0.275042	-1.124878	1.584659
47	6	0	0.762474	-0.231400	2.570707
48	1	0	1.832542	-0.028717	2.418590
49	1	0	0.196611	0.697693	2.467757
50	1	0	0.612309	-0.648149	3.575375
51	6	0	0.924918	-2.393237	1.632154
52	1	0	2.013801	-2.278289	1.551373
53	1	0	0.678187	-2.900553	2.574001
54	1	0	0.551714	-2.965249	0.780548

5 (<sup>1</sup>A):

1	6	0	3.859868	-0.830919	0.939029
2	6	0	2.901226	-0.771408	-0.080654
3	6	0	2.888741	-1.768898	-1.061765
4	6	0	3.819831	-2.799704	-1.026022
5	6	0	4.772766	-2.854661	-0.010850
6	6	0	4.786052	-1.867562	0.971964
7	7	0	1.917429	0.245931	-0.108901
8	6	0	2.295721	1.541813	-0.111036
9	6	0	3.706204	2.013481	-0.219248
10	26	0	-0.000007	-0.083269	-0.000071
11	7	0	-1.917441	0.245953	0.108775
12	6	0	-2.295727	1.541836	0.110786
13	6	0	-1.196602	2.454774	0.055761
14	7	0	-0.000003	1.795374	-0.000162
15	6	0	1.196601	2.454763	-0.056133
16	6	0	1.211712	3.852007	-0.056413

17	6	0	0.000006	4.542733	-0.000278
18	6	0	-1.211703	3.852019	0.055919
19	6	0	-2.901233	-0.771395	0.080759
20	6	0	-3.859998	-0.831063	-0.938799
21	6	0	-4.786167	-1.867729	-0.971478
22	6	0	-4.772744	-2.854694	0.011468
23	6	0	-3.819686	-2.799581	1.026517
24	6	0	-2.888614	-1.768752	1.062005
25	6	0	-3.706201	2.013528	0.219012
26	7	0	-0.000010	-1.869364	-0.000020
27	7	0	-0.000010	-3.008463	0.000006
28	1	0	2.154839	4.388170	-0.092722
29	1	0	0.000009	5.628366	-0.000322
30	1	0	-2.154827	4.388191	0.092190
31	1	0	-4.331087	1.287362	0.744012
32	1	0	-3.750397	2.960456	0.764472
33	1	0	-4.174119	2.186323	-0.758508
34	1	0	4.331112	1.287241	-0.744121
35	1	0	3.750438	2.960338	-0.764828
36	1	0	4.174072	2.186397	0.758274
37	1	0	-2.136323	-1.721895	1.844536
38	1	0	-3.797915	-3.566242	1.795867
39	1	0	-5.495511	-3.664667	-0.017111
40	1	0	-5.517975	-1.906763	-1.773805
41	1	0	-3.854991	-0.069183	-1.714095
42	1	0	2.136546	-1.722162	-1.844396
43	1	0	3.798168	-3.566469	-1.795271
44	1	0	5.495544	-3.664618	0.017926
45	1	0	5.517764	-1.906474	1.774385
46	1	0	3.854751	-0.068931	1.714218

5 (<sup>3</sup>A):

1	6	0	-3.866862	-0.827316	-0.946601
2	6	0	-2.906424	-0.767772	0.070919
3	6	0	-2.891547	-1.764008	1.053030
4	6	0	-3.823894	-2.793796	1.021426
5	6	0	-4.778847	-2.849364	0.008120
6	6	0	-4.793468	-1.863830	-0.976185
7	7	0	-1.921914	0.249096	0.096140
8	6	0	-2.296927	1.541853	0.122519
9	6	0	-3.706882	2.012501	0.239083
10	26	0	-0.000004	-0.085069	-0.000059
11	7	0	1.921900	0.249097	-0.096190
12	6	0	2.296923	1.541850	-0.122532
13	6	0	1.196644	2.449302	-0.066746
14	7	0	-0.000003	1.781674	-0.000026
15	6	0	-1.196644	2.449299	0.066726
16	6	0	-1.209674	3.844690	0.069215
17	6	0	-0.000005	4.539023	0.000014
18	6	0	1.209662	3.844694	-0.069198
19	6	0	2.906418	-0.767770	-0.070932
20	6	0	3.866755	-0.827314	0.946685
21	6	0	4.793377	-1.863809	0.976346
22	6	0	4.778871	-2.849325	-0.007981
23	6	0	3.824021	-2.793753	-1.021382
24	6	0	2.891653	-1.763981	-1.053063
25	6	0	3.706891	2.012477	-0.238990
26	7	0	-0.000008	-1.873925	-0.000102
27	7	0	-0.000011	-3.011749	-0.000130
28	1	0	-2.153123	4.380038	0.116447
29	1	0	-0.000005	5.624351	0.000030
30	1	0	2.153111	4.380046	-0.116412

31	1	0	4.325958	1.289527	-0.775564
32	1	0	3.748614	2.964138	-0.775699
33	1	0	4.183207	2.174157	0.736260
34	1	0	-4.325962	1.289469	0.775527
35	1	0	-3.748564	2.964063	0.775976
36	1	0	-4.183196	2.174386	-0.736133
37	1	0	2.137193	-1.716616	-1.833738
38	1	0	3.801527	-3.559376	-1.791730
39	1	0	5.502166	-3.658897	0.018322
40	1	0	5.526748	-1.903508	1.777191
41	1	0	3.862450	-0.066345	1.722802
42	1	0	-2.137005	-1.716640	1.833627
43	1	0	-3.801307	-3.559434	1.791757
44	1	0	-5.502130	-3.658948	-0.018129
45	1	0	-5.526918	-1.903526	-1.776957
46	1	0	-3.862654	-0.066336	-1.722707

6 (<sup>1</sup>A):

1	6	0	3.083255	-1.657819	0.915155
2	6	0	2.992166	-0.743425	-0.138820
3	6	0	3.873706	-0.857732	-1.220018
4	6	0	4.828780	-1.868074	-1.241304
5	6	0	4.922897	-2.769905	-0.183925
6	6	0	4.045985	-2.659704	0.893132
7	7	0	1.981856	0.249578	-0.119694
8	6	0	2.332708	1.546591	-0.204516
9	6	0	3.734749	2.057091	-0.225197
10	6	0	1.206133	2.417602	-0.278303
11	6	0	1.165209	3.811694	-0.362964
12	6	0	-0.071871	4.452327	-0.424474
13	6	0	-1.257682	3.714589	-0.392847
14	6	0	-1.184268	2.323021	-0.322400
15	7	0	0.033217	1.707306	-0.288558
16	6	0	-2.249912	1.357756	-0.288537
17	6	0	-3.682373	1.768793	-0.344305
18	26	0	0.093945	-0.128135	0.030595
19	6	0	0.065423	0.032979	2.017026
20	7	0	-1.041965	0.826475	2.432872
21	7	0	-1.943799	1.519211	2.255475
22	7	0	-1.809468	0.086601	-0.296128
23	6	0	-2.750162	-0.970226	-0.354931
24	6	0	-3.600998	-1.120663	-1.456477
25	6	0	-4.490296	-2.187935	-1.515057
26	6	0	-4.547200	-3.115381	-0.477215
27	6	0	-3.700522	-2.970516	0.619610
28	6	0	-2.806419	-1.908334	0.680978
29	1	0	-2.222390	4.211003	-0.428634
30	1	0	-0.114226	5.534849	-0.494259
31	1	0	2.087566	4.384435	-0.385051
32	1	0	0.946021	0.577815	2.387727
33	1	0	-0.014797	-0.912527	2.570090
34	1	0	-2.129733	-1.797403	1.524653
35	1	0	-3.732309	-3.691166	1.431937
36	1	0	-5.240517	-3.949682	-0.526612
37	1	0	-5.137966	-2.298099	-2.380570
38	1	0	-3.539998	-0.404534	-2.271771
39	1	0	2.380816	-1.576823	1.740525
40	1	0	4.106138	-3.362715	1.719127
41	1	0	5.668425	-3.559226	-0.203230
42	1	0	5.498848	-1.953699	-2.092340
43	1	0	3.783329	-0.162419	-2.050332
44	1	0	-4.327073	1.034681	0.143823

45	1	0	-3.818771	2.728446	0.160372
46	1	0	-4.045049	1.883984	-1.373462
47	1	0	4.417339	1.382285	0.296424
48	1	0	4.127651	2.182940	-1.242259
49	1	0	3.790215	3.036743	0.258245
50	7	0	0.188144	-1.904962	-0.071742
51	7	0	0.251738	-3.037602	-0.161872

7 (<sup>1</sup>A):

1	6	0	-3.751303	-0.801588	-1.272087
2	6	0	-2.908828	-0.794123	-0.153459
3	6	0	-2.966449	-1.860024	0.751011
4	6	0	-3.875439	-2.892680	0.554230
5	6	0	-4.720381	-2.892232	-0.554001
6	6	0	-4.648907	-1.845426	-1.469227
7	7	0	-1.944042	0.224814	0.017387
8	6	0	-2.303834	1.506834	0.008353
9	6	0	-3.711187	2.005950	-0.026986
10	6	0	-1.192660	2.407725	0.048966
11	6	0	-1.207371	3.797081	-0.056409
12	6	0	-0.000021	4.495924	-0.094379
13	6	0	1.207339	3.797089	-0.056610
14	6	0	1.192656	2.407733	0.048770
15	7	0	0.000008	1.733879	0.150069
16	6	0	2.303828	1.506849	0.007983
17	6	0	3.711174	2.005968	-0.027591
18	26	0	0.000017	-0.126719	0.193830
19	7	0	0.000139	-0.787475	1.871783
20	7	0	0.000211	-1.260684	2.903129
21	7	0	1.944044	0.224827	0.017085
22	6	0	2.908811	-0.794108	-0.153888
23	6	0	2.966577	-1.859983	0.750605
24	6	0	3.875540	-2.892641	0.553714
25	6	0	4.720311	-2.892222	-0.554646
26	6	0	4.648693	-1.845442	-1.469891
27	6	0	3.751114	-0.801601	-1.272644
28	6	0	-0.000061	-1.517081	-0.909382
29	1	0	2.153666	4.325145	-0.131221
30	1	0	-0.000032	5.577213	-0.183152
31	1	0	-2.153715	4.325131	-0.130861
32	1	0	-0.909651	-1.981250	-1.324982
33	1	0	0.909470	-1.981239	-1.325122
34	1	0	3.672368	0.003592	-1.998261
35	1	0	5.288704	-1.842146	-2.347922
36	1	0	5.421397	-3.707072	-0.709015
37	1	0	3.917362	-3.708532	1.269768
38	1	0	2.299038	-1.865243	1.605405
39	1	0	-3.672671	0.003628	-1.997691
40	1	0	-5.289053	-1.842108	-2.347159
41	1	0	-5.421487	-3.707081	-0.708285
42	1	0	-3.917148	-3.708591	1.270267
43	1	0	-2.298776	-1.865307	1.605706
44	1	0	4.033041	2.275990	-1.040601
45	1	0	3.812030	2.903778	0.588655
46	1	0	4.411411	1.254767	0.342040
47	1	0	-4.033202	2.276031	-1.039934
48	1	0	-4.411370	1.254729	0.342707
49	1	0	-3.811954	2.903726	0.589324

8 (<sup>4</sup>A):

1	6	0	-3.036530	-1.808402	0.797380
2	6	0	-3.091745	-0.689876	-0.048951

3	6	0	-4.067175	-0.653579	-1.058787
4	6	0	-4.971027	-1.699607	-1.202113
5	6	0	-4.925991	-2.794512	-0.342233
6	6	0	-3.952836	-2.842326	0.654723
7	7	0	-2.101308	0.292704	0.068622
8	26	0	0.000010	-0.217536	0.551660
9	6	0	0.000076	-0.880664	2.471100
10	7	0	2.101294	0.292815	0.068560
11	6	0	2.358150	1.581744	0.006849
12	6	0	1.180798	2.423136	-0.016121
13	6	0	1.201316	3.809479	-0.162264
14	6	0	-0.000122	4.512282	-0.232288
15	6	0	-1.201522	3.809417	-0.162239
16	6	0	-1.180928	2.423074	-0.016095
17	7	0	-0.000046	1.741705	0.079625
18	6	0	-2.358236	1.581619	0.006907
19	6	0	-3.722838	2.198989	0.012777
20	6	0	3.091779	-0.689710	-0.049051
21	6	0	3.036644	-1.808253	0.797264
22	6	0	3.953003	-2.842124	0.654572
23	6	0	4.926133	-2.794243	-0.342406
24	6	0	4.971089	-1.699323	-1.202271
25	6	0	4.067184	-0.653346	-1.058908
26	6	0	3.722719	2.199188	0.012692
27	7	0	0.000017	-1.729426	-0.750593
28	7	0	-0.000029	-2.696935	-1.327996
29	1	0	-2.149730	4.332067	-0.245529
30	1	0	-0.000152	5.589837	-0.359466
31	1	0	2.149495	4.332179	-0.245574
32	1	0	-0.885785	-0.517177	3.006292
33	1	0	0.885947	-0.517128	3.006242
34	1	0	-2.268156	-1.840286	1.565759
35	1	0	-3.901783	-3.695902	1.324983
36	1	0	-5.635048	-3.609112	-0.455614
37	1	0	-5.711124	-1.660748	-1.996875
38	1	0	-4.082639	0.182350	-1.752717
39	1	0	2.268291	-1.840189	1.565661
40	1	0	3.902012	-3.695713	1.324820
41	1	0	5.635232	-3.608803	-0.455815
42	1	0	5.711166	-1.660412	-1.997049
43	1	0	4.082586	0.182593	-1.752827
44	1	0	-4.476152	1.486607	0.352450
45	1	0	-3.749566	3.069592	0.674157
46	1	0	-4.027001	2.545894	-0.981839
47	1	0	4.476079	1.486845	0.352342
48	1	0	4.026840	2.546119	-0.981927
49	1	0	3.749413	3.069786	0.674079
50	1	0	0.000108	-1.977750	2.523311

9 (<sup>3</sup>A):

1	6	0	-3.774886	-0.805230	1.309382
2	6	0	-2.951532	-0.849433	0.173199
3	6	0	-3.064141	-1.940291	-0.698883
4	6	0	-3.985253	-2.949418	-0.445000
5	6	0	-4.799602	-2.900990	0.684649
6	6	0	-4.684944	-1.824857	1.561871
7	7	0	-1.974725	0.140993	-0.047836
8	6	0	-2.304863	1.427702	-0.037759
9	6	0	-1.176300	2.317803	-0.100179
10	6	0	-1.197791	3.690369	0.131363
11	6	0	0.009525	4.391009	0.208859
12	6	0	1.213278	3.693227	0.119010

13	6	0	1.190671	2.317268	-0.110646
14	7	0	0.005470	1.669526	-0.334780
15	6	0	2.313805	1.427571	-0.046766
16	7	0	1.981452	0.137809	-0.058355
17	6	0	2.949474	-0.858551	0.170321
18	6	0	3.036665	-1.965094	-0.685413
19	6	0	3.946800	-2.982803	-0.426264
20	6	0	4.775828	-2.927027	0.692230
21	6	0	4.686407	-1.835496	1.553493
22	6	0	3.786629	-0.808092	1.296532
23	26	0	0.009271	-0.282380	-0.685886
24	6	0	-0.020201	-1.569254	-2.050555
25	1	0	2.159833	4.204185	0.272654
26	1	0	0.009676	5.458582	0.403451
27	1	0	-2.142753	4.200994	0.295111
28	6	0	-3.702755	1.960584	-0.000846
29	6	0	3.714862	1.952189	-0.017855
30	1	0	-0.066508	-1.354379	-3.126992
31	1	0	-0.012354	-2.657572	-1.894134
32	1	0	2.381394	-1.999150	-1.551780
33	1	0	4.006900	-3.828662	-1.105898
34	1	0	5.480078	-3.728519	0.894713
35	1	0	5.317434	-1.783982	2.436788
36	1	0	3.699458	0.031130	1.981677
37	1	0	-2.418945	-1.971197	-1.572812
38	1	0	-4.065113	-3.783228	-1.137387
39	1	0	-5.512170	-3.696185	0.882821
40	1	0	-5.304829	-1.778529	2.453310
41	1	0	-3.669543	0.023625	2.004679
42	1	0	4.423239	1.204654	-0.380777
43	1	0	3.805941	2.845981	-0.641090
44	1	0	4.038555	2.231912	0.991912
45	1	0	-4.419838	1.214397	-0.348417
46	1	0	-4.012952	2.253531	1.009524
47	1	0	-3.793975	2.848894	-0.631978

**9<sup>+</sup> (<sup>4</sup>A):**

1	6	0	3.970326	-0.762633	-1.235065
2	6	0	3.053886	-0.869334	-0.179415
3	6	0	3.058871	-2.010535	0.630626
4	6	0	3.994698	-3.012720	0.409101
5	6	0	4.906221	-2.906027	-0.639642
6	6	0	4.884439	-1.783480	-1.464556
7	7	0	2.065953	0.120059	0.026053
8	6	0	2.353339	1.389986	0.086589
9	6	0	3.720361	1.982312	0.128526
10	26	0	-0.023858	-0.365175	0.530568
11	6	0	-0.045323	-1.474158	2.034316
12	7	0	-2.057117	0.149074	0.021109
13	6	0	-2.331068	1.426532	-0.016031
14	6	0	-3.693413	2.027454	-0.078907
15	6	0	-3.054329	-0.839967	-0.161987
16	6	0	-3.131898	-1.911831	0.734159
17	6	0	-4.074025	-2.913171	0.534949
18	6	0	-4.920183	-2.874782	-0.571556
19	6	0	-4.826925	-1.821161	-1.478156
20	6	0	-3.905197	-0.801258	-1.275172
21	7	0	0.005800	1.648922	0.180153
22	6	0	1.185565	2.290757	0.114631
23	6	0	1.233985	3.679514	0.000426
24	6	0	0.034184	4.385673	-0.088654
25	6	0	-1.176176	3.699043	-0.088371

26	6	0	-1.158585	2.307771	0.039493
27	1	0	-2.114111	4.232460	-0.200388
28	1	0	0.046153	5.466057	-0.184883
29	1	0	2.185268	4.199076	-0.043992
30	1	0	-0.118300	-1.166888	3.083885
31	1	0	0.015027	-2.569718	1.972367
32	1	0	-2.466186	-1.931517	1.592902
33	1	0	-4.142881	-3.730818	1.245467
34	1	0	-5.644141	-3.667171	-0.731357
35	1	0	-5.471743	-1.792371	-2.350816
36	1	0	-3.813663	0.009582	-1.992659
37	1	0	2.342928	-2.081458	1.444977
38	1	0	4.006991	-3.884949	1.054987
39	1	0	5.624990	-3.698885	-0.819355
40	1	0	5.579603	-1.701581	-2.294158
41	1	0	3.933666	0.101635	-1.892478
42	1	0	-4.467144	1.294404	0.148449
43	1	0	-3.773327	2.856571	0.629787
44	1	0	-3.907383	2.437771	-1.071873
45	1	0	4.478094	1.229857	0.346042
46	1	0	3.983891	2.452590	-0.825157
47	1	0	3.767599	2.765614	0.890454

10 (<sup>1</sup>A):

1	6	0	-3.934213	-0.902176	-1.171572
2	6	0	-3.012949	-0.833396	-0.119209
3	6	0	-3.047787	-1.817266	0.875639
4	6	0	-4.006893	-2.822081	0.837800
5	6	0	-4.929413	-2.878432	-0.205192
6	6	0	-4.881604	-1.919281	-1.213756
7	7	0	-2.004340	0.156730	-0.086903
8	26	0	-0.092211	-0.229749	0.039845
9	6	0	-0.174946	-1.882424	-0.572016
10	6	0	-2.346993	1.451145	-0.191067
11	6	0	-3.744047	1.979605	-0.215784
12	6	0	-1.222091	2.329160	-0.264283
13	6	0	-1.196336	3.720518	-0.390561
14	6	0	0.034937	4.373565	-0.452288
15	6	0	1.227365	3.648944	-0.387205
16	6	0	1.165385	2.258608	-0.274694
17	7	0	-0.044263	1.630343	-0.216651
18	6	0	2.247259	1.309120	-0.234067
19	6	0	3.667581	1.769512	-0.249232
20	7	0	1.843078	0.031600	-0.220278
21	6	0	2.800853	-1.002395	-0.313394
22	6	0	3.701220	-1.066535	-1.384487
23	6	0	4.602102	-2.120639	-1.485683
24	6	0	4.622034	-3.124924	-0.520669
25	6	0	3.719841	-3.073405	0.539953
26	6	0	2.809293	-2.028123	0.638867
27	1	0	-2.123714	4.283203	-0.445477
28	1	0	0.066851	5.453809	-0.555446
29	1	0	2.186884	4.154929	-0.434859
30	1	0	-1.104201	-2.419502	-0.828770
31	1	0	0.701584	-2.445261	-0.938450
32	1	0	-2.300650	-1.789161	1.663107
33	1	0	-4.025227	-3.574018	1.621953
34	1	0	-5.670399	-3.671694	-0.238432
35	1	0	-5.581750	-1.964706	-2.043502
36	1	0	-3.879621	-0.165903	-1.968780
37	1	0	2.079971	-1.995517	1.443076
38	1	0	3.717420	-3.858006	1.291634

39	1	0	5.326367	-3.947636	-0.600744
40	1	0	5.288034	-2.159792	-2.327549
41	1	0	3.668505	-0.293425	-2.147484
42	1	0	-4.444270	1.295390	0.267696
43	1	0	-3.793598	2.941622	0.303061
44	1	0	-4.115988	2.150939	-1.233887
45	1	0	4.337032	1.021872	0.180292
46	1	0	4.028642	1.983574	-1.262934
47	1	0	3.767307	2.691594	0.330027
48	6	0	-0.077172	-0.306933	2.044536
49	1	0	0.222255	-1.260751	2.490194
50	7	0	0.894415	0.637504	2.437758
51	1	0	-1.020312	0.034565	2.490910
52	7	0	1.729084	1.420159	2.394441

11 (<sup>1</sup>A):

1	6	0	3.389239	-1.323127	-1.200928
2	6	0	2.919030	-0.775942	-0.002802
3	6	0	3.424476	-1.252499	1.211095
4	6	0	4.385924	-2.258465	1.223833
5	6	0	4.853295	-2.799652	0.028366
6	6	0	4.351628	-2.328259	-1.182550
7	7	0	1.909053	0.220274	-0.017279
8	26	0	0.000000	-0.110912	-0.020318
9	6	0	-0.000001	-2.009476	-0.708692
10	7	0	-1.909053	0.220275	-0.017279
11	6	0	-2.292040	1.515634	-0.010526
12	6	0	-1.199258	2.440002	-0.010518
13	6	0	-1.215266	3.839189	-0.002617
14	6	0	0.000001	4.526319	0.000324
15	6	0	1.215267	3.839188	-0.002617
16	6	0	1.199259	2.440002	-0.010518
17	7	0	0.000000	1.783447	-0.016044
18	6	0	2.292040	1.515634	-0.010526
19	6	0	3.721639	1.934291	0.004053
20	6	0	-2.919030	-0.775941	-0.002802
21	6	0	-3.389240	-1.323126	-1.200929
22	6	0	-4.351629	-2.328258	-1.182550
23	6	0	-4.853296	-2.799651	0.028366
24	6	0	-4.385923	-2.258465	1.223833
25	6	0	-3.424476	-1.252499	1.211096
26	6	0	-3.721639	1.934292	0.004053
27	6	0	0.000000	-1.996212	0.699899
28	1	0	2.155653	4.381010	0.004095
29	1	0	0.000002	5.612275	0.007179
30	1	0	-2.155651	4.381011	0.004095
31	1	0	0.921822	-2.226592	-1.248781
32	1	0	-0.921823	-2.226591	-1.248781
33	1	0	2.987127	-0.949150	-2.139514
34	1	0	4.709529	-2.745596	-2.119883
35	1	0	5.601872	-3.586362	0.040473
36	1	0	4.769979	-2.621778	2.173235
37	1	0	3.047825	-0.825823	2.137837
38	1	0	-2.987129	-0.949148	-2.139514
39	1	0	-4.709531	-2.745593	-2.119883
40	1	0	-5.601873	-3.586361	0.040473
41	1	0	-4.769978	-2.621779	2.173235
42	1	0	-3.047824	-0.825824	2.137838
43	1	0	4.284034	1.471617	-0.814684
44	1	0	3.820381	3.017260	-0.088209
45	1	0	4.225493	1.629022	0.929223
46	1	0	-4.284034	1.471619	-0.814685

47	1	0	-4.225493	1.629022	0.929222
48	1	0	-3.820381	3.017261	-0.088208
49	1	0	-0.922213	-2.200820	1.244826
50	1	0	0.922212	-2.200820	1.244825

12 (<sup>4</sup>A):

1	6	0	3.057309	-1.905099	-0.703417
2	6	0	3.055308	-0.767743	0.113761
3	6	0	4.002174	-0.663581	1.143943
4	6	0	4.937407	-1.672372	1.342383
5	6	0	4.947185	-2.794131	0.516281
6	6	0	4.003656	-2.903153	-0.503030
7	7	0	2.056620	0.212689	-0.060637
8	6	0	2.367788	1.496062	-0.154082
9	6	0	3.756828	2.038621	-0.272605
10	26	0	-0.022366	-0.246425	-0.319121
11	17	0	-0.369967	-2.180765	-1.367647
12	7	0	-2.021420	0.324126	0.249023
13	6	0	-2.289995	1.614573	0.202696
14	6	0	-1.119686	2.452636	0.036841
15	7	0	0.029489	1.746575	-0.183084
16	6	0	1.235630	2.388891	-0.163533
17	6	0	1.302874	3.780689	-0.079403
18	6	0	0.126353	4.515015	0.042515
19	6	0	-1.094951	3.841856	0.127918
20	6	0	-3.026776	-0.657072	0.332418
21	6	0	-4.155416	-0.660116	-0.497801
22	6	0	-5.078283	-1.696886	-0.419096
23	6	0	-4.893734	-2.736177	0.489097
24	6	0	-3.764876	-2.744410	1.306953
25	6	0	-2.830293	-1.722372	1.219764
26	6	0	-3.641489	2.228623	0.378752
27	1	0	-2.015932	4.395888	0.279196
28	1	0	0.160197	5.597165	0.114070
29	1	0	2.267752	4.278777	-0.076463
30	1	0	4.457320	1.266314	-0.593878
31	1	0	3.788492	2.858447	-0.995515
32	1	0	4.129759	2.437242	0.678308
33	1	0	-4.338175	1.529112	0.843059
34	1	0	-3.579627	3.120300	1.008854
35	1	0	-4.080471	2.544096	-0.574951
36	1	0	2.307536	-1.994695	-1.483506
37	1	0	3.996860	-3.777017	-1.148231
38	1	0	5.679124	-3.581123	0.672336
39	1	0	5.658353	-1.582042	2.150393
40	1	0	3.977488	0.202133	1.800973
41	1	0	-1.931113	-1.732004	1.830391
42	1	0	-3.603157	-3.560773	2.004819
43	1	0	-5.616121	-3.544900	0.547120
44	1	0	-5.941584	-1.695959	-1.078643
45	1	0	-4.280637	0.132235	-1.230427

13 (<sup>4</sup>A):

1	6	0	-3.038276	-1.843150	0.606583
2	6	0	-2.994801	-0.814982	-0.341945
3	6	0	-3.913689	-0.827445	-1.399982
4	6	0	-4.863562	-1.837677	-1.493709
5	6	0	-4.916167	-2.844758	-0.533019
6	6	0	-3.998421	-2.842544	0.515255
7	7	0	-1.988210	0.166303	-0.251408
8	26	0	0.099810	-0.322979	0.018422
9	17	0	0.136900	-2.549973	-0.327168

10	7	0	2.153650	0.273486	-0.087794
11	6	0	2.393674	1.577821	-0.182231
12	6	0	1.216417	2.402609	-0.251794
13	6	0	1.200673	3.801881	-0.349814
14	6	0	-0.017716	4.466296	-0.420821
15	6	0	-1.207843	3.737148	-0.391927
16	6	0	-1.144458	2.344002	-0.301326
17	7	0	0.048220	1.695875	-0.235648
18	6	0	-2.288458	1.451149	-0.290334
19	6	0	-3.669274	2.023845	-0.292851
20	6	0	3.198110	-0.667003	-0.139157
21	6	0	3.218646	-1.714133	0.791606
22	6	0	4.213585	-2.681378	0.741295
23	6	0	5.193847	-2.634950	-0.248001
24	6	0	5.165451	-1.612580	-1.193566
25	6	0	4.179518	-0.634645	-1.141161
26	6	0	3.748100	2.213240	-0.166155
27	6	0	0.038890	-0.255738	2.237898
28	7	0	-0.934538	0.632702	2.528451
29	7	0	-1.765579	1.413866	2.570430
30	1	0	-2.167787	4.238592	-0.455486
31	1	0	-0.044194	5.548386	-0.504321
32	1	0	2.133773	4.355007	-0.384330
33	1	0	1.002197	0.117165	2.589403
34	1	0	-0.222039	-1.254547	2.591557
35	1	0	-2.298433	-1.855782	1.402288
36	1	0	-4.019955	-3.632190	1.260749
37	1	0	-5.658510	-3.633746	-0.607618
38	1	0	-5.562353	-1.839980	-2.325663
39	1	0	-3.854906	-0.052663	-2.159920
40	1	0	2.432030	-1.766352	1.539180
41	1	0	4.214517	-3.484849	1.472311
42	1	0	5.964643	-3.398713	-0.290603
43	1	0	5.911087	-1.578876	-1.983263
44	1	0	4.140065	0.146419	-1.895570
45	1	0	-4.409890	1.286411	0.018580
46	1	0	-3.722772	2.878205	0.388233
47	1	0	-3.962753	2.386809	-1.285248
48	1	0	4.505655	1.531314	0.222775
49	1	0	4.075656	2.526461	-1.165157
50	1	0	3.741334	3.112233	0.457718

14 (<sup>4</sup>A):

1	6	0	4.054298	-0.660185	-1.061399
2	6	0	3.107385	-0.683773	-0.028323
3	6	0	3.103032	-1.756942	0.871096
4	6	0	4.053432	-2.762786	0.760834
5	6	0	5.001962	-2.730223	-0.260063
6	6	0	4.991541	-1.680140	-1.174461
7	7	0	2.104546	0.294628	0.073008
8	6	0	2.356466	1.580112	0.027718
9	6	0	3.720291	2.196669	0.021914
10	26	0	-0.000006	-0.267546	0.390294
11	6	0	-0.000034	-0.690081	2.250544
12	7	0	-2.104550	0.294630	0.072929
13	6	0	-2.356467	1.580113	0.027630
14	6	0	-3.720291	2.196672	0.021775
15	6	0	-3.107386	-0.683771	-0.028435
16	6	0	-3.103062	-1.756939	0.870986
17	6	0	-4.053458	-2.762784	0.760694
18	6	0	-5.001954	-2.730222	-0.260235
19	6	0	-4.991502	-1.680141	-1.174634

20	6	0	-4.054263	-0.660185	-1.061543
21	17	0	0.000015	-2.055101	-0.990773
22	7	0	-0.000002	1.733259	0.116055
23	6	0	1.178308	2.420691	0.025264
24	6	0	1.199387	3.808401	-0.095197
25	6	0	0.000004	4.515380	-0.149667
26	6	0	-1.199382	3.808401	-0.095243
27	6	0	-1.178308	2.420692	0.025219
28	1	0	-2.149048	4.329460	-0.167440
29	1	0	0.000006	5.595098	-0.253777
30	1	0	2.149055	4.329460	-0.167358
31	1	0	-0.000022	0.000495	3.104852
32	1	0	-0.000061	-1.730825	2.608275
33	1	0	-2.344151	-1.779316	1.648991
34	1	0	-4.044788	-3.585423	1.469932
35	1	0	-5.734814	-3.526413	-0.350877
36	1	0	-5.712183	-1.656568	-1.987282
37	1	0	-4.022805	0.142953	-1.792665
38	1	0	2.344095	-1.779319	1.649076
39	1	0	4.044738	-3.585427	1.470070
40	1	0	5.734825	-3.526414	-0.350683
41	1	0	5.712249	-1.656566	-1.987084
42	1	0	4.022863	0.142955	-1.792521
43	1	0	-4.479150	1.479003	0.335593
44	1	0	-3.756587	3.057694	0.694827
45	1	0	-4.002167	2.557006	-0.974061
46	1	0	4.479137	1.479000	0.335762
47	1	0	4.002206	2.557001	-0.973912
48	1	0	3.756563	3.057693	0.694966

15 ( $\delta$ A):

1	6	0	3.035089	-1.775231	0.806032
2	6	0	3.104576	-0.686415	-0.072570
3	6	0	4.113720	-0.651251	-1.044254
4	6	0	5.048220	-1.677763	-1.117432
5	6	0	4.992903	-2.743943	-0.223501
6	6	0	3.982104	-2.787628	0.735414
7	7	0	2.100389	0.294296	-0.006142
8	6	0	2.355674	1.581386	-0.014591
9	6	0	3.719633	2.194210	0.035892
10	6	0	1.179043	2.424122	-0.023915
11	6	0	1.199896	3.815021	-0.103851
12	6	0	0.000004	4.522056	-0.143742
13	6	0	-1.199891	3.815022	-0.103862
14	6	0	-1.179038	2.424124	-0.023924
15	7	0	0.000002	1.736813	0.032319
16	6	0	-2.355673	1.581388	-0.014606
17	6	0	-3.719630	2.194216	0.035873
18	26	0	0.000001	-0.256885	0.306623
19	17	0	0.000002	-2.169351	-0.888848
20	6	0	-0.000010	-0.402267	2.353134
21	7	0	-2.100391	0.294299	-0.006156
22	6	0	-3.104578	-0.686412	-0.072576
23	6	0	-3.035087	-1.775223	0.806033
24	6	0	-3.982101	-2.787620	0.735427
25	6	0	-4.992905	-2.743943	-0.223485
26	6	0	-5.048226	-1.677769	-1.117423
27	6	0	-4.113726	-0.651255	-1.044255
28	1	0	-2.149099	4.339476	-0.153929
29	1	0	0.000005	5.604161	-0.218071
30	1	0	2.149105	4.339475	-0.153909
31	1	0	0.888333	0.090034	2.764983

32	1	0	-0.000019	-1.456073	2.658006
33	1	0	-2.230327	-1.809180	1.535817
34	1	0	-3.922001	-3.623408	1.426314
35	1	0	-5.724356	-3.544361	-0.282816
36	1	0	-5.818500	-1.646353	-1.882902
37	1	0	-4.134475	0.164387	-1.761714
38	1	0	2.230333	-1.809195	1.535819
39	1	0	3.922007	-3.623420	1.426296
40	1	0	5.724355	-3.544360	-0.282840
41	1	0	5.818490	-1.646342	-1.882914
42	1	0	4.134465	0.164396	-1.761706
43	1	0	-4.462481	1.473922	0.380843
44	1	0	-3.731292	3.055383	0.709066
45	1	0	-4.043880	2.551654	-0.948077
46	1	0	4.462480	1.473915	0.380869
47	1	0	4.043890	2.551643	-0.948057
48	1	0	3.731294	3.055379	0.709082
49	1	0	-0.888355	0.090045	2.764970

**16 (<sup>4</sup>A):**

1	6	0	-1.209383	2.195668	-0.618959
2	7	0	-0.024903	1.532303	-0.509927
3	6	0	1.146159	2.223748	-0.613872
4	6	0	1.148510	3.606028	-0.821349
5	6	0	-0.057328	4.284892	-0.937272
6	6	0	-1.251132	3.568673	-0.830826
7	26	0	-0.000740	-0.400077	0.041589
8	17	0	0.044793	-2.510901	-0.748679
9	6	0	2.327438	1.404592	-0.483270
10	6	0	3.684029	2.035496	-0.479028
11	6	0	-2.380249	1.352103	-0.455931
12	6	0	-3.731403	1.983763	-0.355316
13	7	0	2.084427	0.120742	-0.315194
14	6	0	3.111891	-0.837406	-0.257496
15	6	0	4.116716	-0.908366	-1.232048
16	6	0	5.078430	-1.910381	-1.172555
17	6	0	5.056047	-2.847654	-0.142703
18	6	0	4.051457	-2.786869	0.821215
19	6	0	3.079274	-1.797988	0.760792
20	6	0	0.000374	-0.237179	2.110947
21	7	0	-2.121951	0.074019	-0.333983
22	6	0	-3.126725	-0.904895	-0.246556
23	6	0	-2.999854	-1.915461	0.714997
24	6	0	-3.951245	-2.922711	0.797539
25	6	0	-5.024754	-2.954938	-0.090814
26	6	0	-5.137968	-1.970517	-1.069097
27	6	0	-4.198899	-0.948637	-1.148383
28	1	0	-2.207366	4.075617	-0.910979
29	1	0	-0.072322	5.356253	-1.105950
30	1	0	2.090781	4.138858	-0.902240
31	1	0	-1.050420	-0.142678	2.419022
32	1	0	0.367017	-1.207405	2.473541
33	1	0	-2.145110	-1.901700	1.385700
34	1	0	-3.844332	-3.696471	1.551962
35	1	0	-5.759551	-3.752237	-0.031252
36	1	0	-5.957515	-1.999915	-1.781601
37	1	0	-4.267143	-0.197592	-1.930625
38	1	0	2.278340	-1.756947	1.493628
39	1	0	4.016185	-3.522733	1.619197
40	1	0	5.808589	-3.629275	-0.099703
41	1	0	5.844824	-1.961640	-1.940856
42	1	0	4.113899	-0.194589	-2.051347

43	1	0	-4.467593	1.285713	0.043273
44	1	0	-3.683362	2.854557	0.304767
45	1	0	-4.096170	2.331584	-1.328349
46	1	0	4.429357	1.366468	-0.046867
47	1	0	4.022684	2.291870	-1.489383
48	1	0	3.673606	2.963254	0.099721
49	6	0	0.803542	0.869483	2.731859
50	1	0	1.816727	0.973392	2.321875
51	1	0	0.920941	0.807556	3.824042
52	7	0	0.179461	2.265047	2.574465
53	7	0	-0.943300	2.453134	2.275701

16 (<sup>6</sup>A):

1	6	0	-1.204236	2.185794	-0.641065
2	7	0	-0.020478	1.531309	-0.495218
3	6	0	1.149650	2.225462	-0.594042
4	6	0	1.147980	3.607006	-0.814693
5	6	0	-0.057980	4.276959	-0.961938
6	6	0	-1.250826	3.554071	-0.874405
7	26	0	0.016556	-0.400492	0.068804
8	17	0	0.051485	-2.526044	-0.675563
9	6	0	2.331553	1.409799	-0.458767
10	6	0	3.686791	2.044016	-0.450528
11	6	0	-2.376304	1.335782	-0.493529
12	6	0	-3.730692	1.964096	-0.427715
13	7	0	2.091733	0.123378	-0.297016
14	6	0	3.125672	-0.829500	-0.253763
15	6	0	4.115884	-0.889653	-1.243951
16	6	0	5.085627	-1.884805	-1.203403
17	6	0	5.085727	-2.826043	-0.176943
18	6	0	4.096292	-2.775178	0.803050
19	6	0	3.116416	-1.792726	0.762103
20	6	0	0.054815	-0.208924	2.136464
21	7	0	-2.115100	0.063491	-0.348831
22	6	0	-3.117509	-0.918620	-0.263893
23	6	0	-3.008176	-1.907737	0.721341
24	6	0	-3.957423	-2.917057	0.803300
25	6	0	-5.009247	-2.973250	-0.109529
26	6	0	-5.103775	-2.010409	-1.110919
27	6	0	-4.167572	-0.985783	-1.189553
28	1	0	-2.208012	4.053150	-0.985503
29	1	0	-0.075602	5.346124	-1.143880
30	1	0	2.088963	4.143664	-0.885542
31	1	0	-0.995565	-0.194306	2.458923
32	1	0	0.498179	-1.138686	2.517126
33	1	0	-2.169460	-1.875916	1.411402
34	1	0	-3.865303	-3.674070	1.576380
35	1	0	-5.741628	-3.772790	-0.050465
36	1	0	-5.906174	-2.058730	-1.841638
37	1	0	-4.220637	-0.251018	-1.988327
38	1	0	2.328400	-1.758396	1.508728
39	1	0	4.079170	-3.513531	1.599347
40	1	0	5.844278	-3.602517	-0.148451
41	1	0	5.840495	-1.927514	-1.983566
42	1	0	4.095411	-0.172085	-2.059774
43	1	0	-4.475380	1.265348	-0.046974
44	1	0	-3.699046	2.835328	0.232687
45	1	0	-4.069862	2.310680	-1.410276
46	1	0	4.433416	1.374844	-0.020928
47	1	0	4.026015	2.306198	-1.459222
48	1	0	3.673977	2.969181	0.132605
49	6	0	0.774150	0.977153	2.712780

50	1	0	1.730356	1.205638	2.221034
51	1	0	0.999139	0.910077	3.787338
52	7	0	-0.006704	2.293906	2.627721
53	7	0	-1.126271	2.361082	2.263665

**17 (<sup>4</sup>A):**

1	6	0	4.081492	-0.454512	-1.226740
2	6	0	3.161459	-0.595326	-0.179590
3	6	0	3.181175	-1.754982	0.608432
4	6	0	4.136722	-2.734372	0.373384
5	6	0	5.059681	-2.588722	-0.661900
6	6	0	5.020026	-1.452520	-1.465990
7	7	0	2.147762	0.349308	0.042919
8	6	0	2.358232	1.627997	0.150352
9	6	0	3.700403	2.287167	0.198708
10	26	0	0.000368	-0.263713	0.001166
11	6	0	0.078057	-2.081357	-0.232293
12	7	0	-2.168534	0.316397	0.058586
13	6	0	-2.392518	1.587206	0.187192
14	6	0	-3.742030	2.230419	0.245635
15	6	0	-3.168679	-0.641090	-0.165979
16	6	0	-3.171456	-1.797311	0.626092
17	6	0	-4.114241	-2.789985	0.395385
18	6	0	-5.037278	-2.660720	-0.642114
19	6	0	-5.012836	-1.527274	-1.450651
20	6	0	-4.088775	-0.515141	-1.214338
21	17	0	-0.046602	0.024872	-2.308228
22	7	0	-0.015546	1.746104	0.260634
23	6	0	1.151995	2.441531	0.270133
24	6	0	1.164277	3.833766	0.364389
25	6	0	-0.037960	4.527838	0.435425
26	6	0	-1.230495	3.810722	0.396942
27	6	0	-1.193606	2.420603	0.299693
28	1	0	-2.184447	4.326873	0.422400
29	1	0	-0.047213	5.610500	0.502520
30	1	0	2.109063	4.367292	0.364798
31	1	0	0.153574	-2.837044	0.559426
32	1	0	0.092682	-2.486346	-1.249644
33	1	0	-2.434182	-1.893312	1.420791
34	1	0	-4.119656	-3.676546	1.022778
35	1	0	-5.762480	-3.447257	-0.828417
36	1	0	-5.710730	-1.431211	-2.277531
37	1	0	-4.034957	0.352998	-1.865620
38	1	0	2.443722	-1.874919	1.400743
39	1	0	4.150648	-3.623233	0.997338
40	1	0	5.796070	-3.364345	-0.850229
41	1	0	5.716577	-1.343571	-2.292447
42	1	0	4.016011	0.414007	-1.876445
43	1	0	-4.528821	1.485792	0.367970
44	1	0	-3.797040	2.937631	1.078312
45	1	0	-3.954584	2.794626	-0.668992
46	1	0	4.494994	1.553896	0.338488
47	1	0	3.911626	2.834577	-0.726513
48	1	0	3.746287	3.011698	1.016997
49	6	0	-0.024379	-0.443771	2.084958
50	1	0	0.966169	-0.074945	2.385864
51	7	0	-0.262594	-1.739627	2.689141
52	7	0	0.484352	-2.646401	2.830344
53	1	0	-0.814312	0.235093	2.412863

**18 (<sup>3</sup>A):**

1	26	0	0.000000	0.000000	0.252130
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2	7	0	0.000000	0.000000	-1.718280
3	6	0	0.077818	1.196028	-2.355438
4	6	0	0.083503	1.216084	-3.762680
5	6	0	0.000000	0.000000	-4.442776
6	6	0	-0.083503	-1.216084	-3.762680
7	6	0	-0.077818	-1.196028	-2.355438
8	6	0	0.136473	2.295130	-1.438691
9	6	0	0.326858	3.692253	-1.925164
10	6	0	-0.136473	-2.295130	-1.438691
11	6	0	-0.326858	-3.692253	-1.925164
12	7	0	-0.097231	-1.933760	-0.126901
13	6	0	0.000000	-2.844762	0.931786
14	6	0	-0.635510	-2.506558	2.140456
15	6	0	-0.527104	-3.318684	3.260314
16	6	0	0.224152	-4.492290	3.206319
17	6	0	0.871465	-4.830748	2.020019
18	6	0	0.767220	-4.022244	0.893686
19	7	0	0.097231	1.933760	-0.126901
20	6	0	0.000000	2.844762	0.931786
21	6	0	0.635510	2.506558	2.140456
22	6	0	0.527104	3.318684	3.260314
23	6	0	-0.224152	4.492290	3.206319
24	6	0	-0.871465	4.830748	2.020019
25	6	0	-0.767220	4.022244	0.893686
26	1	0	-0.136128	-2.154073	-4.306593
27	1	0	0.000000	0.000000	-5.529430
28	1	0	0.136128	2.154073	-4.306593
29	1	0	0.828899	4.312618	-1.178578
30	1	0	0.938279	3.692810	-2.832768
31	1	0	-0.615142	4.195837	-2.180710
32	1	0	-0.828899	-4.312618	-1.178578
33	1	0	-0.938279	-3.692810	-2.832768
34	1	0	0.615142	-4.195837	-2.180710
35	1	0	1.236344	1.595974	2.170223
36	1	0	1.034814	3.035925	4.178421
37	1	0	-0.312657	5.129045	4.081274
38	1	0	-1.478689	5.730956	1.971279
39	1	0	-1.313084	4.277480	-0.008561
40	1	0	-1.236344	-1.595974	2.170223
41	1	0	-1.034814	-3.035925	4.178421
42	1	0	0.312657	-5.129045	4.081274
43	1	0	1.478689	-5.730956	1.971279
44	1	0	1.313084	-4.277480	-0.008561

**19 (<sup>3</sup>A):**

1	6	0	-3.763206	-0.918035	-1.511301
2	6	0	-2.755073	-0.990229	-0.537132
3	6	0	-2.595363	-2.186544	0.178749
4	6	0	-3.434056	-3.268098	-0.058013
5	6	0	-4.438066	-3.185918	-1.020962
6	6	0	-4.591568	-2.008343	-1.749134
7	7	0	-1.836476	0.050193	-0.329434
8	26	0	0.114630	-0.258811	0.392112
9	6	0	-0.209892	-0.636117	2.375881
10	6	0	-2.209467	1.321654	-0.243861
11	6	0	-3.618123	1.811941	-0.157621
12	6	0	-1.105164	2.260823	-0.220970
13	6	0	-1.171954	3.637041	-0.428097
14	6	0	0.023164	4.358581	-0.533981
15	6	0	1.250558	3.702395	-0.462416
16	6	0	1.269962	2.319336	-0.249573
17	7	0	0.097694	1.652071	-0.069479

18	6	0	2.417051	1.450298	-0.222836
19	6	0	3.799761	2.019258	-0.243705
20	7	0	2.118940	0.152434	-0.118146
21	6	0	3.093527	-0.851937	-0.196701
22	6	0	4.101267	-0.865147	-1.174863
23	6	0	4.984425	-1.935499	-1.261694
24	6	0	4.890512	-3.006630	-0.376294
25	6	0	3.888763	-3.005030	0.593648
26	6	0	2.995871	-1.945477	0.679061
27	1	0	-2.131105	4.134682	-0.537784
28	1	0	-0.006952	5.429267	-0.710248
29	1	0	2.177177	4.253636	-0.596780
30	1	0	0.485603	0.055958	2.869012
31	1	0	-0.076395	-1.643478	2.778289
32	1	0	-1.814134	-2.239323	0.934257
33	1	0	-3.301554	-4.181729	0.514731
34	1	0	-5.089315	-4.034427	-1.207923
35	1	0	-5.358274	-1.938294	-2.515982
36	1	0	-3.864091	-0.014743	-2.105842
37	1	0	2.210210	-1.932738	1.433290
38	1	0	3.800906	-3.836220	1.287866
39	1	0	5.584567	-3.838638	-0.446854
40	1	0	5.748167	-1.934173	-2.034818
41	1	0	4.158473	-0.050630	-1.890968
42	1	0	-4.285896	1.024803	0.197596
43	1	0	-3.678004	2.651132	0.539914
44	1	0	-4.003705	2.159235	-1.123895
45	1	0	4.521584	1.327892	0.196106
46	1	0	4.148960	2.242831	-1.259415
47	1	0	3.837077	2.957629	0.316791
48	7	0	-1.572321	-0.193185	2.724273
49	7	0	-2.090873	0.862266	2.664019

**19 (<sup>5</sup>A):**

1	6	0	-3.749753	-0.975714	-1.528361
2	6	0	-2.791905	-1.015026	-0.503545
3	6	0	-2.698130	-2.168818	0.288127
4	6	0	-3.553130	-3.241958	0.072424
5	6	0	-4.506298	-3.194182	-0.943564
6	6	0	-4.594505	-2.058341	-1.744669
7	7	0	-1.861390	0.020328	-0.318312
8	26	0	0.126865	-0.284896	0.417674
9	6	0	-0.233318	-0.620559	2.435842
10	6	0	-2.226952	1.292505	-0.287946
11	6	0	-3.634218	1.791687	-0.221682
12	6	0	-1.119035	2.224266	-0.265943
13	6	0	-1.185175	3.598083	-0.481521
14	6	0	0.004862	4.324739	-0.588105
15	6	0	1.232786	3.667921	-0.507409
16	6	0	1.251931	2.291534	-0.275642
17	7	0	0.083648	1.617458	-0.090272
18	6	0	2.408411	1.431556	-0.249560
19	6	0	3.787622	2.008307	-0.269175
20	7	0	2.119032	0.135954	-0.149368
21	6	0	3.095324	-0.868398	-0.217368
22	6	0	4.106770	-0.885551	-1.191030
23	6	0	4.989443	-1.956896	-1.268896
24	6	0	4.890089	-3.023874	-0.378990
25	6	0	3.884484	-3.017659	0.586599
26	6	0	2.991448	-1.957304	0.663375
27	1	0	-2.145728	4.091275	-0.600544
28	1	0	-0.027264	5.393273	-0.774942

29	1	0	2.159794	4.215856	-0.652758
30	1	0	0.581310	-0.118423	2.979330
31	1	0	-0.328844	-1.663224	2.750484
32	1	0	-1.961719	-2.189992	1.087882
33	1	0	-3.474801	-4.121920	0.704868
34	1	0	-5.169761	-4.036954	-1.112890
35	1	0	-5.322838	-2.014519	-2.549947
36	1	0	-3.799630	-0.103259	-2.174012
37	1	0	2.205988	-1.941503	1.417881
38	1	0	3.793420	-3.845324	1.284392
39	1	0	5.583688	-3.856732	-0.442871
40	1	0	5.756865	-1.959696	-2.038212
41	1	0	4.167254	-0.074173	-1.910407
42	1	0	-4.310857	1.009615	0.127175
43	1	0	-3.697169	2.633597	0.472614
44	1	0	-4.006579	2.137699	-1.193460
45	1	0	4.512265	1.319626	0.170162
46	1	0	4.134210	2.232448	-1.285375
47	1	0	3.819901	2.946386	0.291349
48	7	0	-1.494845	0.060861	2.653453
49	7	0	-1.685373	1.233303	2.740495

**20 (<sup>4</sup>A):**

1	6	0	4.001440	-0.860734	0.726922
2	6	0	2.912790	-0.809122	-0.155709
3	6	0	2.686251	-1.897829	-1.010168
4	6	0	3.544070	-2.988764	-1.010721
5	6	0	4.634554	-3.024963	-0.142322
6	6	0	4.851516	-1.961471	0.730053
7	7	0	1.970928	0.234805	-0.166918
8	26	0	-0.003541	-0.250650	0.303575
9	6	0	0.014255	-1.898476	1.457759
10	6	0	2.313104	1.521969	-0.096909
11	6	0	3.710828	2.046278	-0.154832
12	6	0	1.183199	2.406010	-0.022499
13	6	0	1.200503	3.790904	-0.186589
14	6	0	-0.005910	4.490869	-0.232386
15	6	0	-1.210848	3.790197	-0.185561
16	6	0	-1.192438	2.404444	-0.021917
17	7	0	-0.003981	1.746237	0.174812
18	6	0	-2.320597	1.519793	-0.097484
19	6	0	-3.718739	2.042027	-0.162082
20	7	0	-1.976914	0.231983	-0.162448
21	6	0	-2.913503	-0.815877	-0.153162
22	6	0	-4.017888	-0.864400	0.710109
23	6	0	-4.860071	-1.971256	0.711630
24	6	0	-4.619592	-3.044584	-0.142235
25	6	0	-3.513017	-3.012077	-0.990342
26	6	0	-2.663665	-1.914764	-0.988418
27	1	0	2.142764	4.317040	-0.306829
28	1	0	-0.006410	5.567841	-0.365976
29	1	0	-2.153685	4.315594	-0.304502
30	1	0	1.821993	-1.864216	-1.671078
31	1	0	3.357100	-3.818950	-1.686032
32	1	0	5.300673	-3.882519	-0.135674
33	1	0	5.684292	-1.991022	1.427478
34	1	0	4.153399	-0.050465	1.433826
35	1	0	-1.786763	-1.883987	-1.633179
36	1	0	-3.306936	-3.849947	-1.650389
37	1	0	-5.279624	-3.906823	-0.136478
38	1	0	-5.705304	-1.997831	1.394032
39	1	0	-4.188697	-0.047556	1.404772

40	1	0	4.382666	1.336394	-0.642051
41	1	0	3.745808	2.984236	-0.715685
42	1	0	4.126761	2.256665	0.838240
43	1	0	-4.385738	1.333582	-0.658131
44	1	0	-4.142447	2.246077	0.829052
45	1	0	-3.751481	2.982836	-0.718111
46	1	0	-0.891356	-1.993062	2.069109
47	1	0	0.060804	-2.776003	0.796537
48	1	0	0.886543	-1.941196	2.121170

**21<sup>+</sup> (<sup>4</sup>A):**

1	6	0	-2.709575	-2.072340	0.489240
2	6	0	-2.996176	-0.881017	-0.191897
3	6	0	-4.067728	-0.846081	-1.093279
4	6	0	-4.842389	-1.983213	-1.294364
5	6	0	-4.566847	-3.159328	-0.600564
6	6	0	-3.498394	-3.199288	0.293270
7	7	0	-2.117440	0.209640	-0.013686
8	6	0	-2.530149	1.454102	0.166935
9	6	0	-3.949127	1.876396	0.342708
10	26	0	-0.082273	-0.105751	0.131357
11	7	0	-0.220645	1.871555	0.159519
12	6	0	-1.460632	2.432335	0.188795
13	6	0	-1.610762	3.818324	0.132525
14	6	0	-0.477825	4.616336	-0.020995
15	6	0	0.774893	4.019103	-0.172477
16	6	0	0.878977	2.630825	-0.103441
17	6	0	2.067938	1.833971	-0.350345
18	6	0	3.398609	2.480424	-0.534002
19	7	0	1.822835	0.539436	-0.459632
20	6	0	2.840800	-0.428749	-0.596781
21	6	0	2.654386	-1.448285	-1.540243
22	6	0	3.582934	-2.476020	-1.653758
23	6	0	4.691913	-2.517349	-0.808579
24	6	0	4.873185	-1.516200	0.143500
25	6	0	3.958760	-0.472080	0.248422
26	1	0	-2.599116	4.265697	0.170296
27	1	0	-0.575105	5.695089	-0.073546
28	1	0	1.652484	4.628271	-0.364038
29	1	0	4.103549	1.817118	-1.036630
30	1	0	3.301342	3.390382	-1.132141
31	1	0	3.845286	2.779919	0.420771
32	1	0	-4.581164	1.040695	0.646637
33	1	0	-4.023247	2.662880	1.097863
34	1	0	-4.371736	2.283813	-0.582815
35	1	0	1.782341	-1.407806	-2.189651
36	1	0	3.439001	-3.249740	-2.401728
37	1	0	5.410470	-3.326335	-0.891533
38	1	0	5.731431	-1.545467	0.807996
39	1	0	4.092773	0.302587	0.999442
40	1	0	-1.887376	-2.086242	1.203478
41	1	0	-3.280375	-4.110876	0.841535
42	1	0	-5.177929	-4.041696	-0.759821
43	1	0	-5.663703	-1.949704	-2.003513
44	1	0	-4.264748	0.058895	-1.660080
45	8	0	0.596669	-1.527367	1.548564
46	6	0	1.334956	-1.041510	2.676359
47	1	0	2.404670	-1.006213	2.437813
48	1	0	0.965914	-0.038580	2.897155
49	1	0	1.166502	-1.693916	3.538713
50	6	0	1.014862	-2.842423	1.157271
51	1	0	2.081997	-2.845366	0.905691

52	1	0	0.816515	-3.547052	1.971403
53	1	0	0.427080	-3.119933	0.279696

7\_D/A (°A):

1	6	0	-3.305816	-1.906848	-0.335363
2	6	0	-2.388901	-1.473616	0.633389
3	6	0	-2.811584	-0.574825	1.621865
4	6	0	-4.133430	-0.150563	1.662541
5	6	0	-5.047147	-0.595305	0.708265
6	6	0	-4.625038	-1.466968	-0.292844
7	7	0	-1.025049	-1.807393	0.563833
8	26	0	0.400289	-0.214872	0.049792
9	6	0	-0.916178	0.651227	-1.156369
10	7	0	2.487917	0.370579	-0.152170
11	6	0	3.370106	-0.595014	-0.296159
12	6	0	2.815639	-1.925904	-0.176481
13	6	0	3.552161	-3.109913	-0.281148
14	6	0	2.903711	-4.331717	-0.147300
15	6	0	1.528116	-4.351158	0.085561
16	6	0	0.835738	-3.146397	0.187466
17	7	0	1.474258	-1.951829	0.064293
18	6	0	-0.597363	-3.033215	0.413829
19	6	0	-1.443929	-4.263870	0.471873
20	6	0	2.829913	1.726647	-0.084265
21	6	0	2.042064	2.654625	-0.782620
22	6	0	2.283847	4.017083	-0.655778
23	6	0	3.301731	4.480319	0.175797
24	6	0	4.076523	3.564836	0.885567
25	6	0	3.848147	2.199667	0.759058
26	6	0	4.820397	-0.405686	-0.609987
27	7	0	0.402499	0.646797	1.830753
28	7	0	0.415089	1.216993	2.806130
29	1	0	0.999930	-5.293936	0.185075
30	1	0	3.460303	-5.260282	-0.222564
31	1	0	4.622478	-3.069272	-0.458408
32	6	0	-1.128543	-0.146815	-2.346719
33	6	0	-1.839848	1.719018	-0.857998
34	1	0	-2.957970	-2.547470	-1.141304
35	1	0	-5.323999	-1.802097	-1.054722
36	1	0	-6.076521	-0.249570	0.734173
37	1	0	-4.447464	0.546094	2.434904
38	1	0	-2.089931	-0.219890	2.351638
39	1	0	1.242342	2.280950	-1.417749
40	1	0	1.664536	4.720556	-1.205944
41	1	0	3.483198	5.545975	0.279034
42	1	0	4.860084	3.915330	1.551847
43	1	0	4.428923	1.488504	1.340463
44	1	0	-2.434065	-4.048299	0.874868
45	1	0	-1.576219	-4.706457	-0.522129
46	1	0	-0.974038	-5.026858	1.099779
47	1	0	5.023520	0.613101	-0.943050
48	1	0	5.460979	-0.602056	0.258186
49	1	0	5.137304	-1.094315	-1.398930
50	6	0	-3.159744	1.745478	-1.371859
51	6	0	-4.056652	2.736713	-1.001942
52	6	0	-3.667232	3.744889	-0.119812
53	6	0	-2.368104	3.750023	0.393536
54	6	0	-1.474516	2.752972	0.036628
55	1	0	-3.487333	0.945340	-2.031082
56	1	0	-5.070739	2.719522	-1.393659
57	1	0	-4.371889	4.520016	0.169324
58	1	0	-2.057367	4.534535	1.078461

59	1	0	-0.460473	2.757092	0.431299
60	8	0	-0.689019	-1.291192	-2.501276
61	1	0	-1.698369	0.329583	-3.186133

**8\_D/A (<sup>4</sup>A):**

1	6	0	-2.385996	-0.200725	2.518831
2	6	0	-1.299356	-0.955988	2.038574
3	6	0	-1.578287	-2.242372	1.534935
4	6	0	-2.881410	-2.730579	1.510743
5	6	0	-3.946596	-1.957105	1.967239
6	6	0	-3.686655	-0.684743	2.476225
7	6	0	0.054493	-0.376978	2.058944
8	6	0	1.253347	-1.186421	2.100508
9	8	0	1.394422	-2.360112	1.745318
10	26	0	0.338609	0.450419	0.080291
11	7	0	0.688519	2.298220	-0.467812
12	7	0	0.886820	3.388800	-0.679487
13	7	0	2.450085	-0.143933	-0.341645
14	6	0	2.558947	-1.405717	-0.680545
15	6	0	3.790398	-2.244234	-0.561376
16	6	0	3.554391	0.662274	-0.037559
17	6	0	3.469651	1.549244	1.046338
18	6	0	4.512582	2.421230	1.328765
19	6	0	5.651879	2.441326	0.525837
20	6	0	5.734740	1.581518	-0.566696
21	6	0	4.699693	0.697523	-0.848242
22	7	0	-1.679290	0.489680	-0.859177
23	6	0	-2.527577	1.600494	-0.781890
24	6	0	-2.432325	2.432923	0.343436
25	6	0	-3.199570	3.585610	0.437928
26	6	0	-4.057186	3.946753	-0.600034
27	6	0	-4.134178	3.144602	-1.736033
28	6	0	-3.381221	1.979777	-1.829767
29	7	0	0.232103	-1.203555	-1.055868
30	6	0	-0.986606	-1.654378	-1.448980
31	6	0	-1.149187	-2.949329	-1.938794
32	6	0	-0.043198	-3.794287	-2.007776
33	6	0	1.198159	-3.329952	-1.583564
34	6	0	1.314007	-2.020988	-1.115255
35	6	0	-2.060971	-0.677992	-1.313270
36	6	0	-3.466135	-1.080494	-1.628278
37	1	0	2.071686	-3.973185	-1.620878
38	1	0	-0.149897	-4.806159	-2.385044
39	1	0	-2.127511	-3.293011	-2.260505
40	1	0	2.572742	1.532913	1.663694
41	1	0	4.432336	3.093525	2.178247
42	1	0	6.462864	3.129609	0.743745
43	1	0	6.609366	1.602211	-1.211028
44	1	0	4.751611	0.049740	-1.719138
45	1	0	-1.749700	2.149040	1.141394
46	1	0	-3.119998	4.211270	1.322369
47	1	0	-4.648526	4.854745	-0.530625
48	1	0	-4.780062	3.430239	-2.561699
49	1	0	-3.417848	1.375765	-2.731920
50	1	0	4.567464	-1.726788	0.001881
51	1	0	3.543563	-3.168220	-0.031234
52	1	0	4.208579	-2.518104	-1.536899
53	1	0	-4.182903	-0.369903	-1.215125
54	1	0	-3.644717	-1.152655	-2.707446
55	1	0	-3.675830	-2.062091	-1.193366
56	1	0	-0.751913	-2.852888	1.187329
57	1	0	-3.063771	-3.731781	1.123641

58	1	0	-4.962677	-2.341105	1.936176
59	1	0	-4.500832	-0.069084	2.850574
60	1	0	-2.194593	0.785433	2.939269
61	1	0	2.149776	-0.613443	2.451430
62	1	0	0.138924	0.523484	2.681494

**9\_D/A (<sup>3</sup>Å):**

1	6	0	-4.486093	-0.844185	-0.627123
2	6	0	-3.328908	-0.715154	0.148812
3	6	0	-3.117884	-1.583525	1.223937
4	6	0	-4.062123	-2.557532	1.524351
5	6	0	-5.216465	-2.684650	0.753951
6	6	0	-5.422460	-1.826992	-0.323969
7	7	0	-2.347061	0.255750	-0.161629
8	26	0	-0.459715	-0.132771	-0.522081
9	6	0	0.431543	-0.629278	1.088447
10	6	0	-2.649721	1.560868	-0.126518
11	6	0	-3.972921	2.100483	0.299141
12	6	0	-1.558877	2.397565	-0.497591
13	6	0	-1.514887	3.784315	-0.605087
14	6	0	-0.338985	4.411582	-1.021091
15	6	0	0.781325	3.643453	-1.347394
16	6	0	0.727618	2.258383	-1.233161
17	7	0	-0.425625	1.654659	-0.771490
18	6	0	1.741055	1.297098	-1.520400
19	6	0	3.120741	1.699237	-1.918906
20	7	0	1.316533	0.036634	-1.394065
21	6	0	2.208136	-1.058358	-1.462393
22	6	0	1.857168	-2.167468	-2.237582
23	6	0	2.671529	-3.293417	-2.248790
24	6	0	3.826606	-3.335474	-1.470070
25	6	0	4.166285	-2.239888	-0.678981
26	6	0	3.365839	-1.103193	-0.675511
27	1	0	-2.401035	4.370639	-0.379288
28	1	0	-0.301664	5.491866	-1.109783
29	1	0	1.694499	4.120533	-1.691432
30	6	0	1.384021	-0.043373	1.986800
31	6	0	0.184984	-1.953762	0.769147
32	1	0	-2.211227	-1.468255	1.811171
33	1	0	-3.893493	-3.223893	2.365726
34	1	0	-5.949195	-3.451064	0.989038
35	1	0	-6.314824	-1.923917	-0.936310
36	1	0	-4.631644	-0.182660	-1.477493
37	1	0	3.603905	-0.262449	-0.028680
38	1	0	5.052507	-2.271464	-0.050908
39	1	0	4.453125	-4.222800	-1.471246
40	1	0	2.393564	-4.148919	-2.857731
41	1	0	0.933511	-2.136405	-2.807099
42	1	0	-4.415348	1.479253	1.082165
43	1	0	-3.874492	3.118957	0.681134
44	1	0	-4.695973	2.128812	-0.524262
45	1	0	3.746863	1.929893	-1.048439
46	1	0	3.622262	0.907761	-2.478951
47	1	0	3.092987	2.598044	-2.541198
48	6	0	2.316267	-0.829942	2.703503
49	6	0	3.277188	-0.243637	3.513378
50	6	0	3.356733	1.145710	3.627402
51	6	0	2.451392	1.940415	2.925331
52	6	0	1.479275	1.358055	2.122108
53	1	0	2.287378	-1.912130	2.596400
54	1	0	3.981249	-0.873246	4.052257
55	1	0	4.117422	1.601629	4.254833

56	1	0	2.502279	3.023454	3.007840
57	1	0	0.767682	1.977672	1.580100
58	8	0	-0.496848	-2.114502	-0.329184
59	1	0	0.489810	-2.856565	1.329585

**10\_D/A (°Å):**

1	6	0	-2.322428	1.028416	2.592004
2	6	0	-2.647613	0.116753	1.581896
3	6	0	-3.973365	0.016136	1.138264
4	6	0	-4.960127	0.810672	1.709032
5	6	0	-4.640198	1.700248	2.732714
6	6	0	-3.321034	1.802513	3.170254
7	7	0	-1.607038	-0.598311	0.940350
8	6	0	-1.728972	-1.882334	0.655971
9	6	0	-2.817050	-2.784810	1.132312
10	6	0	-0.667493	-2.404969	-0.176775
11	6	0	-0.495553	-3.715579	-0.619391
12	6	0	0.569452	-4.008814	-1.475868
13	6	0	1.438927	-2.997937	-1.878778
14	6	0	1.241176	-1.696170	-1.413823
15	7	0	0.199005	-1.426249	-0.567877
16	6	0	2.004537	-0.516697	-1.702114
17	6	0	3.179416	-0.570456	-2.618009
18	26	0	-0.033156	0.289832	0.022645
19	6	0	1.520706	-0.108076	2.070109
20	7	0	0.683950	-0.829563	2.812452
21	7	0	-0.082867	-1.413919	3.420186
22	7	0	1.524808	0.577399	-1.105608
23	6	0	2.162687	1.831569	-1.277175
24	6	0	1.383106	2.932039	-1.648177
25	6	0	1.969097	4.184120	-1.784238
26	6	0	3.327201	4.363236	-1.528528
27	6	0	4.106545	3.270263	-1.157929
28	6	0	3.533598	2.007620	-1.042867
29	6	0	-1.479314	1.030314	-1.062039
30	1	0	2.272639	-3.215141	-2.539888
31	1	0	0.713897	-5.023281	-1.833073
32	1	0	-1.192106	-4.490192	-0.314566
33	6	0	-1.430023	2.159016	-0.292411
34	6	0	-2.536478	0.496368	-1.867870
35	1	0	4.139989	1.153294	-0.759126
36	1	0	5.168025	3.396593	-0.962077
37	1	0	3.776140	5.348130	-1.619405
38	1	0	1.355498	5.029619	-2.082151
39	1	0	0.328710	2.773349	-1.846669
40	1	0	-1.288730	1.147152	2.900238
41	1	0	-3.058380	2.504959	3.955839
42	1	0	-5.413025	2.320666	3.177601
43	1	0	-5.979576	0.742987	1.338792
44	1	0	-4.210101	-0.639208	0.304162
45	1	0	4.094900	-0.876574	-2.094266
46	1	0	3.007703	-1.300399	-3.414372
47	1	0	3.376729	0.398896	-3.079183
48	1	0	-3.350052	-2.358598	1.982880
49	1	0	-3.549798	-2.985084	0.341561
50	1	0	-2.397352	-3.749919	1.432623
51	6	0	1.479538	1.349516	2.341275
52	6	0	2.717855	-0.827102	1.584274
53	8	0	0.828404	1.876806	3.218330
54	1	0	2.121120	1.917546	1.635280
55	6	0	3.942936	-0.157066	1.461532
56	6	0	5.071484	-0.829996	1.004669

57	6	0	5.009555	-2.185543	0.690789
58	6	0	3.802957	-2.865127	0.840196
59	6	0	2.668239	-2.194082	1.278426
60	1	0	4.020178	0.893207	1.725707
61	1	0	6.009797	-0.289655	0.911976
62	1	0	5.895647	-2.709266	0.344725
63	1	0	3.735132	-3.922931	0.601226
64	1	0	1.725929	-2.732014	1.364075
65	6	0	-3.768281	1.184304	-2.010918
66	6	0	-4.822897	0.637997	-2.723419
67	6	0	-4.704489	-0.620308	-3.320453
68	6	0	-3.500302	-1.311034	-3.204360
69	6	0	-2.435338	-0.764842	-2.496368
70	1	0	-3.890326	2.150873	-1.527272
71	1	0	-5.755521	1.191667	-2.805745
72	1	0	-5.537502	-1.050045	-3.869531
73	1	0	-3.385587	-2.285623	-3.673979
74	1	0	-1.493245	-1.302022	-2.437121
75	8	0	-0.394375	2.170733	0.519692
76	1	0	-2.144241	2.998624	-0.240951

**13\_D/A (<sup>4</sup>A):**

1	6	0	1.404378	2.256170	1.788092
2	6	0	1.411464	0.891406	2.113149
3	6	0	2.644936	0.242069	2.279910
4	6	0	3.830077	0.950889	2.119575
5	6	0	3.816713	2.307531	1.804853
6	6	0	2.595120	2.955378	1.638553
7	6	0	0.147367	0.153949	2.278366
8	7	0	-0.972900	0.861276	2.258489
9	7	0	-1.948701	1.458616	2.272130
10	26	0	-0.447304	-0.533783	-0.580409
11	17	0	-0.820865	-2.710363	-0.257790
12	7	0	-2.450376	0.316110	-0.512348
13	6	0	-2.532024	1.619099	-0.707137
14	6	0	-1.273983	2.266646	-1.005529
15	7	0	-0.203345	1.416187	-1.019082
16	6	0	1.034325	1.890969	-1.348189
17	6	0	1.229737	3.237328	-1.653014
18	6	0	0.146628	4.114989	-1.612855
19	6	0	-1.116621	3.624916	-1.286549
20	6	0	2.071526	0.879458	-1.347908
21	6	0	3.489969	1.272361	-1.611164
22	6	0	-3.610528	-0.455017	-0.303277
23	6	0	-4.684183	-0.430648	-1.204001
24	6	0	-5.793743	-1.241858	-0.995549
25	6	0	-5.853352	-2.080718	0.114889
26	6	0	-4.785911	-2.113078	1.009714
27	6	0	-3.669114	-1.315697	0.798465
28	6	0	-3.778211	2.435655	-0.580318
29	7	0	1.654506	-0.336298	-1.057775
30	6	0	2.521267	-1.446005	-1.116309
31	6	0	3.318120	-1.703210	-2.241168
32	6	0	4.118764	-2.838653	-2.287946
33	6	0	4.141772	-3.726343	-1.214679
34	6	0	3.341510	-3.479684	-0.100883
35	6	0	2.525620	-2.356724	-0.053224
36	1	0	-1.977993	4.285080	-1.272842
37	1	0	0.283075	5.165821	-1.847145
38	1	0	2.219367	3.594059	-1.920270
39	6	0	-0.045215	-1.235245	2.708882
40	1	0	-2.819275	-1.358284	1.474199

41	1	0	-4.815628	-2.773533	1.871389
42	1	0	-6.720592	-2.714177	0.275328
43	1	0	-6.613573	-1.220538	-1.708218
44	1	0	-4.625532	0.211061	-2.079475
45	1	0	1.881595	-2.178909	0.802055
46	1	0	3.336868	-4.173361	0.734793
47	1	0	4.767946	-4.612948	-1.253243
48	1	0	4.721946	-3.032204	-3.170749
49	1	0	3.279368	-1.022382	-3.087478
50	1	0	-4.551718	1.894457	-0.033862
51	1	0	-3.568319	3.366869	-0.046054
52	1	0	-4.196369	2.712550	-1.555229
53	1	0	4.183998	0.514302	-1.245132
54	1	0	3.689802	1.416576	-2.679655
55	1	0	3.718019	2.216004	-1.107308
56	1	0	2.664823	-0.808300	2.539795
57	1	0	4.775045	0.430504	2.248831
58	1	0	4.748301	2.853683	1.686167
59	1	0	2.561958	4.010984	1.381448
60	1	0	0.461442	2.776491	1.631588
61	8	0	0.857616	-2.017890	2.939579
62	1	0	-1.113631	-1.522978	2.819129

14\_D/A (<sup>4</sup>A):

1	6	0	-1.436334	-0.079634	2.136861
2	6	0	-1.326470	-1.288602	1.408323
3	6	0	-2.240551	-2.324654	1.718150
4	6	0	-3.214036	-2.149838	2.689746
5	6	0	-3.303775	-0.945571	3.389345
6	6	0	-2.405832	0.088519	3.112242
7	6	0	-0.378071	-1.396681	0.330416
8	26	0	0.406460	0.137664	-0.615673
9	17	0	1.087316	-0.314000	-2.722187
10	7	0	-1.581383	1.001769	-0.895274
11	6	0	-1.715642	2.280838	-0.621021
12	6	0	-0.510663	2.914147	-0.141698
13	7	0	0.552279	2.063248	0.002480
14	6	0	1.737730	2.549904	0.473792
15	6	0	1.890905	3.890332	0.805872
16	6	0	0.810025	4.764434	0.660603
17	6	0	-0.397403	4.267056	0.187155
18	6	0	2.789398	1.549762	0.596602
19	6	0	4.137883	1.935892	1.114708
20	6	0	-2.662111	0.154121	-1.188660
21	6	0	-2.495699	-0.824175	-2.179679
22	6	0	-3.495609	-1.761655	-2.405231
23	6	0	-4.661246	-1.753492	-1.639306
24	6	0	-4.820440	-0.795849	-0.640750
25	6	0	-3.832093	0.155382	-0.415074
26	6	0	-2.969394	3.076636	-0.802369
27	7	0	2.431071	0.342839	0.259537
28	6	0	3.315512	-0.749823	0.217562
29	6	0	4.495605	-0.707623	-0.536757
30	6	0	5.297728	-1.838407	-0.631999
31	6	0	4.936093	-3.015536	0.020378
32	6	0	3.758921	-3.059656	0.764447
33	6	0	2.946244	-1.937015	0.860026
34	1	0	-1.255561	4.922318	0.074524
35	1	0	0.912547	5.813713	0.915808
36	1	0	2.845586	4.252163	1.173977
37	6	0	-0.070515	-2.708415	-0.235756
38	1	0	-3.927776	0.860995	0.405904

39	1	0	-5.709492	-0.799589	-0.015745
40	1	0	-5.433077	-2.498125	-1.810360
41	1	0	-3.357332	-2.511412	-3.179088
42	1	0	-1.572002	-0.832245	-2.754329
43	1	0	2.020737	-1.967769	1.426696
44	1	0	3.454615	-3.976380	1.260768
45	1	0	5.562066	-3.898907	-0.064165
46	1	0	6.203263	-1.802501	-1.231063
47	1	0	4.747195	0.199906	-1.079226
48	1	0	-3.685295	2.545532	-1.430648
49	1	0	-3.463589	3.293060	0.151934
50	1	0	-2.747903	4.038776	-1.272812
51	1	0	4.723424	1.055848	1.382397
52	1	0	4.707549	2.499610	0.367761
53	1	0	4.045780	2.576129	1.996423
54	1	0	-2.174587	-3.261643	1.174487
55	1	0	-3.913349	-2.953640	2.903503
56	1	0	-4.067830	-0.813549	4.150925
57	1	0	-2.466182	1.023382	3.663512
58	1	0	-0.732440	0.720048	1.908244
59	8	0	0.160860	-3.697245	0.456712
60	1	0	0.049692	-2.746407	-1.343235

15\_D/A (<sup>4</sup>A):

1	6	0	2.188960	1.278210	1.956274
2	6	0	0.788723	1.415987	1.890811
3	6	0	0.271564	2.720072	1.766427
4	6	0	1.102584	3.829786	1.701090
5	6	0	2.488145	3.676303	1.771012
6	6	0	3.018843	2.395745	1.908317
7	6	0	-0.126271	0.269839	1.895415
8	26	0	-0.336363	-0.581095	-0.130470
9	7	0	-0.091064	1.211937	-1.023930
10	6	0	1.174681	1.642909	-1.268444
11	6	0	1.422993	2.949115	-1.687120
12	6	0	0.354552	3.819016	-1.884249
13	6	0	-0.939032	3.368881	-1.634915
14	6	0	-1.135130	2.060512	-1.193291
15	6	0	2.191603	0.619145	-1.101135
16	6	0	3.632000	0.969672	-1.284406
17	6	0	-2.430253	1.481023	-0.867990
18	6	0	-3.655587	2.336526	-0.921257
19	7	0	1.733760	-0.565108	-0.773633
20	6	0	2.578499	-1.696719	-0.745889
21	6	0	3.342397	-2.040069	-1.869198
22	6	0	4.126233	-3.187207	-1.854042
23	6	0	4.162113	-3.994782	-0.719476
24	6	0	3.398593	-3.653587	0.394805
25	6	0	2.596600	-2.518530	0.384971
26	17	0	-0.832119	-2.754411	-0.250430
27	7	0	-2.389612	0.230443	-0.485807
28	6	0	-3.548403	-0.508414	-0.182710
29	6	0	-4.640845	-0.565452	-1.058077
30	6	0	-5.742505	-1.354610	-0.747859
31	6	0	-5.772213	-2.084280	0.437726
32	6	0	-4.681503	-2.038333	1.304457
33	6	0	-3.568751	-1.269756	0.992169
34	1	0	-1.789680	4.025900	-1.785704
35	1	0	0.527784	4.834826	-2.223166
36	1	0	2.441965	3.276304	-1.866618
37	6	0	0.134585	-0.936957	2.658100
38	1	0	-2.699920	-1.257155	1.647176

39	1	0	-4.687908	-2.618597	2.222125
40	1	0	-6.633949	-2.699620	0.677968
41	1	0	-6.577979	-1.403009	-1.440323
42	1	0	-4.601605	-0.018087	-1.995954
43	1	0	2.003249	-2.254589	1.255829
44	1	0	3.416721	-4.279432	1.281998
45	1	0	4.774820	-4.891443	-0.708176
46	1	0	4.705619	-3.452556	-2.733907
47	1	0	3.290716	-1.416821	-2.758464
48	1	0	-4.479902	1.885412	-0.368433
49	1	0	-3.448636	3.323187	-0.497434
50	1	0	-3.996438	2.495910	-1.950363
51	1	0	4.279179	0.204169	-0.854704
52	1	0	3.899479	1.077219	-2.341524
53	1	0	3.844245	1.922669	-0.790387
54	1	0	-1.183328	0.559570	1.952900
55	1	0	-0.809890	2.850343	1.718159
56	1	0	0.668012	4.821840	1.599296
57	1	0	3.141259	4.543755	1.729742
58	1	0	4.096175	2.259288	1.976157
59	1	0	2.609778	0.283284	2.064785
60	8	0	1.214167	-1.327392	3.096107
61	1	0	-0.782278	-1.564944	2.804199

**20\_D/A (°Å):**

1	6	0	1.871224	-1.040866	2.612024
2	6	0	0.884987	-1.595613	1.775211
3	6	0	-0.374773	-0.946730	1.744262
4	6	0	-0.590758	0.249810	2.435543
5	6	0	0.423829	0.811695	3.203897
6	6	0	1.644258	0.138894	3.308912
7	6	0	1.145860	-2.752395	0.941303
8	6	0	0.687360	-2.860119	-0.339487
9	8	0	-0.015894	-1.977346	-1.007462
10	26	0	-0.172040	-0.113463	-0.542688
11	7	0	1.849663	0.604660	-0.657682
12	6	0	2.941213	-0.278196	-0.752525
13	6	0	2.953344	-1.218671	-1.790774
14	6	0	3.978742	-2.151332	-1.880571
15	6	0	4.998276	-2.173637	-0.930989
16	6	0	4.987967	-1.245540	0.108175
17	6	0	3.974026	-0.298294	0.195602
18	7	0	-2.291023	0.281361	-0.550738
19	6	0	-2.657661	1.554714	-0.498937
20	6	0	-1.563808	2.494685	-0.456456
21	6	0	-1.692108	3.883571	-0.350448
22	6	0	-0.544276	4.669826	-0.282008
23	6	0	0.710699	4.064656	-0.334240
24	6	0	0.794300	2.674623	-0.455619
25	7	0	-0.332554	1.909000	-0.505656
26	6	0	2.018750	1.912695	-0.553715
27	6	0	3.336662	2.616970	-0.601104
28	6	0	-3.218321	-0.766896	-0.430103
29	6	0	-3.104206	-1.876703	-1.280211
30	6	0	-3.960737	-2.960302	-1.134999
31	6	0	-4.929588	-2.970926	-0.132584
32	6	0	-5.031173	-1.884178	0.732582
33	6	0	-4.186248	-0.789789	0.587781
34	6	0	-4.068421	2.050804	-0.537627
35	1	0	-2.677046	4.337618	-0.304891
36	1	0	-0.626265	5.747959	-0.185275
37	1	0	1.614545	4.662467	-0.274199

38	1	0	-4.248740	0.046318	1.279870
39	1	0	-5.768019	-1.888929	1.531259
40	1	0	-5.590667	-3.824882	-0.018347
41	1	0	-3.863694	-3.809074	-1.806238
42	1	0	-2.326038	-1.878095	-2.036408
43	1	0	3.946536	0.409603	1.019876
44	1	0	5.773744	-1.258680	0.859117
45	1	0	5.792595	-2.911395	-0.996898
46	1	0	3.974622	-2.873562	-2.692484
47	1	0	2.135720	-1.215758	-2.505681
48	1	0	-4.421867	2.386753	0.445170
49	1	0	-4.152717	2.908898	-1.211455
50	1	0	-4.754571	1.275455	-0.881531
51	1	0	3.677404	2.915601	0.397929
52	1	0	4.113331	1.982993	-1.031557
53	1	0	3.266500	3.530449	-1.198502
54	1	0	-1.211982	-1.451077	1.262853
55	1	0	-1.566719	0.727845	2.376244
56	1	0	0.261059	1.744308	3.735921
57	1	0	2.434314	0.551405	3.932693
58	1	0	2.839061	-1.533635	2.675318
59	1	0	0.970825	-3.752495	-0.913249
60	1	0	1.849157	-3.502951	1.291224

TS[6-7] (<sup>1</sup>A):

1	6	0	3.101818	-1.634188	0.915984
2	6	0	2.999530	-0.734601	-0.149196
3	6	0	3.874079	-0.855523	-1.235024
4	6	0	4.835300	-1.860122	-1.249870
5	6	0	4.940929	-2.748542	-0.182140
6	6	0	4.070916	-2.630217	0.899667
7	7	0	1.989984	0.259462	-0.133792
8	6	0	2.342485	1.557103	-0.198395
9	6	0	3.747753	2.058018	-0.215171
10	6	0	1.215838	2.424832	-0.252800
11	6	0	1.168383	3.816964	-0.357259
12	6	0	-0.068082	4.453519	-0.438389
13	6	0	-1.252386	3.708410	-0.422185
14	6	0	-1.175836	2.322490	-0.330658
15	7	0	0.043211	1.713630	-0.243106
16	6	0	-2.239321	1.354273	-0.333132
17	6	0	-3.673407	1.754383	-0.409863
18	26	0	0.108350	-0.113780	0.082279
19	6	0	0.148214	-0.004841	1.938995
20	7	0	-1.327139	0.785873	2.610865
21	7	0	-2.164783	1.460773	2.238169
22	7	0	-1.794635	0.088128	-0.334221
23	6	0	-2.727315	-0.975906	-0.392912
24	6	0	-3.555777	-1.147172	-1.508059
25	6	0	-4.437828	-2.220541	-1.565967
26	6	0	-4.508166	-3.131465	-0.514421
27	6	0	-3.683441	-2.963937	0.595945
28	6	0	-2.796506	-1.895753	0.658586
29	1	0	-2.218005	4.199800	-0.491425
30	1	0	-0.113523	5.534481	-0.524170
31	1	0	2.089320	4.391994	-0.388512
32	1	0	0.815608	0.749706	2.384852
33	1	0	0.136832	-0.888366	2.594964
34	1	0	-2.138178	-1.762510	1.513357
35	1	0	-3.727631	-3.671129	1.419407
36	1	0	-5.195991	-3.970355	-0.563209
37	1	0	-5.068948	-2.348130	-2.441208

38	1	0	-3.483771	-0.443254	-2.333125
39	1	0	2.405078	-1.543517	1.745747
40	1	0	4.141471	-3.322043	1.734217
41	1	0	5.690620	-3.534028	-0.197008
42	1	0	5.500889	-1.951996	-2.103728
43	1	0	3.774818	-0.169545	-2.072090
44	1	0	-4.313732	1.027486	0.094812
45	1	0	-3.822164	2.725659	0.067287
46	1	0	-4.028129	1.833929	-1.444692
47	1	0	4.412837	1.406085	0.356770
48	1	0	4.165683	2.125543	-1.227406
49	1	0	3.800033	3.059969	0.219231
50	7	0	0.196255	-1.901317	-0.023492
51	7	0	0.256637	-3.031492	-0.115244

TS[7-8] (°A):

1	6	0	2.062708	4.161986	0.766193
2	6	0	2.477333	3.303573	1.785975
3	6	0	1.547720	2.535404	2.471610
4	6	0	0.175954	2.593925	2.158000
5	6	0	-0.219788	3.447040	1.113080
6	6	0	0.709790	4.231223	0.439869
7	6	0	-0.763839	1.724102	2.861986
8	6	0	-2.236454	1.849502	2.602083
9	6	0	-0.040378	-0.698088	2.046443
10	26	0	-0.153126	-0.785065	0.096633
11	7	0	-2.154996	-0.202542	-0.600970
12	6	0	-3.290817	-0.957330	-0.282479
13	6	0	-3.406154	-1.493164	1.009274
14	6	0	-4.479075	-2.310982	1.339068
15	6	0	-5.446869	-2.627126	0.386921
16	6	0	-5.327719	-2.117465	-0.904080
17	6	0	-4.263831	-1.288233	-1.239553
18	6	0	-2.218284	0.919720	-1.292104
19	6	0	-3.477573	1.656212	-1.632159
20	6	0	-0.934896	1.472526	-1.647763
21	6	0	-0.755616	2.608196	-2.440658
22	6	0	0.531651	3.042631	-2.738403
23	6	0	1.619389	2.337289	-2.224152
24	6	0	1.398315	1.197788	-1.453094
25	7	0	0.134861	0.770880	-1.165000
26	6	0	2.452422	0.330605	-0.968388
27	6	0	3.878176	0.782643	-1.063683
28	7	0	2.031505	-0.793336	-0.430690
29	6	0	2.892979	-1.857818	-0.137793
30	6	0	3.925641	-2.241168	-1.012304
31	6	0	4.705493	-3.358620	-0.742038
32	6	0	4.478562	-4.117740	0.403482
33	6	0	3.442614	-3.759006	1.264063
34	6	0	2.649177	-2.651586	0.994473
35	1	0	-1.620433	3.131477	-2.838215
36	1	0	0.688004	3.915915	-3.363771
37	1	0	2.635016	2.654577	-2.441273
38	1	0	0.955694	-0.611753	2.503549
39	1	0	-0.665267	-1.315719	2.708128
40	1	0	-2.642719	-1.244112	1.741312
41	1	0	-4.556944	-2.709337	2.347025
42	1	0	-6.280124	-3.273543	0.645679
43	1	0	-6.065330	-2.371762	-1.660509
44	1	0	-4.155642	-0.916989	-2.255131
45	1	0	1.823127	-2.383012	1.646542
46	1	0	3.241605	-4.353886	2.150861

47	1	0	5.090357	-4.989968	0.613801
48	1	0	5.490214	-3.642611	-1.438161
49	1	0	4.082168	-1.678667	-1.928089
50	1	0	-4.315429	1.301975	-1.028941
51	1	0	-3.354758	2.729004	-1.452476
52	1	0	-3.762553	1.541074	-2.684704
53	1	0	4.523344	0.194560	-0.409485
54	1	0	4.281665	0.702836	-2.080036
55	1	0	3.954171	1.834630	-0.771019
56	1	0	-0.468059	0.504224	2.343019
57	1	0	-0.498038	1.553579	3.907956
58	1	0	-2.618309	2.848586	2.849934
59	1	0	-2.470802	1.663282	1.546295
60	1	0	-2.804151	1.123997	3.190562
61	1	0	1.873524	1.870471	3.269789
62	1	0	-1.270705	3.505028	0.836574
63	1	0	3.530299	3.239046	2.049548
64	1	0	0.376835	4.892673	-0.355801
65	1	0	2.787430	4.771321	0.232000
66	7	0	-0.375386	-2.651183	-0.481362
67	7	0	-0.539228	-3.748307	-0.689210

TS[8-5] ( $^3A$ ):

1	6	0	-2.062432	-3.061399	1.590543
2	6	0	-2.139818	-1.845948	2.303715
3	6	0	-3.212924	-0.980094	1.995564
4	6	0	-4.161012	-1.315763	1.042424
5	6	0	-4.070529	-2.528516	0.353786
6	6	0	-3.012466	-3.393322	0.633696
7	6	0	-1.120117	-1.429668	3.234133
8	6	0	-0.181815	-2.404727	3.862253
9	6	0	0.243341	-0.335515	1.821016
10	26	0	0.677656	0.603639	-0.030635
11	7	0	2.559734	-0.371297	-0.359152
12	6	0	3.775236	0.179229	0.050142
13	6	0	3.818182	0.890216	1.262065
14	6	0	4.981973	1.521842	1.677395
15	6	0	6.132277	1.472830	0.890536
16	6	0	6.096904	0.790416	-0.323417
17	6	0	4.937325	0.149235	-0.742288
18	7	0	-1.449046	1.016672	-0.797621
19	6	0	-1.946766	0.064055	-1.543147
20	6	0	-1.036529	-1.042337	-1.820153
21	6	0	-1.392294	-2.185045	-2.527535
22	6	0	-0.433522	-3.185380	-2.733263
23	6	0	0.846248	-3.013787	-2.229581
24	6	0	1.171713	-1.844337	-1.526271
25	7	0	0.221362	-0.871322	-1.332267
26	6	0	2.468298	-1.543164	-0.989374
27	6	0	3.578432	-2.543674	-1.099193
28	6	0	-2.133458	2.208192	-0.523572
29	6	0	-2.130909	2.698882	0.790984
30	6	0	-2.734788	3.911777	1.094141
31	6	0	-3.329011	4.674660	0.089979
32	6	0	-3.309066	4.210909	-1.222951
33	6	0	-2.721737	2.988898	-1.530785
34	6	0	-3.340495	0.032409	-2.090027
35	7	0	1.144419	2.456400	-0.204134
36	1	0	1.604562	-3.773839	-2.393171
37	1	0	-0.689999	-4.084107	-3.285097
38	1	0	-2.399869	-2.301725	-2.913095
39	1	0	-0.703942	0.183016	1.680406

40	1	0	0.916911	0.004886	2.600354
41	1	0	2.915330	0.929046	1.868341
42	1	0	4.990663	2.059829	2.621554
43	1	0	7.040934	1.971480	1.214103
44	1	0	6.978804	0.763883	-0.958240
45	1	0	4.907614	-0.346986	-1.707961
46	1	0	-1.645370	2.112649	1.568043
47	1	0	-2.731157	4.269563	2.119965
48	1	0	-3.789388	5.629005	0.326996
49	1	0	-3.749048	4.806829	-2.017928
50	1	0	-2.681811	2.643252	-2.560075
51	1	0	4.361147	-2.344461	-0.365033
52	1	0	3.204294	-3.557305	-0.926938
53	1	0	4.055441	-2.546837	-2.087295
54	1	0	-3.984176	0.746658	-1.574791
55	1	0	-3.360673	0.275493	-3.158754
56	1	0	-3.774022	-0.963475	-1.974165
57	1	0	0.377252	-1.332561	1.419616
58	1	0	-1.386478	-0.570319	3.849307
59	1	0	-0.705510	-3.102874	4.531317
60	1	0	0.341206	-3.015848	3.117976
61	1	0	0.582721	-1.896250	4.455076
62	1	0	-3.287513	-0.030501	2.524438
63	1	0	-1.244536	-3.749257	1.792374
64	1	0	-4.978187	-0.629411	0.831616
65	1	0	-2.926347	-4.335902	0.098204
66	1	0	-4.816842	-2.795232	-0.390361
67	7	0	1.448885	3.546898	-0.200424

TS[8-5] ( $^{\circ}$ A):

1	6	0	-1.858785	-3.331272	1.291700
2	6	0	-2.066803	-2.212772	2.127571
3	6	0	-3.267032	-1.488184	1.954863
4	6	0	-4.215322	-1.873635	1.020605
5	6	0	-3.995553	-2.990811	0.210962
6	6	0	-2.808842	-3.710370	0.352989
7	6	0	-1.076941	-1.754646	3.069670
8	6	0	0.039815	-2.632746	3.525188
9	6	0	-0.000621	-0.225395	1.819469
10	26	0	0.635997	0.726317	-0.034623
11	7	0	2.420675	-0.459773	-0.477563
12	6	0	3.687702	-0.072868	-0.036618
13	6	0	3.798748	0.551761	1.217256
14	6	0	5.022069	1.030282	1.666083
15	6	0	6.161203	0.911355	0.871208
16	6	0	6.058501	0.313137	-0.382934
17	6	0	4.839562	-0.177489	-0.835381
18	7	0	-1.373353	1.370779	-0.678268
19	6	0	-2.066173	0.443027	-1.317551
20	6	0	-1.296431	-0.715544	-1.705305
21	6	0	-1.804996	-1.806765	-2.408443
22	6	0	-0.967292	-2.874278	-2.727952
23	6	0	0.360258	-2.845776	-2.307670
24	6	0	0.837598	-1.738191	-1.605397
25	7	0	0.020145	-0.675049	-1.331968
26	6	0	2.186598	-1.596922	-1.112923
27	6	0	3.175694	-2.709472	-1.277594
28	6	0	-1.901016	2.611133	-0.315300
29	6	0	-1.542623	3.149521	0.933239
30	6	0	-1.976131	4.412046	1.314268
31	6	0	-2.764086	5.176835	0.455632
32	6	0	-3.105360	4.664056	-0.794167

33	6	0	-2.684820	3.396651	-1.178723
34	6	0	-3.537677	0.495850	-1.588459
35	7	0	1.474169	2.430723	-0.389717
36	1	0	1.026991	-3.671290	-2.539322
37	1	0	-1.349014	-3.723031	-3.286393
38	1	0	-2.847775	-1.820108	-2.710928
39	1	0	-0.998187	0.180941	1.714171
40	1	0	0.626363	0.118973	2.635582
41	1	0	2.903251	0.645857	1.829062
42	1	0	5.085888	1.503856	2.641943
43	1	0	7.116210	1.291828	1.220647
44	1	0	6.934419	0.234315	-1.021397
45	1	0	4.758547	-0.608358	-1.829248
46	1	0	-0.916696	2.554243	1.595858
47	1	0	-1.691494	4.804231	2.286828
48	1	0	-3.097086	6.166990	0.751745
49	1	0	-3.699249	5.259560	-1.482528
50	1	0	-2.924100	3.019738	-2.168714
51	1	0	3.994712	-2.616317	-0.561953
52	1	0	2.697845	-3.681289	-1.125955
53	1	0	3.622852	-2.728969	-2.278931
54	1	0	-4.035498	1.188797	-0.906518
55	1	0	-3.766405	0.824977	-2.609506
56	1	0	-3.987158	-0.491974	-1.455741
57	1	0	0.264385	-1.142354	1.308437
58	1	0	-1.437671	-1.031431	3.799386
59	1	0	-0.328200	-3.487704	4.110421
60	1	0	0.609638	-3.049214	2.686359
61	1	0	0.745880	-2.085555	4.154696
62	1	0	-3.442336	-0.611897	2.577908
63	1	0	-0.939112	-3.905181	1.381894
64	1	0	-5.133946	-1.300465	0.918831
65	1	0	-2.620679	-4.574906	-0.279063
66	1	0	-4.738877	-3.294274	-0.521593
67	7	0	1.978810	3.441130	-0.458701

TS[9-20] ( $^{\circ}$ A):

1	6	0	4.072765	-1.987974	-1.047137
2	6	0	3.030021	-1.670142	-0.158973
3	6	0	2.854425	-2.473331	0.978004
4	6	0	3.715605	-3.532395	1.233906
5	6	0	4.756702	-3.830942	0.356659
6	6	0	4.921625	-3.057580	-0.789933
7	7	0	2.107092	-0.650918	-0.442729
8	6	0	2.492510	0.509363	-0.962703
9	6	0	1.407131	1.326310	-1.448314
10	6	0	1.528911	2.446683	-2.265937
11	6	0	0.375990	3.024825	-2.806616
12	6	0	-0.869334	2.458461	-2.538545
13	6	0	-0.947328	1.347740	-1.696848
14	7	0	0.178181	0.849576	-1.106269
15	6	0	-2.126231	0.581453	-1.405302
16	7	0	-1.890091	-0.548674	-0.740495
17	6	0	-2.901216	-1.499112	-0.529229
18	6	0	-3.032252	-2.099073	0.732326
19	6	0	-3.978258	-3.094640	0.943423
20	6	0	-4.802143	-3.522348	-0.095984
21	6	0	-4.667233	-2.942635	-1.355844
22	6	0	-3.730498	-1.939721	-1.574050
23	26	0	0.042492	-0.655216	0.172873
24	6	0	0.001141	-0.935156	2.097256
25	1	0	-1.767438	2.854087	-3.005642

26	1	0	0.455120	3.881317	-3.468692
27	1	0	2.511494	2.839565	-2.513118
28	6	0	3.897074	1.024871	-1.016944
29	6	0	-3.483936	1.097861	-1.767162
30	1	0	0.894890	-0.637816	2.666868
31	1	0	-0.441901	-1.812508	2.588707
32	1	0	-2.388780	-1.755280	1.536801
33	1	0	-4.071432	-3.540266	1.930201
34	1	0	-5.536850	-4.304179	0.071774
35	1	0	-5.292039	-3.277461	-2.179611
36	1	0	-3.606141	-1.510840	-2.564701
37	1	0	2.030702	-2.244759	1.648599
38	1	0	3.566586	-4.134703	2.126070
39	1	0	5.422669	-4.665118	0.556562
40	1	0	5.712345	-3.292223	-1.497649
41	1	0	4.184155	-1.413070	-1.961992
42	1	0	-4.257749	0.636723	-1.149238
43	1	0	-3.531722	2.182276	-1.628189
44	1	0	-3.750356	0.898713	-2.812194
45	1	0	4.552165	0.466945	-0.345936
46	1	0	4.334694	0.964341	-2.020773
47	1	0	3.917157	2.079736	-0.724273
48	1	0	-0.769635	0.077686	2.518152
49	6	0	-1.329185	1.202161	3.022745
50	6	0	-2.784661	1.064280	2.682524
51	1	0	-1.093013	1.087547	4.083746
52	1	0	-3.353790	1.980087	2.891083
53	1	0	-2.919160	0.835121	1.616779
54	1	0	-3.249207	0.251609	3.247386
55	6	0	-0.529793	2.227760	2.351788
56	6	0	0.822164	2.400729	2.708393
57	6	0	-1.017545	2.980084	1.270207
58	6	0	1.643499	3.283097	2.021568
59	1	0	1.222218	1.819603	3.537844
60	6	0	-0.198712	3.877040	0.592046
61	1	0	-2.054017	2.862354	0.959969
62	6	0	1.136407	4.030193	0.956650
63	1	0	2.684101	3.392899	2.317554
64	1	0	-0.603031	4.449519	-0.239104
65	1	0	1.776777	4.721919	0.415010

TS[10-11] (<sup>1</sup>A):

1	6	0	-4.046144	-0.891117	-0.956492
2	6	0	-3.027963	-0.850771	0.005158
3	6	0	-2.958209	-1.872402	0.958971
4	6	0	-3.910226	-2.884486	0.976161
5	6	0	-4.929168	-2.912041	0.026377
6	6	0	-4.985883	-1.915940	-0.945479
7	7	0	-2.024129	0.145467	-0.025521
8	26	0	-0.110414	-0.233403	-0.076663
9	6	0	-0.244601	-1.860291	-0.738801
10	6	0	-2.378199	1.437698	-0.109095
11	6	0	-3.770937	1.967010	-0.004127
12	6	0	-1.263222	2.318829	-0.264464
13	6	0	-1.246528	3.713848	-0.320680
14	6	0	-0.022768	4.375804	-0.428006
15	6	0	1.172659	3.656070	-0.459963
16	6	0	1.116446	2.262551	-0.412052
17	7	0	-0.084251	1.626909	-0.347062
18	6	0	2.211139	1.319162	-0.427603
19	6	0	3.627725	1.778079	-0.531509
20	7	0	1.822662	0.048524	-0.418047

21	6	0	2.795782	-0.979412	-0.377506
22	6	0	2.974679	-1.813239	-1.485738
23	6	0	3.897883	-2.852416	-1.432672
24	6	0	4.643649	-3.076701	-0.277405
25	6	0	4.466799	-2.246919	0.827315
26	6	0	3.551704	-1.199887	0.779246
27	1	0	-2.174840	4.275287	-0.272920
28	1	0	0.000181	5.460307	-0.470297
29	1	0	2.129318	4.167452	-0.504988
30	1	0	-1.195810	-2.362769	-0.975988
31	1	0	0.616610	-2.479520	-1.035857
32	1	0	-2.140810	-1.865909	1.671824
33	1	0	-3.846358	-3.665124	1.729090
34	1	0	-5.664354	-3.711369	0.034233
35	1	0	-5.761633	-1.938462	-1.706010
36	1	0	-4.073705	-0.128013	-1.729367
37	1	0	3.417146	-0.540586	1.633896
38	1	0	5.047428	-2.410193	1.731174
39	1	0	5.359985	-3.892040	-0.239018
40	1	0	4.033221	-3.492073	-2.300483
41	1	0	2.381608	-1.630050	-2.376821
42	1	0	-4.427024	1.274014	0.526022
43	1	0	-3.772424	2.917893	0.537327
44	1	0	-4.230162	2.160010	-0.981767
45	1	0	4.279933	0.984387	-0.899281
46	1	0	3.708066	2.633005	-1.209640
47	1	0	4.014897	2.101217	0.441421
48	6	0	0.212138	-0.596173	1.742018
49	1	0	0.981317	-1.336377	2.003481
50	7	0	1.033955	0.732154	2.461376
51	1	0	-0.607419	-0.664962	2.467786
52	7	0	1.748199	1.582487	2.194610

TS[19-9] ( $^{\circ}\text{A}$ ):

1	6	0	-3.740552	-0.861989	-1.550142
2	6	0	-2.752671	-0.952216	-0.555834
3	6	0	-2.608280	-2.163151	0.139151
4	6	0	-3.445003	-3.237570	-0.133122
5	6	0	-4.431102	-3.135901	-1.112662
6	6	0	-4.566552	-1.945621	-1.823428
7	7	0	-1.837855	0.082912	-0.312256
8	26	0	0.114547	-0.242439	0.450106
9	6	0	-0.130084	-0.846592	2.316489
10	6	0	-2.203549	1.358196	-0.255369
11	6	0	-3.611031	1.859097	-0.197996
12	6	0	-1.094137	2.285605	-0.206858
13	6	0	-1.147651	3.659680	-0.426576
14	6	0	0.051152	4.375723	-0.517318
15	6	0	1.272773	3.708436	-0.424906
16	6	0	1.280217	2.330221	-0.198776
17	7	0	0.102429	1.669423	-0.014491
18	6	0	2.422814	1.454733	-0.178217
19	6	0	3.810076	2.014086	-0.193587
20	7	0	2.115016	0.159626	-0.091192
21	6	0	3.088004	-0.845047	-0.201889
22	6	0	4.058646	-0.843839	-1.216760
23	6	0	4.946646	-1.905745	-1.343815
24	6	0	4.893516	-2.982601	-0.461901
25	6	0	3.928702	-2.994146	0.544492
26	6	0	3.030062	-1.942919	0.670668
27	1	0	-2.102220	4.159674	-0.564722
28	1	0	0.030724	5.444437	-0.705423

29	1	0	2.205681	4.249653	-0.557793
30	1	0	0.439669	-0.262826	3.049932
31	1	0	-0.121090	-1.895960	2.630045
32	1	0	-1.840098	-2.234107	0.905262
33	1	0	-3.324317	-4.161922	0.424832
34	1	0	-5.080945	-3.979033	-1.326850
35	1	0	-5.316960	-1.859991	-2.604708
36	1	0	-3.826403	0.050100	-2.133310
37	1	0	2.270553	-1.938971	1.450768
38	1	0	3.873485	-3.830049	1.236513
39	1	0	5.590795	-3.808857	-0.562896
40	1	0	5.681555	-1.893340	-2.144299
41	1	0	4.082781	-0.022815	-1.927624
42	1	0	-4.292040	1.076149	0.141491
43	1	0	-3.680913	2.699591	0.497648
44	1	0	-3.975976	2.210476	-1.170635
45	1	0	4.528559	1.306987	0.225875
46	1	0	4.155454	2.257860	-1.205831
47	1	0	3.858007	2.938837	0.388323
48	7	0	-1.709638	-0.380964	2.812218
49	7	0	-2.162310	0.678560	2.780117

**TS[20-18] ( $^3A$ ):**

1	6	0	-2.497121	-2.722395	-2.325396
2	6	0	-2.543813	-2.812196	-0.916869
3	6	0	-3.736746	-2.400726	-0.281997
4	6	0	-4.821860	-1.940324	-1.012232
5	6	0	-4.753827	-1.856492	-2.404926
6	6	0	-3.582106	-2.249691	-3.051531
7	6	0	-1.411875	-3.237631	-0.132755
8	6	0	-0.328462	-4.082611	-0.719419
9	6	0	-0.275739	-1.381771	0.238906
10	26	0	0.653717	0.484769	0.426928
11	7	0	2.622071	-0.135573	0.296868
12	6	0	2.973346	-1.405273	0.771205
13	6	0	3.460715	-2.425430	-0.063496
14	6	0	3.695405	-3.699930	0.440557
15	6	0	3.447151	-3.990621	1.780806
16	6	0	2.945626	-2.989880	2.613309
17	6	0	2.706243	-1.715775	2.115560
18	7	0	-0.713305	2.005688	0.471232
19	6	0	-0.432876	3.101776	-0.239626
20	6	0	0.872358	3.102206	-0.845032
21	6	0	1.501930	4.173544	-1.483040
22	6	0	2.811829	4.007094	-1.940527
23	6	0	3.493842	2.817134	-1.696813
24	6	0	2.839408	1.776909	-1.023826
25	7	0	1.514395	1.907718	-0.705983
26	6	0	3.420157	0.562654	-0.535213
27	6	0	4.830315	0.190834	-0.859433
28	6	0	-1.970599	1.897702	1.111635
29	6	0	-2.927801	0.991279	0.638495
30	6	0	-4.141184	0.848828	1.305777
31	6	0	-4.417371	1.602270	2.443604
32	6	0	-3.466844	2.506635	2.914402
33	6	0	-2.252051	2.656128	2.255290
34	6	0	-1.394651	4.230061	-0.411675
35	1	0	4.529607	2.707078	-2.003674
36	1	0	3.316255	4.824992	-2.445957
37	1	0	0.995974	5.127731	-1.592661
38	1	0	-1.185105	-1.029972	0.725731
39	1	0	0.420707	-1.999821	0.796256

40	1	0	3.620895	-2.215484	-1.117487
41	1	0	4.064376	-4.476354	-0.224719
42	1	0	3.630832	-4.987601	2.169652
43	1	0	2.738721	-3.203936	3.658447
44	1	0	2.308693	-0.931456	2.757349
45	1	0	-2.719767	0.410993	-0.258694
46	1	0	-4.872361	0.142285	0.921600
47	1	0	-5.365305	1.486191	2.960595
48	1	0	-3.670515	3.098458	3.802851
49	1	0	-1.501180	3.351014	2.623486
50	1	0	4.927645	-0.337340	-1.816707
51	1	0	5.457081	1.084788	-0.929057
52	1	0	5.256502	-0.459180	-0.091838
53	1	0	-2.412237	3.855536	-0.558620
54	1	0	-1.432534	4.882403	0.469553
55	1	0	-1.131518	4.849705	-1.270744
56	1	0	-0.215536	-1.360946	-0.848162
57	1	0	-1.638562	-3.437027	0.914199
58	1	0	-0.704771	-5.064425	-1.039651
59	1	0	0.131326	-3.618271	-1.600404
60	1	0	0.475661	-4.254706	0.002135
61	1	0	-3.793837	-2.452062	0.804906
62	1	0	-1.595791	-3.031037	-2.850027
63	1	0	-5.734387	-1.649688	-0.495937
64	1	0	-3.516753	-2.192014	-4.135276
65	1	0	-5.603279	-1.494526	-2.976527

TS[20-18] ( $^{\circ}$ A):

1	6	0	3.636281	2.582423	-1.959219
2	6	0	3.403726	2.065679	-0.668215
3	6	0	4.172312	0.954001	-0.259594
4	6	0	5.125612	0.394192	-1.094093
5	6	0	5.348603	0.925330	-2.366748
6	6	0	4.597304	2.020988	-2.790361
7	6	0	2.388889	2.593415	0.210612
8	6	0	1.706948	3.890013	-0.071105
9	6	0	0.721840	1.128110	0.047613
10	26	0	-0.788086	-0.349649	0.162401
11	7	0	-2.574938	0.629953	-0.058961
12	6	0	-2.795595	1.962008	0.347919
13	6	0	-2.018995	3.001440	-0.181591
14	6	0	-2.191674	4.308359	0.264008
15	6	0	-3.136755	4.601914	1.243902
16	6	0	-3.912550	3.572286	1.774692
17	6	0	-3.747163	2.264960	1.333062
18	7	0	0.252700	-2.071097	0.577624
19	6	0	-0.236812	-3.205450	0.031727
20	6	0	-1.505917	-3.039024	-0.591196
21	6	0	-2.343529	-4.044084	-1.082605
22	6	0	-3.621525	-3.719915	-1.534396
23	6	0	-4.078536	-2.400847	-1.439009
24	6	0	-3.223886	-1.416291	-0.951841
25	7	0	-1.922884	-1.725126	-0.629049
26	6	0	-3.550111	-0.052142	-0.677239
27	6	0	-4.852717	0.560967	-1.072464
28	6	0	1.511616	-2.006085	1.189244
29	6	0	2.674795	-2.588404	0.657124
30	6	0	3.900636	-2.430773	1.295100
31	6	0	4.004414	-1.680788	2.464690
32	6	0	2.862178	-1.069226	2.984072
33	6	0	1.635712	-1.225301	2.352946
34	6	0	0.422850	-4.541531	0.129448

35	1	0	-5.103608	-2.155694	-1.702361
36	1	0	-4.280396	-4.497929	-1.906120
37	1	0	-2.011087	-5.078242	-1.088278
38	1	0	1.505822	0.427662	0.312232
39	1	0	0.256159	1.742191	0.816228
40	1	0	-1.291492	2.770727	-0.954999
41	1	0	-1.584745	5.102153	-0.164760
42	1	0	-3.268228	5.622285	1.591244
43	1	0	-4.650715	3.787575	2.542759
44	1	0	-4.337755	1.457403	1.758341
45	1	0	2.615605	-3.140664	-0.275361
46	1	0	4.786536	-2.889521	0.863307
47	1	0	4.964771	-1.559712	2.956809
48	1	0	2.927457	-0.469459	3.887995
49	1	0	0.739256	-0.750365	2.750691
50	1	0	-4.711498	1.587563	-1.424468
51	1	0	-5.330419	-0.009315	-1.871453
52	1	0	-5.564430	0.617403	-0.239518
53	1	0	1.084157	-4.761554	-0.718515
54	1	0	1.032315	-4.618416	1.033648
55	1	0	-0.325206	-5.337632	0.161277
56	1	0	0.632996	1.441998	-0.988210
57	1	0	2.536559	2.359018	1.264441
58	1	0	2.405492	4.737322	-0.015523
59	1	0	1.264325	3.913761	-1.074196
60	1	0	0.900691	4.080389	0.642935
61	1	0	3.996725	0.528081	0.728114
62	1	0	3.064891	3.440609	-2.304847
63	1	0	5.701517	-0.462251	-0.751402
64	1	0	4.764555	2.443192	-3.778048
65	1	0	6.098152	0.488828	-3.020591

TS[13-14] (<sup>4</sup>A):

1	6	0	-1.203866	2.304846	-0.512437
2	7	0	-0.048094	1.586143	-0.431222
3	6	0	1.148439	2.217813	-0.589245
4	6	0	1.216696	3.589359	-0.814378
5	6	0	0.038935	4.331858	-0.894608
6	6	0	-1.180796	3.681649	-0.739704
7	26	0	-0.091857	-0.369285	0.029802
8	17	0	-0.255016	-2.418454	-0.908658
9	6	0	2.297761	1.342024	-0.476457
10	6	0	3.669699	1.931924	-0.404409
11	6	0	-2.405755	1.514654	-0.353218
12	6	0	-3.740709	2.188132	-0.306450
13	7	0	2.007579	0.063792	-0.381976
14	6	0	2.989625	-0.941428	-0.376235
15	6	0	4.044531	-0.959073	-1.300312
16	6	0	4.959297	-2.005534	-1.299728
17	6	0	4.840070	-3.045359	-0.381066
18	6	0	3.781879	-3.043024	0.525454
19	6	0	2.856271	-2.008661	0.521910
20	6	0	0.000039	-0.449693	2.127898
21	7	0	-2.196874	0.226081	-0.209124
22	6	0	-3.237328	-0.715533	-0.133130
23	6	0	-3.148781	-1.731601	0.827333
24	6	0	-4.131909	-2.707774	0.905822
25	6	0	-5.202017	-2.704740	0.012852
26	6	0	-5.277824	-1.716900	-0.965535
27	6	0	-4.306081	-0.725546	-1.040328
28	1	0	-2.112095	4.235138	-0.805913
29	1	0	0.073736	5.400354	-1.078044

30	1	0	2.181988	4.071000	-0.933943
31	1	0	-0.974506	-0.115934	2.504891
32	1	0	0.080766	-1.536796	2.269749
33	1	0	-2.297811	-1.745475	1.502550
34	1	0	-4.053256	-3.485316	1.659900
35	1	0	-5.962625	-3.477749	0.068115
36	1	0	-6.093771	-1.720075	-1.682798
37	1	0	-4.346008	0.024155	-1.825476
38	1	0	2.009192	-2.021193	1.202046
39	1	0	3.665868	-3.860399	1.230986
40	1	0	5.556269	-3.861491	-0.383912
41	1	0	5.764532	-2.010900	-2.028967
42	1	0	4.117379	-0.167482	-2.040624
43	1	0	-4.494706	1.540540	0.142473
44	1	0	-3.683153	3.110858	0.276851
45	1	0	-4.097217	2.462087	-1.305942
46	1	0	4.385571	1.217985	0.004470
47	1	0	4.040654	2.243074	-1.387689
48	1	0	3.658827	2.819084	0.234676
49	6	0	1.109235	0.230433	2.836132
50	1	0	2.091605	-0.207522	2.638253
51	1	0	0.982074	0.399765	3.910098
52	7	0	1.264944	1.759293	2.271858
53	7	0	0.618983	2.641041	2.676125

TS[14-15] (<sup>4</sup>A):

1	6	0	2.972843	-2.310868	1.091733
2	6	0	3.140395	-1.546356	-0.071500
3	6	0	4.220865	-1.835686	-0.920035
4	6	0	5.123410	-2.840483	-0.594135
5	6	0	4.968562	-3.572356	0.580620
6	6	0	3.886537	-3.304061	1.416824
7	7	0	2.173877	-0.584834	-0.404612
8	6	0	2.486832	0.593399	-0.911273
9	6	0	3.865016	1.176062	-0.974111
10	6	0	1.362540	1.357085	-1.391391
11	6	0	1.464845	2.554049	-2.104525
12	6	0	0.321436	3.146850	-2.626173
13	6	0	-0.917897	2.549922	-2.388594
14	6	0	-0.981105	1.372638	-1.649019
15	7	0	0.145577	0.776399	-1.163565
16	6	0	-2.213986	0.678388	-1.324623
17	6	0	-3.530898	1.298510	-1.677813
18	26	0	0.056463	-0.921135	-0.065758
19	17	0	-0.105901	-3.128152	-0.495853
20	6	0	0.158198	-0.504620	1.858008
21	7	0	-2.056618	-0.438600	-0.660379
22	6	0	-3.114900	-1.291108	-0.315148
23	6	0	-3.118741	-1.854574	0.968447
24	6	0	-4.118448	-2.741151	1.341777
25	6	0	-5.112673	-3.105377	0.434603
26	6	0	-5.093166	-2.578186	-0.853891
27	6	0	-4.105474	-1.674974	-1.230275
28	6	0	-1.146438	1.582694	2.707077
29	6	0	-2.623091	1.477133	2.460142
30	6	0	-0.370290	2.656203	2.083238
31	6	0	0.973674	2.845037	2.456492
32	6	0	1.761097	3.810719	1.846962
33	6	0	1.224258	4.623345	0.847561
34	6	0	-0.105495	4.453264	0.468201
35	6	0	-0.890616	3.475669	1.067877
36	1	0	-1.827033	2.992705	-2.783824

37	1	0	0.389989	4.062621	-3.204435
38	1	0	2.441198	2.999441	-2.270530
39	1	0	1.072448	-0.018731	2.227614
40	1	0	-0.143292	-1.275606	2.584523
41	1	0	-2.320295	-1.585115	1.655094
42	1	0	-4.112021	-3.164476	2.342100
43	1	0	-5.885908	-3.810492	0.724565
44	1	0	-5.846753	-2.877417	-1.577010
45	1	0	-4.068557	-1.294765	-2.247137
46	1	0	2.111206	-2.117966	1.724152
47	1	0	3.743003	-3.883240	2.324514
48	1	0	5.674640	-4.358002	0.832887
49	1	0	5.946536	-3.058700	-1.269061
50	1	0	4.321268	-1.293824	-1.856023
51	1	0	-4.341357	0.864329	-1.090091
52	1	0	-3.507436	2.377104	-1.496763
53	1	0	-3.781889	1.158022	-2.735159
54	1	0	4.545163	0.653049	-0.300353
55	1	0	4.299269	1.123548	-1.979477
56	1	0	3.842711	2.233040	-0.691332
57	1	0	-0.646331	0.483201	2.109997
58	1	0	-0.852594	1.388837	3.741262
59	1	0	-3.155532	2.364958	2.825240
60	1	0	-2.850599	1.374685	1.393625
61	1	0	-3.047912	0.606170	2.964746
62	1	0	1.392808	2.216364	3.240266
63	1	0	-1.924450	3.349934	0.752973
64	1	0	2.796057	3.936354	2.154481
65	1	0	-0.532008	5.080069	-0.310826
66	1	0	1.836373	5.384216	0.370763

TS[14-16] (<sup>4</sup>A):

1	6	0	-1.219651	2.326342	-0.465400
2	7	0	-0.079507	1.569951	-0.437706
3	6	0	1.127474	2.171695	-0.656856
4	6	0	1.220586	3.543167	-0.885856
5	6	0	0.063683	4.319788	-0.901680
6	6	0	-1.165258	3.701726	-0.686657
7	26	0	-0.190010	-0.376529	0.085447
8	17	0	-0.363561	-2.383171	-0.945694
9	6	0	2.262709	1.274113	-0.610329
10	6	0	3.652953	1.833073	-0.646265
11	6	0	-2.437670	1.573037	-0.274152
12	6	0	-3.756957	2.278352	-0.213069
13	7	0	1.953892	0.007625	-0.441552
14	6	0	2.900996	-1.024086	-0.452166
15	6	0	3.946782	-1.090942	-1.386893
16	6	0	4.824715	-2.168198	-1.382948
17	6	0	4.683362	-3.192085	-0.449154
18	6	0	3.633039	-3.145515	0.465509
19	6	0	2.739723	-2.083131	0.455989
20	6	0	-0.154683	-0.456716	2.005994
21	7	0	-2.258794	0.278762	-0.120320
22	6	0	-3.324020	-0.632417	-0.038765
23	6	0	-3.284134	-1.632621	0.941415
24	6	0	-4.296558	-2.578738	1.018278
25	6	0	-5.350651	-2.561192	0.106555
26	6	0	-5.381173	-1.587135	-0.888217
27	6	0	-4.379282	-0.626460	-0.962420
28	1	0	-2.082725	4.281914	-0.705565
29	1	0	0.119289	5.387475	-1.085174
30	1	0	2.189913	3.998723	-1.062189

31	1	0	-0.644157	0.293071	2.642897
32	1	0	-0.045394	-1.394265	2.571730
33	1	0	-2.442663	-1.650307	1.629361
34	1	0	-4.254716	-3.344635	1.787466
35	1	0	-6.134309	-3.311060	0.161110
36	1	0	-6.185546	-1.577644	-1.618624
37	1	0	-4.384430	0.113647	-1.757862
38	1	0	1.886881	-2.064914	1.130100
39	1	0	3.493678	-3.953705	1.177620
40	1	0	5.372224	-4.031453	-0.449931
41	1	0	5.619796	-2.210671	-2.122211
42	1	0	4.037691	-0.315754	-2.141752
43	1	0	-4.518876	1.650187	0.250374
44	1	0	-3.673565	3.202839	0.365167
45	1	0	-4.123997	2.556159	-1.207889
46	1	0	4.369768	1.130358	-0.216871
47	1	0	3.989897	2.055812	-1.665021
48	1	0	3.703261	2.768017	-0.081227
49	6	0	1.889194	0.334138	2.873397
50	1	0	2.548417	-0.207694	2.202293
51	1	0	1.830376	0.046463	3.916406
52	7	0	1.813730	1.623552	2.654946
53	7	0	1.610525	2.723529	2.392791

**TS[15-12] (<sup>4</sup>A):**

1	6	0	-2.163262	2.656334	0.689533
2	6	0	-2.212804	2.129934	-0.608083
3	6	0	-2.889000	2.842835	-1.606973
4	6	0	-3.526109	4.040829	-1.302966
5	6	0	-3.505277	4.539027	-0.003230
6	6	0	-2.818849	3.841954	0.989839
7	7	0	-1.501518	0.946841	-0.874108
8	6	0	-2.009842	-0.054502	-1.542763
9	6	0	-3.414868	-0.132629	-2.051305
10	6	0	-1.096252	-1.169793	-1.762829
11	6	0	-1.438492	-2.346117	-2.421170
12	6	0	-0.478929	-3.351718	-2.572131
13	6	0	0.798886	-3.146877	-2.073164
14	6	0	1.109580	-1.941127	-1.432564
15	7	0	0.157191	-0.971203	-1.269617
16	6	0	2.415519	-1.581646	-0.946131
17	6	0	3.538525	-2.569326	-1.012737
18	26	0	0.638007	0.676908	-0.197482
19	17	0	1.199242	2.839777	-0.020208
20	6	0	0.323326	-0.101473	1.757558
21	7	0	2.496817	-0.367359	-0.424801
22	6	0	3.723095	0.203242	-0.043710
23	6	0	3.801578	0.889379	1.175293
24	6	0	4.984817	1.507055	1.556883
25	6	0	6.102384	1.469263	0.724948
26	6	0	6.023671	0.811409	-0.500109
27	6	0	4.846094	0.181054	-0.884309
28	6	0	-1.098888	-1.138444	3.316673
29	6	0	-0.104626	-1.915135	4.107590
30	6	0	-2.017995	-1.752694	2.399641
31	6	0	-3.156221	-1.037920	1.958944
32	6	0	-4.009645	-1.560707	1.001748
33	6	0	-3.755213	-2.813748	0.437438
34	6	0	-2.638525	-3.537104	0.858276
35	6	0	-1.785064	-3.021196	1.823033
36	1	0	1.566620	-3.904288	-2.197887
37	1	0	-0.729312	-4.276600	-3.081465

38	1	0	-2.442166	-2.482432	-2.809687
39	1	0	-0.711747	0.072164	1.465905
40	1	0	0.750030	0.560971	2.503782
41	1	0	2.917111	0.934543	1.803711
42	1	0	5.030078	2.032711	2.506368
43	1	0	7.023290	1.961791	1.022766
44	1	0	6.881226	0.794948	-1.167180
45	1	0	4.773857	-0.303606	-1.854128
46	1	0	-1.593683	2.128889	1.450913
47	1	0	-2.776954	4.234386	2.001656
48	1	0	-4.004430	5.474441	0.231271
49	1	0	-4.035638	4.589742	-2.089934
50	1	0	-2.878148	2.470668	-2.627424
51	1	0	4.348258	-2.293885	-0.335651
52	1	0	3.187378	-3.568772	-0.739517
53	1	0	3.968449	-2.648118	-2.018464
54	1	0	-4.064546	0.566598	-1.522779
55	1	0	-3.468985	0.109429	-3.119009
56	1	0	-3.815181	-1.140222	-1.922792
57	1	0	0.708799	-1.111363	1.687092
58	1	0	-1.447715	-0.211133	3.770052
59	1	0	-0.589904	-2.502801	4.901254
60	1	0	0.458588	-2.625413	3.492962
61	1	0	0.622191	-1.257252	4.590478
62	1	0	-3.354037	-0.055531	2.385438
63	1	0	-0.916582	-3.597996	2.132163
64	1	0	-4.881505	-0.990294	0.689377
65	1	0	-2.429734	-4.512033	0.424249
66	1	0	-4.424002	-3.224301	-0.315131

TS[15-20] (<sup>4</sup>A):

1	6	0	-2.877758	-1.834842	-1.302897
2	6	0	-3.013863	-0.581163	-0.683379
3	6	0	-4.119289	-0.367863	0.161495
4	6	0	-5.053646	-1.375861	0.373822
5	6	0	-4.914078	-2.611194	-0.254868
6	6	0	-3.821640	-2.830881	-1.093753
7	7	0	-1.981531	0.351650	-0.821437
8	6	0	-2.188922	1.649521	-0.918884
9	6	0	-3.516197	2.309870	-1.134284
10	6	0	-0.991197	2.456644	-0.837751
11	6	0	-0.988421	3.846398	-0.729958
12	6	0	0.220290	4.517346	-0.534336
13	6	0	1.399173	3.781515	-0.456305
14	6	0	1.357736	2.391969	-0.598732
15	7	0	0.171924	1.742609	-0.802734
16	6	0	2.499216	1.518935	-0.520289
17	6	0	3.879510	2.088041	-0.403570
18	26	0	0.143390	-0.246976	-1.145007
19	17	0	0.217422	-2.247207	0.282566
20	6	0	0.078871	-0.975947	-3.049496
21	7	0	2.206891	0.232889	-0.620983
22	6	0	3.165914	-0.772103	-0.449672
23	6	0	3.166849	-1.863497	-1.331163
24	6	0	4.046586	-2.920169	-1.138782
25	6	0	4.925679	-2.923764	-0.056377
26	6	0	4.915361	-1.854901	0.836391
27	6	0	4.048278	-0.785239	0.642657
28	6	0	-0.476559	-1.838303	2.301644
29	6	0	-1.815038	-2.490602	2.360474
30	6	0	-0.331491	-0.399119	2.428347
31	6	0	0.955199	0.157113	2.557483

32	6	0	1.130830	1.528783	2.645964
33	6	0	0.025757	2.380818	2.595944
34	6	0	-1.252245	1.845863	2.450527
35	6	0	-1.431075	0.470876	2.358293
36	1	0	2.347070	4.278672	-0.270687
37	1	0	0.237326	5.596727	-0.421851
38	1	0	-1.924763	4.395846	-0.760130
39	1	0	-0.818863	-0.611263	-3.564158
40	1	0	0.064221	-2.073338	-3.070362
41	1	0	2.461868	-1.861868	-2.158802
42	1	0	4.038037	-3.754169	-1.835111
43	1	0	5.605372	-3.757135	0.095176
44	1	0	5.584103	-1.853129	1.693258
45	1	0	4.023380	0.037215	1.353967
46	1	0	-2.014258	-2.008575	-1.938713
47	1	0	-3.696416	-3.792471	-1.583579
48	1	0	-5.645001	-3.396645	-0.087208
49	1	0	-5.891472	-1.194763	1.042037
50	1	0	-4.214147	0.580006	0.684935
51	1	0	4.634269	1.359801	-0.704952
52	1	0	3.988140	2.975161	-1.033923
53	1	0	4.119554	2.396236	0.622137
54	1	0	-4.257228	1.600015	-1.505137
55	1	0	-3.918712	2.749785	-0.212698
56	1	0	-3.426255	3.123559	-1.859319
57	1	0	0.955361	-0.632357	-3.612241
58	1	0	0.335444	-2.407074	2.751540
59	1	0	-2.235412	-2.384678	3.369774
60	1	0	-2.521885	-2.044001	1.656131
61	1	0	-1.744077	-3.555473	2.134371
62	1	0	1.815012	-0.511045	2.564580
63	1	0	-2.430308	0.061607	2.233945
64	1	0	2.132017	1.943209	2.742138
65	1	0	-2.114425	2.507314	2.395077
66	1	0	0.163755	3.457221	2.651170

TS[7-8]\_D/A ( $^{\circ}$ A):

1	6	0	-3.498363	1.914158	0.538964
2	6	0	-3.536218	1.124384	-0.619508
3	6	0	-4.614121	1.287150	-1.506125
4	6	0	-5.628689	2.194089	-1.224977
5	6	0	-5.595383	2.952099	-0.056612
6	6	0	-4.522171	2.808661	0.820917
7	7	0	-2.453370	0.287534	-0.911391
8	6	0	-2.611232	-0.923720	-1.392204
9	6	0	-3.899277	-1.682769	-1.460579
10	6	0	-1.384386	-1.557597	-1.841352
11	6	0	-1.325886	-2.783469	-2.502183
12	6	0	-0.099907	-3.249804	-2.970822
13	6	0	1.040093	-2.467913	-2.788561
14	6	0	0.940068	-1.254495	-2.108947
15	7	0	-0.256109	-0.828190	-1.611114
16	6	0	2.041545	-0.337907	-1.869736
17	6	0	3.381551	-0.610124	-2.475479
18	26	0	-0.318243	0.658639	-0.264924
19	7	0	-0.486621	2.613446	-0.567587
20	7	0	-0.536191	3.738183	-0.554898
21	6	0	-0.526270	-0.052379	1.633505
22	7	0	1.732914	0.691074	-1.115704
23	6	0	2.625046	1.734617	-0.824148
24	6	0	2.598653	2.256214	0.477696
25	6	0	3.424705	3.315951	0.825665

26	6	0	4.271259	3.892577	-0.120725
27	6	0	4.269963	3.407801	-1.426352
28	6	0	3.456101	2.336841	-1.781174
29	6	0	1.640160	-1.258847	2.599391
30	6	0	1.849745	-0.438954	3.841040
31	6	0	2.772916	-1.508305	1.709932
32	6	0	2.790401	-2.654630	0.891184
33	6	0	3.877914	-2.940980	0.077899
34	6	0	4.976702	-2.080516	0.046668
35	6	0	4.963291	-0.922831	0.823591
36	6	0	3.879412	-0.641089	1.645508
37	1	0	1.997203	-2.797440	-3.180133
38	1	0	-0.036033	-4.198807	-3.493212
39	1	0	-2.234354	-3.356160	-2.663345
40	6	0	-1.495252	-1.156721	1.728272
41	6	0	-0.619590	1.084476	2.532063
42	1	0	1.910652	1.831723	1.208910
43	1	0	3.391210	3.701421	1.841180
44	1	0	4.910274	4.727844	0.150833
45	1	0	4.900796	3.870680	-2.180455
46	1	0	3.433646	1.989565	-2.809630
47	1	0	-2.648869	1.810216	1.208453
48	1	0	-4.474776	3.404504	1.728082
49	1	0	-6.390430	3.659063	0.160631
50	1	0	-6.447488	2.314167	-1.929230
51	1	0	-4.625918	0.722913	-2.434624
52	1	0	4.175838	-0.105697	-1.923735
53	1	0	3.601215	-1.679465	-2.472309
54	1	0	3.425977	-0.270528	-3.517282
55	1	0	-4.672378	-1.201879	-0.859997
56	1	0	-4.278014	-1.775920	-2.485111
57	1	0	-3.751388	-2.695545	-1.071578
58	1	0	0.694368	-0.580147	1.888603
59	1	0	1.044689	-2.161052	2.773110
60	1	0	2.592060	-0.908076	4.499178
61	1	0	2.190112	0.576299	3.618897
62	1	0	0.919083	-0.340799	4.406112
63	1	0	1.944091	-3.339469	0.928708
64	1	0	3.889863	0.258968	2.253939
65	1	0	3.875579	-3.844630	-0.527651
66	1	0	5.805313	-0.235530	0.793208
67	1	0	5.829787	-2.304664	-0.588362
68	6	0	-2.785352	-1.028872	2.284564
69	6	0	-3.674882	-2.097029	2.296655
70	6	0	-3.315516	-3.334143	1.763134
71	6	0	-2.050749	-3.480259	1.196626
72	6	0	-1.165541	-2.409264	1.172476
73	1	0	-3.108872	-0.075760	2.693294
74	1	0	-4.662577	-1.959368	2.729914
75	1	0	-4.013497	-4.166414	1.781113
76	1	0	-1.752621	-4.430620	0.758779
77	1	0	-0.189865	-2.522335	0.699975
78	8	0	0.236883	1.957281	2.687201
79	1	0	-1.574201	1.167351	3.111400

**TS[9-20]\_D/A (<sup>3</sup>A):**

1	6	0	-1.447822	-2.563352	-0.814718
2	6	0	-1.596077	-1.317760	-1.452648
3	6	0	-2.744524	-1.128189	-2.243342
4	6	0	-3.710490	-2.121806	-2.359308
5	6	0	-3.556384	-3.339268	-1.695410
6	6	0	-2.413382	-3.557315	-0.927966

7	6	0	-0.577474	-0.284801	-1.243979
8	6	0	-0.830037	1.079335	-1.490280
9	8	0	0.002042	1.937911	-0.949479
10	26	0	-0.335437	0.695757	0.500832
11	7	0	1.475438	0.822304	1.282022
12	6	0	2.406420	1.787400	0.836424
13	6	0	3.642430	1.427073	0.292170
14	6	0	4.510925	2.411256	-0.166565
15	6	0	4.160287	3.756012	-0.080866
16	6	0	2.920299	4.114229	0.447944
17	6	0	2.040999	3.136442	0.891702
18	7	0	-2.365202	0.610643	0.939038
19	6	0	-2.731529	-0.534516	1.500234
20	6	0	-1.614860	-1.258335	2.047407
21	6	0	-1.646980	-2.376622	2.877550
22	6	0	-0.460946	-2.856179	3.436310
23	6	0	0.734631	-2.177442	3.208651
24	6	0	0.743171	-1.064791	2.368114
25	7	0	-0.411193	-0.682702	1.727975
26	6	0	1.834459	-0.188742	2.071770
27	6	0	3.185408	-0.387065	2.667910
28	6	0	-3.249506	1.521835	0.335131
29	6	0	-4.358112	1.157723	-0.445122
30	6	0	-5.114661	2.137381	-1.081114
31	6	0	-4.788549	3.484320	-0.948265
32	6	0	-3.682723	3.851358	-0.181524
33	6	0	-2.915627	2.881021	0.445927
34	6	0	-4.124441	-1.046471	1.643912
35	6	0	1.506130	-1.479428	-2.426639
36	6	0	2.837669	-1.482107	-1.852928
37	6	0	3.119415	-2.257136	-0.704287
38	6	0	4.396348	-2.316589	-0.164082
39	6	0	5.445835	-1.591728	-0.738100
40	6	0	5.185077	-0.805021	-1.860251
41	6	0	3.907406	-0.741669	-2.402662
42	6	0	1.269848	-0.828126	-3.757660
43	1	0	1.654844	-2.499950	3.686070
44	1	0	-0.478265	-3.726701	4.083526
45	1	0	-2.593642	-2.858273	3.101215
46	1	0	3.901041	0.376973	0.196067
47	1	0	5.462793	2.116228	-0.600576
48	1	0	4.841890	4.522409	-0.438758
49	1	0	2.632018	5.160143	0.501946
50	1	0	1.057400	3.395144	1.275586
51	1	0	-4.589680	0.109921	-0.600713
52	1	0	-5.961818	1.840496	-1.693589
53	1	0	-5.384067	4.242789	-1.447694
54	1	0	-3.410341	4.898027	-0.082149
55	1	0	-2.033637	3.148450	1.023239
56	1	0	3.817331	-1.025966	2.038886
57	1	0	3.105862	-0.861931	3.649451
58	1	0	3.709308	0.563931	2.784972
59	1	0	-4.852266	-0.232986	1.674071
60	1	0	-4.229590	-1.630485	2.561661
61	1	0	-4.395624	-1.706245	0.808410
62	1	0	0.588317	-0.749650	-1.574469
63	1	0	0.987109	-2.434782	-2.299982
64	1	0	1.859570	-1.280154	-4.567667
65	1	0	1.522296	0.239386	-3.733063
66	1	0	0.214712	-0.899256	-4.041195
67	1	0	2.311241	-2.833795	-0.253440
68	1	0	3.731044	-0.130172	-3.283744

69	1	0	4.582880	-2.944589	0.705226
70	1	0	5.990017	-0.237549	-2.322335
71	1	0	6.447335	-1.647118	-0.321266
72	1	0	-2.882455	-0.187069	-2.771064
73	1	0	-4.589276	-1.946743	-2.975672
74	1	0	-4.313161	-4.113471	-1.786943
75	1	0	-2.274564	-4.504140	-0.411560
76	1	0	-0.561046	-2.727057	-0.203629
77	1	0	-1.751651	1.473946	-1.950505

TS[10-11]\_D/A (<sup>1</sup>A):

1	6	0	-3.317835	-1.434365	1.260209
2	6	0	-2.916706	-1.145390	-0.045349
3	6	0	-3.857043	-0.723402	-0.986957
4	6	0	-5.189011	-0.575151	-0.618418
5	6	0	-5.594999	-0.866335	0.682190
6	6	0	-4.656428	-1.295874	1.615734
7	7	0	-1.556856	-1.331726	-0.446625
8	6	0	-1.283747	-2.527868	-0.950915
9	6	0	-2.290256	-3.618581	-1.109354
10	6	0	0.069114	-2.687862	-1.432139
11	6	0	0.631129	-3.798472	-2.057311
12	6	0	1.958916	-3.736744	-2.484654
13	6	0	2.702137	-2.578682	-2.275062
14	6	0	2.109612	-1.485246	-1.640903
15	7	0	0.801174	-1.555795	-1.230479
16	6	0	2.717600	-0.235864	-1.311518
17	6	0	4.188115	-0.045297	-1.500799
18	26	0	0.068123	-0.119451	-0.281387
19	6	0	0.634953	-0.682092	1.570517
20	7	0	1.872545	0.630557	-0.745706
21	6	0	2.293976	1.956632	-0.484005
22	6	0	3.061482	2.684488	-1.406485
23	6	0	3.377274	4.016035	-1.169925
24	6	0	2.935670	4.650065	-0.011600
25	6	0	2.149091	3.944990	0.895766
26	6	0	1.817802	2.619352	0.653660
27	6	0	-0.834403	1.469918	-0.666166
28	7	0	0.097823	-2.246160	1.814428
29	7	0	-0.267046	-3.211312	1.336797
30	1	0	3.736035	-2.516699	-2.600867
31	1	0	2.408646	-4.589603	-2.982388
32	1	0	0.042333	-4.695876	-2.215142
33	6	0	-0.200194	2.355341	-1.676494
34	6	0	-2.199976	1.896342	-0.349228
35	1	0	1.143030	2.086484	1.312582
36	1	0	1.764922	4.437413	1.784331
37	1	0	3.175413	5.694019	0.166267
38	1	0	3.953562	4.566365	-1.907954
39	1	0	3.357916	2.217692	-2.340434
40	1	0	-2.581374	-1.739786	1.995147
41	1	0	-4.960915	-1.519764	2.634442
42	1	0	-6.636756	-0.749388	0.967142
43	1	0	-5.910103	-0.221828	-1.350549
44	1	0	-3.525848	-0.490212	-1.995723
45	1	0	4.579673	0.717493	-0.825349
46	1	0	4.708799	-0.982849	-1.282950
47	1	0	4.460058	0.246757	-2.522019
48	1	0	-2.953196	-3.671497	-0.243257
49	1	0	-2.926580	-3.444326	-1.984348
50	1	0	-1.805152	-4.588031	-1.231686
51	6	0	-0.183503	0.054825	2.542544

52	6	0	2.102321	-0.793525	1.818166
53	6	0	-3.031886	2.507204	-1.316801
54	6	0	-4.318751	2.920559	-1.008061
55	6	0	-4.819176	2.755712	0.283232
56	6	0	-4.018628	2.162993	1.256810
57	6	0	-2.735093	1.737268	0.942359
58	1	0	-2.655709	2.650741	-2.324450
59	1	0	-4.935885	3.379027	-1.776782
60	1	0	-5.825982	3.085111	0.527558
61	1	0	-4.397773	2.020242	2.265480
62	1	0	-2.127919	1.267776	1.707821
63	8	0	-0.428148	3.549570	-1.817216
64	1	0	0.532277	1.857043	-2.352087
65	8	0	-1.143823	-0.388570	3.155994
66	1	0	0.124038	1.117837	2.660175
67	6	0	2.802340	0.198623	2.523608
68	6	0	4.182650	0.127309	2.675335
69	6	0	4.898580	-0.949995	2.159615
70	6	0	4.213062	-1.960193	1.489918
71	6	0	2.837026	-1.878930	1.314016
72	1	0	2.270904	1.041492	2.952747
73	1	0	4.697096	0.915611	3.217561
74	1	0	5.975251	-1.007248	2.289592
75	1	0	4.750146	-2.817460	1.091209
76	1	0	2.322889	-2.674483	0.781669

TS[13-14]\_D/A (<sup>4</sup>A):

1	6	0	2.509969	0.227216	2.340326
2	6	0	1.292404	0.812445	1.931181
3	6	0	1.301161	2.186045	1.633425
4	6	0	2.464154	2.941160	1.737699
5	6	0	3.661813	2.346614	2.124346
6	6	0	3.671095	0.985185	2.422137
7	6	0	0.085843	-0.028425	1.764782
8	7	0	-1.288084	0.861508	2.321695
9	7	0	-1.671067	1.908057	2.050736
10	26	0	-0.340643	-0.467995	-0.269945
11	7	0	-0.195955	1.410387	-1.009701
12	6	0	1.028963	1.887114	-1.363078
13	6	0	1.196736	3.217232	-1.755611
14	6	0	0.096837	4.065846	-1.784929
15	6	0	-1.158248	3.566225	-1.432313
16	6	0	-1.277622	2.230545	-1.058218
17	6	0	2.087474	0.899843	-1.311974
18	6	0	3.503972	1.326113	-1.526145
19	6	0	-2.535238	1.574397	-0.723941
20	6	0	-3.784790	2.389228	-0.631525
21	7	0	1.687921	-0.316189	-1.011868
22	6	0	2.560127	-1.420402	-1.070023
23	6	0	3.384928	-1.645626	-2.181473
24	6	0	4.190067	-2.777033	-2.235244
25	6	0	4.188227	-3.690233	-1.183180
26	6	0	3.358604	-3.474203	-0.084694
27	6	0	2.536770	-2.356080	-0.030162
28	7	0	-2.439601	0.293208	-0.485909
29	6	0	-3.574204	-0.506355	-0.253358
30	6	0	-3.575096	-1.374174	0.843274
31	6	0	-4.663815	-2.202184	1.078456
32	6	0	-5.751756	-2.198267	0.207439
33	6	0	-5.743178	-1.356941	-0.902328
34	6	0	-4.664712	-0.510601	-1.132756
35	17	0	-0.803017	-2.622652	-0.641577

36	1	0	-2.035591	4.203874	-1.462531
37	1	0	0.208843	5.101132	-2.089604
38	1	0	2.181608	3.576661	-2.036837
39	6	0	-0.094470	-1.280254	2.512908
40	1	0	-2.710301	-1.388759	1.501323
41	1	0	-4.653916	-2.865845	1.937811
42	1	0	-6.595218	-2.858659	0.384814
43	1	0	-6.577451	-1.361918	-1.597995
44	1	0	-4.641839	0.128258	-2.011644
45	1	0	1.875035	-2.203450	0.817805
46	1	0	3.335107	-4.187897	0.733462
47	1	0	4.817871	-4.574071	-1.227871
48	1	0	4.814563	-2.948525	-3.107547
49	1	0	3.360875	-0.947485	-3.013940
50	1	0	-4.572395	1.848127	-0.106734
51	1	0	-3.582764	3.319296	-0.093078
52	1	0	-4.169989	2.662584	-1.620109
53	1	0	4.201354	0.568421	-1.167276
54	1	0	3.730442	1.516687	-2.581467
55	1	0	3.695057	2.253716	-0.976916
56	1	0	0.381998	2.675501	1.322678
57	1	0	2.427655	4.003182	1.505589
58	1	0	4.572098	2.934996	2.197842
59	1	0	4.593416	0.501651	2.733234
60	1	0	2.533331	-0.828574	2.581490
61	8	0	0.754750	-2.130747	2.723830
62	1	0	-1.148360	-1.435336	2.847434

TS[14-15]\_D/A ( $^{\circ}$ A):

1	6	0	-2.482038	1.048418	-2.170226
2	6	0	-1.310539	1.108237	-1.383722
3	6	0	-1.220987	2.165391	-0.456013
4	6	0	-2.239407	3.099924	-0.311269
5	6	0	-3.400872	2.999619	-1.071963
6	6	0	-3.512028	1.964099	-2.000167
7	6	0	-0.222311	0.120048	-1.474601
8	26	0	-0.051381	-1.107137	0.184520
9	17	0	-0.194396	-3.295713	-0.326174
10	7	0	2.093254	-1.097161	0.805141
11	6	0	2.420454	-0.120925	1.617084
12	6	0	3.818046	0.263038	1.994119
13	7	0	-2.104288	-0.856058	0.925138
14	6	0	-3.184868	-1.643586	0.492685
15	6	0	-3.254471	-2.029123	-0.850999
16	6	0	-4.289741	-2.838561	-1.297202
17	6	0	-5.257499	-3.299974	-0.406896
18	6	0	-5.176540	-2.948255	0.938271
19	6	0	-4.151289	-2.124738	1.387908
20	7	0	0.082162	0.209855	1.707716
21	6	0	-1.053185	0.770441	2.213719
22	6	0	-0.986541	1.827779	3.122598
23	6	0	0.254269	2.308143	3.527544
24	6	0	1.411328	1.699757	3.038018
25	6	0	1.300020	0.640496	2.140760
26	6	0	-2.277779	0.170786	1.729156
27	6	0	-3.595819	0.771668	2.102891
28	6	0	3.024542	-2.045637	0.344845
29	6	0	2.960366	-2.458588	-0.991995
30	6	0	3.838510	-3.424624	-1.463022
31	6	0	4.763858	-4.019186	-0.606543
32	6	0	4.803491	-3.641343	0.733236
33	6	0	3.943693	-2.658512	1.209346

34	6	0	1.872661	1.616986	-2.088027
35	6	0	3.151740	0.854533	-1.896901
36	6	0	1.709807	2.927106	-1.462461
37	6	0	2.289037	3.233920	-0.217187
38	6	0	2.057309	4.457235	0.396803
39	6	0	1.251670	5.413905	-0.222196
40	6	0	0.678150	5.132236	-1.461706
41	6	0	0.897477	3.903337	-2.068061
42	1	0	2.389867	2.037079	3.365536
43	1	0	0.322829	3.131575	4.230725
44	1	0	-1.901636	2.264236	3.510826
45	6	0	-0.129286	-0.749620	-2.645659
46	1	0	2.220538	-2.015696	-1.653675
47	1	0	3.783204	-3.727094	-2.504472
48	1	0	5.436952	-4.787104	-0.976464
49	1	0	5.500422	-4.118909	1.416228
50	1	0	3.948405	-2.391351	2.262390
51	1	0	-2.479229	-1.688549	-1.530010
52	1	0	-4.330528	-3.124017	-2.344402
53	1	0	-6.059195	-3.943961	-0.756014
54	1	0	-5.910608	-3.323278	1.646005
55	1	0	-4.069238	-1.875919	2.442378
56	1	0	4.545899	-0.165203	1.302961
57	1	0	3.930926	1.351737	1.989696
58	1	0	4.083365	-0.076426	3.001530
59	1	0	-4.385032	0.434876	1.429461
60	1	0	-3.898925	0.517253	3.125017
61	1	0	-3.538863	1.862583	2.039793
62	1	0	0.920514	0.819141	-1.533946
63	1	0	1.514772	1.589869	-3.120557
64	1	0	3.995505	1.422289	-2.309368
65	1	0	3.377973	0.662361	-0.843677
66	1	0	3.099147	-0.105626	-2.410358
67	1	0	0.427819	3.673891	-3.022592
68	1	0	2.913530	2.491096	0.274812
69	1	0	0.047399	5.869878	-1.950112
70	1	0	2.507802	4.669494	1.363681
71	1	0	1.074888	6.372207	0.257900
72	1	0	-0.320719	2.260062	0.143678
73	1	0	-2.117590	3.908198	0.407558
74	1	0	-4.205824	3.719145	-0.951540
75	1	0	-4.407428	1.874422	-2.609775
76	1	0	-2.598561	0.263571	-2.911869
77	8	0	0.902317	-1.077732	-3.219919
78	1	0	-1.101541	-1.180306	-2.993499

TS[14-16]\_D/A (<sup>4</sup>A):

1	6	0	2.344697	0.213625	1.303434
2	6	0	2.016006	0.769296	0.050013
3	6	0	3.085723	1.244311	-0.740169
4	6	0	4.405126	1.112566	-0.326489
5	6	0	4.703002	0.547957	0.912115
6	6	0	3.661081	0.112767	1.732179
7	6	0	0.617587	0.888512	-0.376261
8	26	0	-0.535531	-0.887494	-0.303414
9	17	0	-0.962280	-1.557259	-2.424011
10	7	0	1.058249	-2.353308	0.034013
11	6	0	1.248651	-2.704949	1.290543
12	6	0	0.230912	-2.243679	2.205828
13	7	0	-0.733265	-1.473842	1.622921
14	6	0	-1.834740	-1.120672	2.335580
15	6	0	-1.936631	-1.402810	3.693537

16	6	0	-0.913630	-2.116944	4.321017
17	6	0	0.165525	-2.560037	3.566109
18	6	0	-2.899153	-0.521552	1.542397
19	6	0	-4.099442	0.035515	2.236768
20	6	0	1.863064	-2.873478	-0.995556
21	6	0	2.133617	-4.246468	-1.091859
22	6	0	2.880955	-4.743442	-2.152749
23	6	0	3.375230	-3.881987	-3.129067
24	6	0	3.095407	-2.519451	-3.046847
25	6	0	2.334038	-2.019773	-1.999557
26	6	0	2.428641	-3.463647	1.812626
27	7	0	-2.679873	-0.495546	0.254047
28	6	0	-3.696928	-0.207874	-0.675377
29	6	0	-4.963155	-0.799387	-0.560563
30	6	0	-5.936308	-0.567799	-1.525407
31	6	0	-5.661961	0.257538	-2.612746
32	6	0	-4.398488	0.832639	-2.738287
33	6	0	-3.414279	0.591553	-1.789806
34	6	0	-0.050868	2.608135	0.639715
35	6	0	0.911707	3.670094	0.270199
36	6	0	0.590898	4.594677	-0.734495
37	6	0	1.497999	5.577155	-1.105733
38	6	0	2.743144	5.661037	-0.484370
39	6	0	3.070551	4.748421	0.512203
40	6	0	2.166441	3.760304	0.889110
41	7	0	-1.360174	2.819037	0.271669
42	7	0	-2.438096	2.416291	0.344206
43	1	0	0.942095	-3.169218	4.018092
44	1	0	-0.978445	-2.353683	5.377935
45	1	0	-2.814144	-1.087925	4.248508
46	6	0	0.364842	1.336746	-1.742551
47	1	0	2.093255	-0.963693	-1.942132
48	1	0	3.458634	-1.840280	-3.812838
49	1	0	3.959344	-4.271981	-3.957362
50	1	0	3.069707	-5.811289	-2.219958
51	1	0	1.719135	-4.922578	-0.349206
52	1	0	-2.425269	1.024828	-1.903198
53	1	0	-4.166991	1.463060	-3.591601
54	1	0	-6.422391	0.437602	-3.367065
55	1	0	-6.908923	-1.042297	-1.429294
56	1	0	-5.163612	-1.470667	0.270186
57	1	0	3.262631	-3.421047	1.110258
58	1	0	2.759199	-3.037528	2.764729
59	1	0	2.205150	-4.520835	1.995949
60	1	0	-4.704055	0.635735	1.557006
61	1	0	-4.739661	-0.746076	2.660267
62	1	0	-3.767325	0.671187	3.063501
63	6	0	-0.084513	2.068865	2.033822
64	1	0	-0.371317	4.520797	-1.231481
65	1	0	1.229520	6.281543	-1.887761
66	1	0	3.451078	6.430871	-0.777248
67	1	0	4.040223	4.792699	1.000175
68	1	0	2.465186	3.042082	1.647382
69	1	0	2.871267	1.729697	-1.690220
70	1	0	5.205257	1.477426	-0.964869
71	1	0	5.734224	0.458221	1.241049
72	1	0	3.877712	-0.314125	2.708688
73	1	0	1.535880	-0.133753	1.941888
74	8	0	-0.452045	2.162992	-2.134852
75	1	0	0.958476	0.759597	-2.494634
76	8	0	-1.074130	1.673147	2.610874
77	1	0	0.919732	2.025756	2.498212

TS[15-12]\_D/A ( $^{\circ}$ A):

1	6	0	-2.253195	1.802551	-1.717255
2	6	0	-1.039332	1.668960	-1.003995
3	6	0	-0.776677	2.602904	0.019147
4	6	0	-1.678854	3.613696	0.329352
5	6	0	-2.873630	3.724291	-0.376963
6	6	0	-3.150109	2.812115	-1.399658
7	6	0	-0.067663	0.639880	-1.280575
8	26	0	-0.175928	-1.546460	0.438492
9	17	0	-0.411479	-3.529509	-0.524516
10	7	0	1.979371	-1.378595	0.781605
11	6	0	2.353176	-0.374132	1.554024
12	6	0	3.768996	0.033590	1.818518
13	7	0	-2.215311	-0.880320	0.855642
14	6	0	-3.339366	-1.511507	0.284080
15	6	0	-3.352524	-1.743765	-1.095356
16	6	0	-4.431012	-2.402391	-1.672363
17	6	0	-5.486033	-2.860860	-0.885850
18	6	0	-5.460621	-2.654005	0.491524
19	6	0	-4.396324	-1.978436	1.077090
20	7	0	0.026367	-0.048231	1.783053
21	6	0	-1.073141	0.598899	2.251855
22	6	0	-0.961704	1.647937	3.160243
23	6	0	0.305666	2.083453	3.549219
24	6	0	1.430056	1.465075	3.013202
25	6	0	1.270087	0.387243	2.135792
26	6	0	-2.330931	0.122961	1.688441
27	6	0	-3.593304	0.854772	2.006242
28	6	0	2.913395	-2.323328	0.311259
29	6	0	2.855696	-2.745972	-1.022485
30	6	0	3.740146	-3.707228	-1.493323
31	6	0	4.677521	-4.283559	-0.638823
32	6	0	4.719668	-3.892568	0.697472
33	6	0	3.848764	-2.919061	1.171158
34	6	0	1.757834	1.733457	-2.584573
35	6	0	2.760596	0.632109	-2.596722
36	6	0	1.906996	2.881116	-1.755802
37	6	0	2.819282	2.905454	-0.671794
38	6	0	2.924863	4.019672	0.145367
39	6	0	2.134284	5.148302	-0.089640
40	6	0	1.226300	5.143573	-1.149046
41	6	0	1.103616	4.027096	-1.961187
42	1	0	2.425587	1.799866	3.286619
43	1	0	0.412849	2.905268	4.249555
44	1	0	-1.855253	2.136415	3.535465
45	6	0	-0.167743	-0.379023	-2.288207
46	1	0	2.101193	-2.320695	-1.677977
47	1	0	3.683284	-4.019075	-2.531966
48	1	0	5.358810	-5.044601	-1.007308
49	1	0	5.428624	-4.353292	1.379646
50	1	0	3.859757	-2.637814	2.220670
51	1	0	-2.523652	-1.399522	-1.707329
52	1	0	-4.435594	-2.569400	-2.745374
53	1	0	-6.318185	-3.389412	-1.341787
54	1	0	-6.268876	-3.024631	1.115807
55	1	0	-4.358657	-1.834167	2.153986
56	1	0	4.449011	-0.397128	1.081447
57	1	0	3.860033	1.123541	1.779961
58	1	0	4.119729	-0.279424	2.808624
59	1	0	-4.404351	0.556369	1.342096
60	1	0	-3.920711	0.684562	3.038259

61	1	0	-3.429145	1.931540	1.886366
62	1	0	0.793766	0.583047	-0.618637
63	1	0	1.092750	1.826949	-3.440798
64	1	0	3.764576	1.014218	-2.829688
65	1	0	2.844202	0.126561	-1.623682
66	1	0	2.515633	-0.132645	-3.335927
67	1	0	0.374402	4.015102	-2.768929
68	1	0	3.446733	2.035871	-0.487525
69	1	0	0.597827	6.011189	-1.330419
70	1	0	3.635156	4.019064	0.969293
71	1	0	2.226642	6.022205	0.548773
72	1	0	0.163444	2.529944	0.565941
73	1	0	-1.436875	4.320785	1.120475
74	1	0	-3.581529	4.514374	-0.140500
75	1	0	-4.078951	2.893103	-1.958462
76	1	0	-2.463044	1.102064	-2.517706
77	8	0	-1.027594	-0.488840	-3.165491
78	1	0	0.669185	-1.119479	-2.243348

TS[15-20]\_D/A (<sup>4</sup>A):

1	6	0	0.281033	1.630084	2.863632
2	6	0	-0.922246	1.968918	2.225904
3	6	0	-2.045061	1.146128	2.432557
4	6	0	-1.972386	0.042358	3.267976
5	6	0	-0.772627	-0.273916	3.907846
6	6	0	0.351197	0.522500	3.700283
7	6	0	-1.023543	3.098808	1.314808
8	6	0	0.071595	4.103631	1.205756
9	17	0	-1.130204	2.191266	-0.643989
10	26	0	-0.231406	-0.054360	-0.605416
11	7	0	-2.272715	-0.865011	-0.243539
12	6	0	-3.424656	-0.282628	-0.794659
13	6	0	-3.362490	0.206140	-2.106917
14	6	0	-4.459899	0.855152	-2.657271
15	6	0	-5.619021	1.054882	-1.908110
16	6	0	-5.673955	0.598427	-0.593399
17	6	0	-4.588462	-0.071142	-0.038430
18	7	0	1.739473	0.348742	0.346797
19	6	0	2.215838	-0.714524	0.957599
20	6	0	1.225286	-1.725573	1.281041
21	6	0	1.477460	-2.839308	2.080450
22	6	0	0.433332	-3.707780	2.394519
23	6	0	-0.839863	-3.450774	1.888175
24	6	0	-1.043000	-2.336959	1.073446
25	7	0	-0.019070	-1.486399	0.781427
26	6	0	-2.310425	-1.962678	0.480243
27	6	0	-3.510826	-2.836005	0.677822
28	6	0	2.499448	1.498034	0.116448
29	6	0	2.330084	2.185738	-1.095821
30	6	0	2.978531	3.391873	-1.323122
31	6	0	3.795777	3.951180	-0.341118
32	6	0	3.960475	3.285809	0.872058
33	6	0	3.325821	2.069521	1.100792
34	6	0	3.651398	-0.962676	1.295593
35	6	0	0.389900	-0.895554	-2.480139
36	1	0	-1.669887	-4.107906	2.130134
37	1	0	0.607597	-4.569758	3.030383
38	1	0	2.477399	-3.015333	2.465653
39	6	0	1.645929	-1.616762	-2.214976
40	6	0	0.309300	0.152104	-3.477257
41	1	0	-2.447538	0.090926	-2.688855
42	1	0	-4.396422	1.223086	-3.677334

43	1	0	-6.468536	1.575744	-2.340477
44	1	0	-6.564048	0.766262	0.007300
45	1	0	-4.621082	-0.405761	0.996205
46	1	0	1.669000	1.761628	-1.848153
47	1	0	2.832715	3.903869	-2.269927
48	1	0	4.292979	4.900405	-0.516559
49	1	0	4.582387	3.718350	1.651227
50	1	0	3.430246	1.570829	2.061391
51	1	0	-4.279572	-2.627000	-0.067275
52	1	0	-3.235498	-3.891611	0.603021
53	1	0	-3.967066	-2.696344	1.665632
54	1	0	4.308806	-0.276604	0.760164
55	1	0	3.851432	-0.852676	2.369093
56	1	0	3.927219	-1.983188	1.011486
57	1	0	-0.491824	-1.549778	-2.507902
58	1	0	-2.029479	3.507020	1.230102
59	1	0	0.140645	4.674305	2.141543
60	1	0	1.044014	3.637762	1.026302
61	1	0	-0.119769	4.807985	0.395023
62	1	0	-2.968649	1.377375	1.903721
63	1	0	1.164225	2.242492	2.702269
64	1	0	-2.848853	-0.584926	3.415449
65	1	0	1.292545	0.271827	4.184915
66	1	0	-0.711200	-1.147067	4.551899
67	8	0	-0.718861	0.574209	-4.003217
68	1	0	1.289704	0.614570	-3.760088
69	6	0	2.924796	-1.055443	-2.410108
70	6	0	4.080169	-1.775557	-2.132420
71	6	0	4.010469	-3.076080	-1.632202
72	6	0	2.756234	-3.641849	-1.411115
73	6	0	1.600022	-2.925632	-1.698991
74	1	0	3.017227	-0.036536	-2.777925
75	1	0	5.048723	-1.311371	-2.304301
76	1	0	4.916902	-3.635734	-1.418497
77	1	0	2.673708	-4.650797	-1.012739
78	1	0	0.625229	-3.377869	-1.516635