Supporting information

Understanding the Reaction Mechanism of the Oxidative Addition of Ammonia by [(PXP)Ir(I)] Complexes: The role of the X group

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Table of Contents

Table S1. B3LYP-D3BJ/def2TZVP absolute energetic values for B3LYP-D3BJ/def2SVP optimized structures (metallic fragment, reactant, transition structure and product). Energies in a.u. The lowest vibrational frequency (cm^{-1}) is also presented. We made sure that for transition states there is only one imaginary frequency.

		E(TZ)	Lowest frequency
1	F	-1129.22604	27.9
(X = B)	R	-1185.83672	28.6
	TS	-1185.79304	-863.8
	P	-1185.85251	43.1
2	F	-1143.05127	33.9
(X = CH)	R	-1199.67333	22.3
	TS	-1199.63844	-1090.4
	P	-1199.68100	44.64
3	F	-1159.07716	35.9
(X = N)	R	-1215.71025	29.3
	TS	-1215.68131	-985.9
	P	-1215.71205	45.0
4	F	-1179.33806	34.6
(X = O)	R	-1236.01354	23.7
	TS	-1235.96585	-920.7
	P	-1236.00523	41.6
5	F	-1394.50659	31.6
(X = SiH)	R	-1451.12367	21.9
	TS	-1451.08305	-893.9
	P	-1451.13442	39.6
NH$_3$		-56.58656	1062.6

Table 2. Integrated ELF basins electron populations for the stationary points (R, TS and P) for complexes **1**-**5**.

| comple	structur	V(Ir)	V(Ir,X)	V(Ir,N_{NH3})	V(N,H_1)	V(Ir,H_1)	V(Ir,P_1)	V(Ir,P_2)
1	R	14.9	2.47	1.90	1.97	-----	2.43	2.44
(X = B)	TS	13.9	2.70	3.23	-----	1.52	2.35	2.34
	P	14.0	2.01	3.65	-----	1.78	2.31	2.31
2	R	15.6	1.64	1.88	1.98	-----	2.49	2.50
(X = CH)	TS	14.7	1.67	3.27	-----	1.52	2.40	2.43
	P	14.3	1.47	3.64	-----	1.77	2.39	2.39
3	R	15.8	1.80	1.82	2.00	-----	2.40	2.41
(X = N)	TS	14.9	1.77	3.27	-----	1.50	2.36	2.36
	P	14.4	1.57	3.65	-----	1.77	2.33	2.33
4	R	15.7	2.27	1.77	2.00	-----	2.36	2.37
(X = O)	TS	15.0	2.23	3.11	-----	1.43	2.29	2.34
	P	14.4	2.19	3.40	-----	1.78	2.28	2.28
5	R	15.0	2.31	1.86	1.98	-----	2.47	2.47
(X = CH)	TS	14.0	2.63	3.23	-----	1.50	2.34	2.34
	P	14.2	1.83	3.67	-----	1.77	2.36	2.36

Figure S1. Integrated electron density for some ELF basins along the calculated IRC path for the oxidative addition of NH_3 to [(PBP)Ir] fragment (complex **1**, X = B). Bifurcation points separating the SSDs indicated by vertical lines. Basin populations in electrons. Right axis for V(Ir) basin and left axis for the other basins (disynaptic).
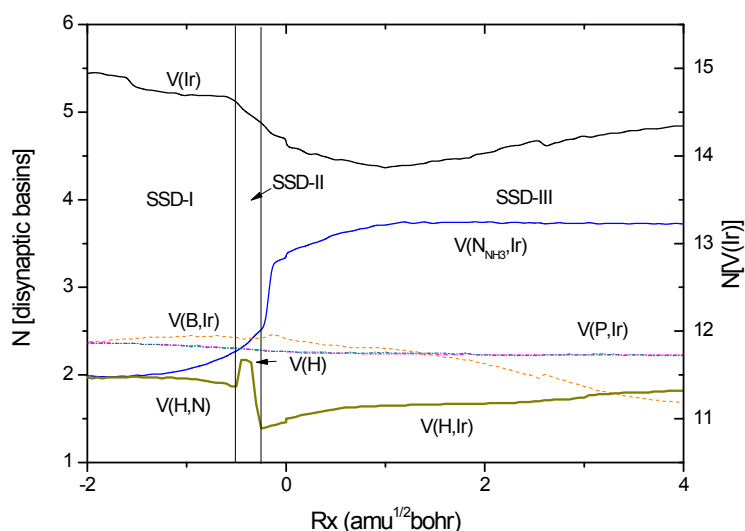
Table S3. Reaction coordinates (IRC, $amu^{1/2}bohr$), energy relative to the reactant (B3LYP-D3BJ/def2-SVP, in kcal/mol), some geometrical parameters (in Å) and selected ELF basin populations for the initial and final points of SSDs defined on the reaction path for NH3 oxidative addition at complex **1** (X = B).

| B	SDD I		SDD II		SDD III	
Rx	-4.95	-0.3	-0.25	-0.1	-0.05	4.95
E(DZ)	0.2	17.6	19.5	25.3	26.8	-1
dN-H	1.022	1.33	1.444	1.548	1.601	3.518
dIr-H	2.878	1.694	1.659	1.63	1.618	1.645
dIr-N	2.389	2.186	2.186	2.185	2.184	2
dXIr	2.021	2.055	2.056	2.058	2.059	2.091
V(N1,Ir)	1.97	2.27	2.31	2.47	2.51	3.73
V(P1,Ir)	2.38	2.31	2.3	2.29	2.28	2.22
V(P2,Ir)	2.36	2.3	2.3	2.28	2.28	2.22
V(C1,Ir)	2.38	2.43	2.41	2.42	2.42	1.61
V(H,N)	1.96	1.87				
V(H)			2.17	1.67		
V(H,Ir)					1.39	1.85
V(Ir)	14.93	14.62	14.55	14.42	14.38	14.38

Figure S2. Integrated electron density for some ELF basins along the calculated IRC path for the oxidative addition of NH_3 to [(PNP)Ir] fragment (complex **3**, X = N). Bifurcation points separating the SSDs indicated by vertical lines. Basin populations in electrons. Right axis for V(Ir) basin and left axis for the other basins (disynaptic).
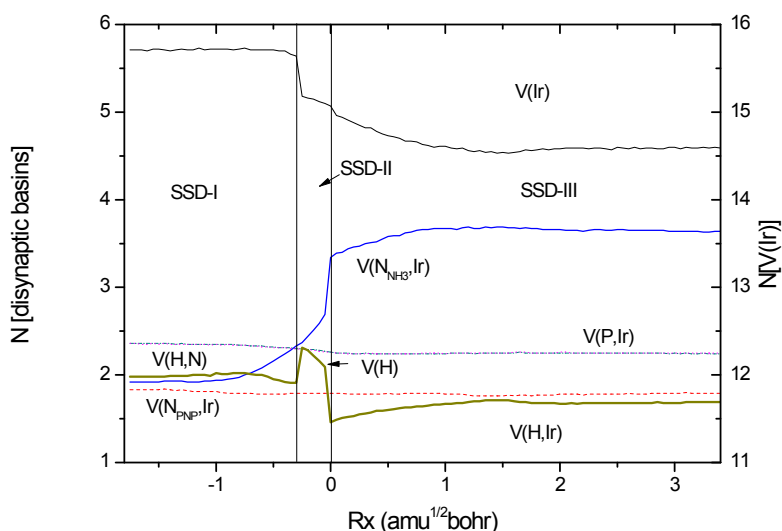
Table S4. Reaction coordinates (IRC, $amu^{1/2}bohr$), energy relative to the reactant (B3LYP-D3BJ/def2-SVP, in kcal/mol), some geometrical parameters (in Å) and selected ELF basin populations for the initial and final points of SSDs defined on the reaction path for NH3 oxidative addition at complex **3** (X = N).

| N	SDD I		SDD II		SDD III	
Rx	-1.75	-0.25	-0.2	-0.15	-0.1	3.4
E(DZ)	0	16.1	17	18.7	19.3	6.7
dN-H	1.02	1.219	1.265	1.313	1.363	2.354
dIr-H	2.731	1.732	1.707	1.686	1.666	1.568
dIr-N	2.186	2.175	2.175	2.174	2.174	2.09
dXIr	2.071	2.049	2.049	2.049	2.049	2.046
V(N1,Ir)	1.83	1.79	1.79	1.79	1.79	1.79
V(P1,Ir)	2.36	2.3	2.3	2.29	2.28	2.24
V(P2,Ir)	2.36	2.3	2.29	2.28	2.27	2.25
V(C1,Ir)	1.92	2.33	2.37	2.51	2.59	3.64
V(H,N)	1.98	1.91				
V(H)			2.31	2.22		
V(H,Ir)					2.16	1.69
V(Ir)	15.71	15.64	15.18	15.15	15.12	14.59

Figure S3. Integrated electron density for some ELF basins along the calculated IRC path for the oxidative addition of NH_3 to [(POP)Ir] fragment (complex **4**, X = O). Bifurcation points separating the SSDs indicated by vertical lines. Basin populations in electrons. Right axis for V(Ir) basin and left axis for the other basins (disynaptic).
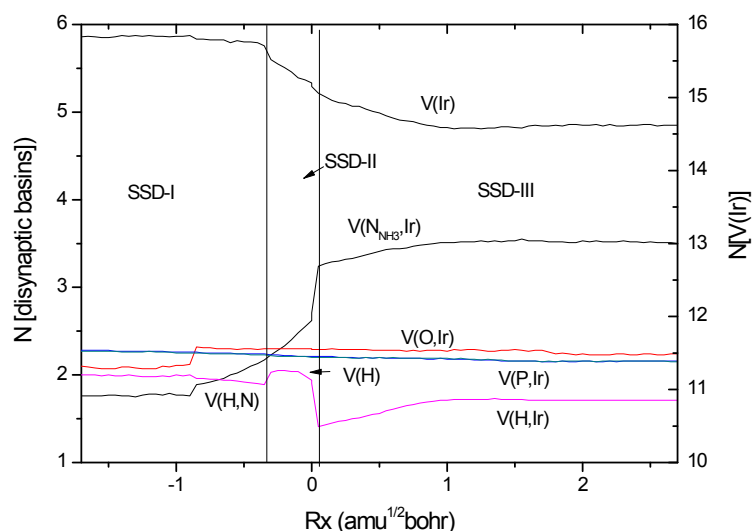
Table S5. Reaction coordinates (IRC, $amu^{1/2}bohr$), energy relative to the reactant (B3LYP-D3BJ/def2-SVP, in kcal/mol), some geometrical parameters (in Å) and selected ELF basin populations for the initial and final points of SSDs defined on the reaction path for NH3 oxidative addition at complex **4** (X = O).

| O	SDD I		SDD II		SDD III	
Rx	-1.7	-0.4	-0.3	-0.2	-0.1	2.7
E(DZ)	0.0	24.6	26.3	30.4	31.1	8.0
dN-H	1.026	1.176	1.218	1.359	1.408	3.028
dIr-H	2.635	1.754	1.726	1.661	1.643	1.572
dIr-N	2.089	2.039	2.038	2.037	2.037	1.922
dXIr	2.164	2.169	2.170	2.171	2.172	2.247
V(N1,Ir)	1.76	2.17	2.23	2.40	2.48	3.51
V(P1,Ir)	2.28	2.24	2.23	2.22	2.21	2.16
V(P2,Ir)	2.27	2.23	2.22	2.21	2.21	2.15
V(O,Ir)	2.10	2.30	2.30	2.30	2.30	2.24
V(H,N)	2.00	1.89				
V(H)			2.03	2.04		
V(H,Ir)					2.04	1.71
V(Ir)	15.83	15.71	15.52	15.35	15.27	14.62

Figure S4. Integrated electron density for some ELF basins along the calculated IRC path for the oxidative addition of NH_3 to [(PSiHP)Ir] fragment (complex **5**, X = SiH). Bifurcation points separating the SSDs indicated by vertical lines. Basin populations in electrons. Right axis for V(Ir) basin and left axis for the other basins (disynaptic).
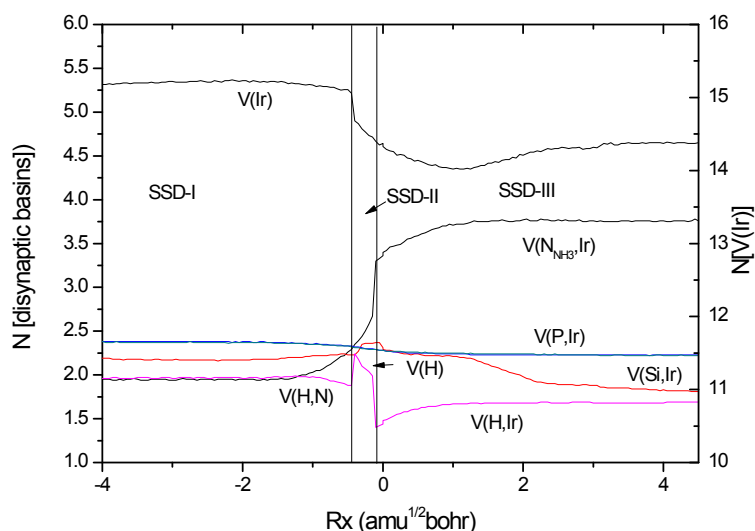
Table S6. Reaction coordinates (IRC, $amu^{1/2}$bohr), energy relative to the reactant (B3LYP-D3BJ/def2-SVP, in kcal/mol), some geometrical parameters (in Å) and selected ELF basin populations for the initial and final points of SSDs defined on the reaction path for NH3 oxidative addition at complex **5** (X = SiH).

SIH	SDD I		SDD II		SDD III	
Rx	-4.0	-0.5	-0.4	-0.3	-0.3	5.0
E(DZ)	0.2	17.5	19.1	22.5	24.0	0.5
dN-H	1.022	1.148	1.191	1.288	1.339	3.391
dIr-H	2.821	1.780	1.752	1.705	1.686	1.598
dIr-N	2.313	2.176	2.175	2.173	2.173	2.008
dXIr	2.321	2.360	2.361	2.362	2.363	2.368
V(N1,Ir)	1.95	2.29	2.35	2.44	2.50	3.76
V(P1,Ir)	2.38	2.33	2.32	2.31	2.30	2.23
V(P2,Ir)	2.38	2.32	2.31	2.30	2.30	2.22
V(Si,Ir)	2.19	2.23	2.23	2.35	2.36	1.81
V(H,N)	1.96	1.88				
V(H)			2.24	2.10		
V(H,Ir)					2.07	1.70
V(Ir)	15.18	15.06	14.68	14.57	14.53	14.39

Figure S5. Geometrical representation of R (up), TS (middle) and P (down) for complex 1 (X = CH).
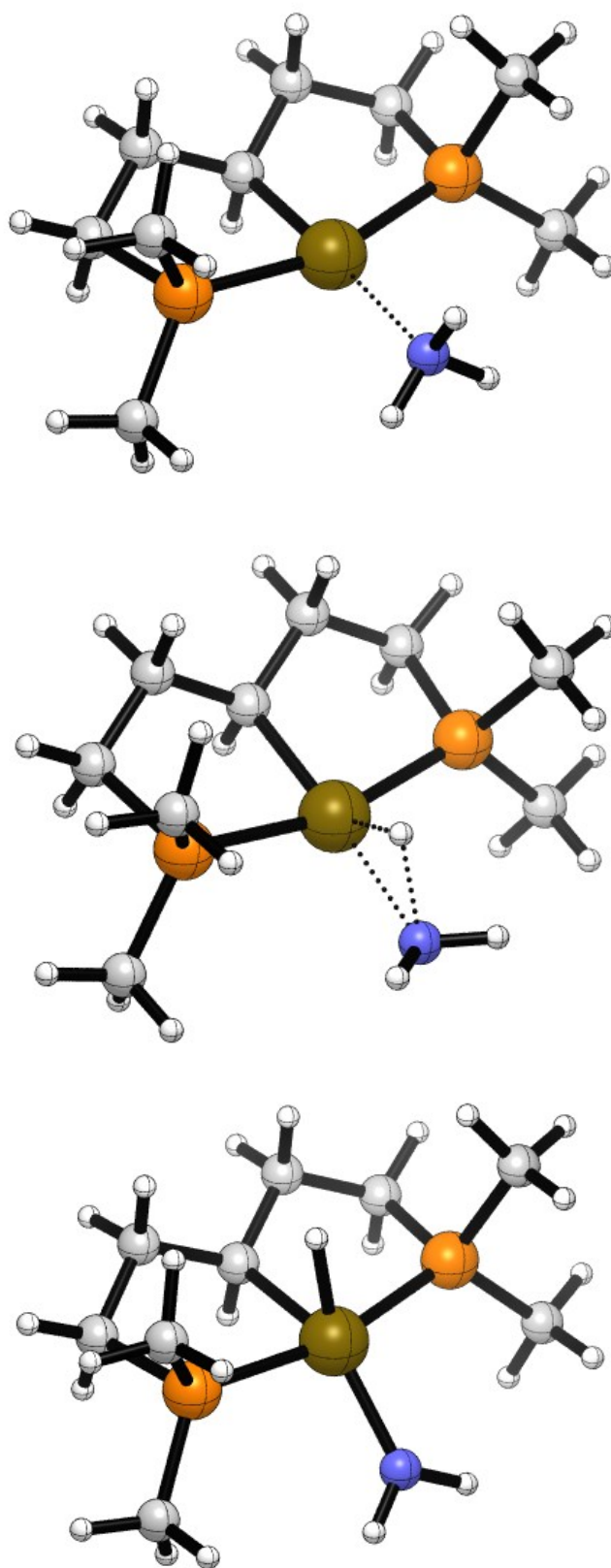
Table S7. Cartesian coordinates (Å) of fragment, reactant, transition state and product for different X groups:

F (X=CH)

6	0.000007	1.549256	-0.419203
1	0.000007	1.597959	-1.530839
6	1.266710	2.259352	0.085799
1	1.275096	3.310954	-0.259831
1	1.249511	2.297951	1.189439
6	-1.266698	2.259346	0.085799
1	-1.275085	3.310950	-0.259829
1	-1.249503	2.297943	1.189439
6	2.530687	1.536285	-0.384391
1	2.621601	1.603598	-1.481674
1	3.456068	1.940725	0.057205
6	-2.530673	1.536283	-0.384396
1	-3.456056	1.940729	0.057194
1	-2.621582	1.603593	-1.481680
15	2.281519	-0.251720	0.034103
15	-2.281535	-0.251727	0.034097
77	0.000008	-0.487429	-0.057813
6	-3.091825	-0.423036	1.685095
1	-4.152710	-0.125724	1.650323
1	-3.016154	-1.467013	2.023810
1	-2.555086	0.207293	2.408301
6	-3.472733	-1.148166	-1.054276
1	-3.461352	-2.219936	-0.804093
1	-4.498688	-0.762342	-0.938681
1	-3.153489	-1.036773	-2.100573
6	3.091853	-0.423037	1.685079
1	3.016067	-1.466982	2.023867
1	4.152772	-0.125850	1.650250
1	2.555217	0.207405	2.408264
6	3.472643	-1.148208	-1.054310
1	4.498625	-0.762445	-0.938752
1	3.461207	-2.219979	-0.804130
1	3.153363	-1.036796	-2.100594

R (X=CH)

6	-0.002322	1.717447	-0.411995
1	-0.001650	1.814704	-1.521717
6	1.260439	2.441680	0.091371
1	1.285040	3.496088	-0.248977
1	1.248431	2.477963	1.196449
6	-1.266703	2.439956	0.089682
1	-1.292930	3.494009	-0.251635
1	-1.255582	2.477244	1.194738
6	2.522245	1.715035	-0.376323
1	2.610768	1.777297	-1.474480
1	3.454691	2.109391	0.061510
6	-2.526751	1.710419	-0.378216

1	-3.460293	2.103399	0.058517
1	-2.614519	1.771250	-1.476506
15	2.255796	-0.069231	0.041117
15	-2.256540	-0.072712	0.041515
77	-0.000345	-0.383335	-0.101188
6	-2.998586	-0.218499	1.730666
1	-4.054251	0.099426	1.743081
1	-2.928902	-1.260690	2.077300
1	-2.417334	0.407693	2.422194
6	-3.526947	-0.964784	-0.969840
1	-3.535536	-2.033090	-0.700611
1	-4.538118	-0.554824	-0.812449
1	-3.261363	-0.879869	-2.033772
6	2.997988	-0.215527	1.730211
1	2.932706	-1.258833	2.074461
1	4.052400	0.106488	1.743741
1	2.413971	0.406619	2.423055
6	3.528739	-0.957197	-0.970762
1	4.538897	-0.544830	-0.813113
1	3.539545	-2.025560	-0.701886
1	3.263171	-0.872232	-2.034717
1	0.106087	-2.941102	1.004371
1	-0.842460	-3.055728	-0.333672
1	0.787702	-3.040074	-0.490480
7	0.011234	-2.634280	0.033981

TS (X=CH)

6	-0.000001	1.733938	-0.370097
1	0.000013	1.828788	-1.482618
6	1.269767	2.440532	0.135390
1	1.303053	3.499592	-0.188859
1	1.258408	2.459546	1.240391
6	-1.269782	2.440531	0.135357
1	-1.303069	3.499586	-0.188908
1	-1.258443	2.459562	1.240358
6	2.529529	1.715936	-0.346095
1	2.620032	1.801928	-1.442652
1	3.462002	2.102802	0.097196
6	-2.529531	1.715921	-0.346140
1	-3.462016	2.102793	0.097123
1	-2.620011	1.801888	-1.442701
15	2.278299	-0.080836	0.024055
15	-2.278298	-0.080841	0.024056
77	0.000000	-0.381993	-0.092625
6	-3.039857	-0.313480	1.685851
1	-4.106608	-0.037938	1.689381
1	-2.932821	-1.366233	1.988050
1	-2.495155	0.305989	2.412263

6 -3.467074 -0.965067 -1.072021
1 -3.431901 -2.042362 -0.850144
1 -4.498088 -0.599720 -0.938807
1 -3.159169 -0.824598 -2.118252
6   3.039869 -0.313523 1.685838
1   2.932837 -1.366287 1.988006
1   4.106621 -0.037980 1.689368
1   2.495173 0.305922 2.412272
6   3.467067 -0.965030 -1.072056
1   4.498081 -0.599683 -0.938843
1   3.431900 -2.042331 -0.850207
1   3.159151 -0.824535 -2.118281
1   0.000001 -1.486067 1.081630
1 -0.812738 -3.054905 0.336220
1   0.812745 -3.054904 0.336224
7   0.000004 -2.561543 -0.036276

P (X=CH)
6   0.000033 1.639362 -0.611321
1   0.000066 1.509858 -1.713493
6   1.274666 2.407822 -0.241755
1   1.316227 3.383905 -0.763460
1   1.267132 2.631674 0.839811
6 -1.274621 2.407832 -0.241832
1 -1.316176 3.383891 -0.763582
1 -1.267116 2.631727 0.839726
6   2.524403 1.590487 -0.588379
1   2.604861 1.473915 -1.682762
1   3.461619 2.048201 -0.231257
6 -2.524332 1.590474 -0.588475
1 -3.461578 2.048253 -0.231519
1 -2.604656 1.473781 -1.682858
15   2.284634 -0.112737 0.102800
15 -2.284643 -0.112703 0.102834
77 -0.000003 -0.398142 0.060351
6 -3.092248 -0.057961 1.754232
1 -4.158420 0.208009 1.676569
1 -2.990757 -1.039230 2.240501
1 -2.568965 0.684530 2.372836
6 -3.429013 -1.181580 -0.864480
1 -3.423481 -2.196646 -0.438849
1 -4.459902 -0.793863 -0.852047
1 -3.070896 -1.239704 -1.902667
6   3.092085 -0.058092 1.754285
1   2.990308 -1.039334 2.240554
1   4.158321 0.207659 1.676774
1   2.568845 0.684499 2.372803
6   3.429146 -1.181514 -0.864466
1   4.459917 -0.793472 -0.852199
1   3.423976 -2.196501 -0.438647

1   3.070957 -1.239918 -1.902611
1   0.000043 0.483605 1.402969
1 -0.824000 -2.783268 -0.961855
1   0.823790 -2.783335 -0.961985
7 -0.000063 -2.235805 -0.723025

F (X=N)
6 1.190677 2.216620 0.020674
1 1.143317 3.243604 -0.391698
1 1.247677 2.341055 1.129186
6 -1.190677 2.216620 0.020673
1 -1.143318 3.243604 -0.391699
1 -1.247678 2.341055 1.129185
6 2.455873 1.516727 -0.472648
1 2.488548 1.540966 -1.573472
1 3.373914 1.981826 -0.078826
6 -2.455873 1.516727 -0.472649
1 -3.373914 1.981826 -0.078828
1 -2.488547 1.540965 -1.573474
15 2.285500 -0.253597 0.033203
15 -2.285500 -0.253597 0.033203
77 0.000000 -0.489891 -0.038662
6 -3.125148 -0.324006 1.674394
1 -4.174476 0.007392 1.610697
1 -3.089337 -1.354029 2.058759
1 -2.576637 0.319276 2.377241
6 -3.469014 -1.168507 -1.043238
1 -3.485988 -2.229119 -0.749681
1 -4.488443 -0.757151 -0.965591
1 -3.123886 -1.104481 -2.085142
6 3.125149 -0.324007 1.674394
1 3.089336 -1.354030 2.058760
1 4.174478 0.007388 1.610695
1 2.576641 0.319277 2.377240
6 3.469014 -1.168505 -1.043240
1 4.488442 -0.757145 -0.965597
1 3.485992 -2.229117 -0.749680
1 3.123883 -1.104483 -2.085143
7 0.000000 1.494404 -0.404604

R (X=N)
6   1.187763 2.407128 -0.015080
1   1.147991 3.416116 -0.479149
1   1.294263 2.600946 1.084893
6 -1.187773 2.407130 -0.015100
1 -1.147998 3.416114 -0.479177
1 -1.294286 2.600957 1.084871
6   2.440178 1.678387 -0.502990
1   2.456382 1.666106 -1.604717
1   3.372913 2.138682 -0.137252

```
 6  -2.440184  1.678381 -0.503015
 1  -3.372923  2.138679 -0.137291
 1  -2.456374  1.666087 -1.604741
15   2.260188 -0.076105  0.046713
15  -2.260182 -0.076100  0.046716
77  -0.000005 -0.395911 -0.069676
 6  -3.033324 -0.080262  1.725466
 1  -4.076901  0.274381  1.699033
 1  -3.004743 -1.097947  2.142902
 1  -2.439300  0.572410  2.380993
 6  -3.529055 -0.994924 -0.937247
 1  -3.575373 -2.043162 -0.601159
 1  -4.531063 -0.548304 -0.830270
 1  -3.236078 -0.982368 -1.997225
 6   3.033313 -0.080282  1.725472
 1   3.004752 -1.097975  2.142892
 1   4.076882  0.274384  1.699057
 1   2.439266  0.572366  2.381003
 6   3.529096 -0.994877 -0.937255
 1   4.531091 -0.548237 -0.830242
 1   3.575429 -2.043127 -0.601207
 1   3.236140 -0.982286 -1.997238
 1   0.000342 -2.933423  0.943015
 1  -0.817982 -2.977414 -0.482621
 1   0.817716 -2.977376 -0.483178
 7   0.000015 -2.580017 -0.016654
 7  -0.000003  1.656953 -0.350645
```

TS (X=N)
```
 6   1.192955  2.405688 -0.000200
 1   1.146062  3.408387 -0.474094
 1   1.295541  2.603825  1.096008
 6  -1.192980  2.405681 -0.000213
 1  -1.146092  3.408378 -0.474112
 1  -1.295576  2.603823  1.095993
 6   2.445899  1.678634 -0.490706
 1   2.467342  1.678923 -1.592481
 1   3.376835  2.137826 -0.120276
 6  -2.445914  1.678612 -0.490724
 1  -3.376857  2.137799 -0.120306
 1  -2.467346  1.678892 -1.592499
15   2.279419 -0.085485  0.031077
15  -2.279420 -0.085499  0.031078
77   0.000001 -0.381818 -0.041971
 6  -3.089923 -0.159309  1.683318
 1  -4.146301  0.150505  1.636706
 1  -3.026900 -1.186583  2.072490
 1  -2.541100  0.499357  2.371349
 6  -3.457582 -1.017806 -1.032598
 1  -3.467755 -2.074904 -0.726330
 1  -4.479809 -0.612530 -0.963364
 1  -3.108734 -0.968002 -2.073958
 6   3.089926 -0.159314  1.683314
 1   3.026902 -1.186592  2.072474
 1   4.146306  0.150496  1.636701
 1   2.541108  0.499345  2.371354
 6   3.457575 -1.017777 -1.032616
 1   4.479808 -0.612516 -0.963367
 1   3.467731 -2.074883 -0.726377
 1   3.108733 -0.967940 -2.073977
 1   0.000015 -1.687803  0.964537
 1  -0.818065 -3.087115  0.136824
 1   0.818135 -3.087094  0.136913
 7   0.000045 -2.553102 -0.153101
 7  -0.000009  1.648347 -0.319504
```

P (X=N)
```
 6   1.188961  2.382991 -0.175541
 1   1.185951  3.374965 -0.674528
 1   1.261351  2.602684  0.921770
 6  -1.188950  2.382990 -0.175506
 1  -1.185937  3.374976 -0.674470
 1  -1.261324  2.602657  0.921811
 6   2.441850  1.614995 -0.606525
 1   2.458851  1.528766 -1.705058
 1   3.374712  2.100319 -0.276622
 6  -2.441848  1.615013 -0.606495
 1  -3.374704  2.100336 -0.276575
 1  -2.458858  1.528807 -1.705030
15   2.288482 -0.103302  0.057921
15  -2.288484 -0.103300  0.057911
77  -0.000001 -0.406664  0.049515
 6  -3.132763 -0.056338  1.689993
 1  -4.188102  0.244056  1.593200
 1  -3.073708 -1.048902  2.160295
 1  -2.603279  0.659904  2.334111
 6  -3.421324 -1.128395 -0.964741
 1  -3.448002 -2.153644 -0.565050
 1  -4.444504 -0.720648 -0.971688
 1  -3.032477 -1.167848 -1.992411
 6   3.132762 -0.056302  1.690002
 1   3.073710 -1.048856  2.160325
 1   4.188101  0.244093  1.593205
 1   2.603275  0.659951  2.334106
 6   3.421317 -1.128421 -0.964710
 1   4.444500 -0.720681 -0.971660
 1   3.447985 -2.153664 -0.565003
 1   3.032473 -1.167890 -1.992380
 1  -0.000010  0.342671  1.443722
 1  -0.822594 -2.915720 -0.469048
```

1   0.822715 -2.915551 -0.469717
7   -0.000004 -2.316176 -0.476684
7   0.000000 1.645065 -0.526497

F (X=B)
6 1.381333 2.335900 -0.046016
1 1.300167 3.281691 -0.612201
1 1.534059 2.644494 1.007997
6 -1.381335 2.335900 -0.046023
1 -1.300166 3.281687 -0.612215
1 -1.534063 2.644502 1.007987
6 2.583172 1.512220 -0.529408
1 2.605237 1.485687 -1.631118
1 3.563917 1.884396 -0.186962
6 -2.583174 1.512218 -0.529413
1 -3.563919 1.884394 -0.186967
1 -2.605239 1.485682 -1.631122
15 2.288495 -0.230320 0.011108
15 -2.288494 -0.230321 0.011107
77 0.000000 -0.467435 -0.037012
6 -3.093720 -0.317314 1.671388
1 -4.162121 -0.052047 1.617967
1 -2.990400 -1.333534 2.080216
1 -2.576025 0.375901 2.349539
6 -3.445709 -1.239840 -1.012820
1 -3.413983 -2.288600 -0.680157
1 -4.480836 -0.869770 -0.934517
1 -3.121938 -1.200890 -2.063057
6 3.093726 -0.317319 1.671385
1 2.990403 -1.333539 2.080212
1 4.162127 -0.052056 1.617960
1 2.576036 0.375898 2.349539
6 3.445707 -1.239835 -1.012827
1 4.480833 -0.869760 -0.934533
1 3.413990 -2.288595 -0.680161
1 3.121928 -1.200890 -2.063061
5 -0.000001 1.511174 -0.075242

R (X=B)
6   1.367234 2.517461 -0.160838
1   1.287936 3.427118 -0.784335
1   1.507867 2.890517 0.874539
6 -1.367172 2.517475 -0.160801
1 -1.287883 3.427178 -0.784230
1 -1.507810 2.890449 0.874605
6   2.578010 1.673717 -0.579215
1   2.618311 1.586725 -1.677780
1   3.557621 2.055708 -0.241580
6 -2.577950 1.673759 -0.579230
1 -3.557568 2.055776 -0.241643

1 -2.618197 1.586761 -1.677797
15 2.260352 -0.036180 0.048179
15 -2.260349 -0.036138 0.048182
77 0.000003 -0.363977 -0.047158
6 -2.992394 -0.006324 1.747263
1 -4.056586 0.280760 1.727700
1 -2.890993 -0.997575 2.214229
1 -2.428062 0.714295 2.355785
6 -3.505216 -1.079297 -0.844171
1 -3.495473 -2.102676 -0.436052
1 -4.525283 -0.673005 -0.746856
1 -3.235970 -1.127277 -1.909839
6   2.992336 -0.006369 1.747289
1   2.890960 -0.997629 2.214240
1   4.056517 0.280755 1.727764
1   2.427954 0.714221 2.355799
6   3.505238 -1.079340 -0.844142
1   4.525332 -0.673152 -0.746669
1   3.495338 -2.102770 -0.436158
1   3.236104 -1.127164 -1.909847
1   0.000840 -3.148007 0.759622
1 -0.821668 -3.102238 -0.664556
1   0.820519 -3.102177 -0.666188
7 -0.000107 -2.742659 -0.178424
5   0.000028 1.657309 -0.140598

TS (X=B)
6 1.372621 2.512468 0.184524
1 1.314298 3.522961 -0.260280
1 1.494699 2.686674 1.273379
6 -1.372525 2.512452 0.184496
1 -1.314163 3.522917 -0.260378
1 -1.494562 2.686720 1.273343
6 2.586314 1.748190 -0.362021
1 2.633698 1.853398 -1.459087
1 3.563412 2.068787 0.039889
6 -2.586286 1.748246 -0.361961
1 -3.563326 2.068859 0.040074
1 -2.633798 1.853503 -1.459016
15 2.285503 -0.050602 -0.051253
15 -2.285499 -0.050551 -0.051255
77 -0.000001 -0.371726 -0.101490
6 -3.090729 -0.368489 1.577160
1 -4.166454 -0.132224 1.556852
1 -2.953180 -1.425360 1.851395
1 -2.593405 0.248284 2.339445
6 -3.411819 -0.933080 -1.213098
1 -3.367575 -2.014037 -1.012091
1 -4.452735 -0.585752 -1.112821
1 -3.068192 -0.762895 -2.243901

6   3.090700 -0.368487 1.577188
1   2.952838 -1.425265 1.851619
1   4.166495 -0.132548 1.556804
1   2.593583   0.248575 2.339375
6   3.411828 -0.933166 -1.213063
1   4.452699 -0.585654 -1.112958
1   3.367776 -2.014093 -1.011851
1   3.068064 -0.763223 -2.243860
1   -0.000127 -1.165446 1.295784
1   -0.816444 -2.984963 0.724524
1   0.816158 -2.985049 0.724642
7   -0.000089 -2.510593 0.335309
5   0.000057   1.684279   0.014993

P (X=B)

6   1.385451   2.426409 -0.434438
1   1.312008   3.240039 -1.177552
1   1.560080   2.934059   0.535237
6   -1.385453   2.426407 -0.434441
1   -1.312010   3.240037 -1.177556
1   -1.560084   2.934058   0.535233
6   2.571853   1.505935 -0.764185
1   2.570844   1.270091 -1.841424
1   3.561794   1.928714 -0.521301
6   -2.571854   1.505933 -0.764188
1   -3.561795   1.928711 -0.521306
1   -2.570843   1.270087 -1.841427
15 2.299938 -0.114604   0.086410
15 -2.299938 -0.114604   0.086411
77 0.000000 -0.361241   0.121845
6   -3.148327   0.060549   1.708946
1   -4.217751   0.294425   1.585746
1   -3.038362 -0.872421   2.281078
1   -2.655637   0.865549   2.272400
6   -3.378737 -1.307290 -0.805427
1   -3.333329 -2.285956 -0.304666
1   -4.424161 -0.962314 -0.833290
1   -3.009073 -1.425283 -1.834612
6   3.148327   0.060546   1.708946
1   3.038366 -0.872426   2.281074
1   4.217750   0.294426   1.585745
1   2.655635   0.865542   2.272403
6   3.378736 -1.307287 -0.805430
1   4.424162 -0.962316 -0.833287
1   3.333322 -2.285956 -0.304675
1   3.009076 -1.425273 -1.834617
1   -0.000001   0.675628   1.400891
1   -0.820828 -2.479042 -1.350563
1   0.820841 -2.479063 -1.350527
7   0.000000 -2.114665 -0.871367

5   -0.000001   1.627567 -0.271307

F (X=SiH)

1   0.000095   2.114161 -1.906487
6   1.620851   2.380319   0.294739
1   1.814294   3.422947 -0.010119
1   1.541229   2.372377   1.395361
6   -1.620912   2.380344   0.294578
1   -1.814360   3.422931 -0.010415
1   -1.541343   2.372539   1.395204
6   2.758935   1.455252 -0.166111
1   2.926367   1.573834 -1.250444
1   3.722450   1.654249   0.335042
6   -2.758961   1.455210 -0.166224
1   -3.722490   1.654221   0.334896
1   -2.926377   1.573711 -1.250569
15 2.277062 -0.329967   0.081445
15 -2.277054 -0.329979   0.081460
77 0.000000 -0.570662 -0.165755
6   -2.883566 -0.679456   1.791716
1   -3.960013 -0.463865   1.889646
1   -2.698701 -1.735133   2.039810
1   -2.316578 -0.059204   2.500210
6   -3.527100 -1.228921 -0.940592
1   -3.432587 -2.311247 -0.765092
1   -4.554488 -0.912702 -0.697230
1   -3.325869 -1.034155 -2.004020
6   2.883605 -0.679565   1.791665
1   2.698770 -1.735267   2.039675
1   3.960049 -0.463957   1.889597
1   2.316614 -0.059384   2.500219
6   3.527111 -1.228808 -0.940692
1   4.554496 -0.912584 -0.697321
1   3.432624 -2.311150 -0.765272
1   3.325861 -1.033967 -2.004102
14 0.000002   1.684684 -0.456680

R (X=SiH)

1   -0.000899   2.277462 -1.947993
6   1.621239   2.575434   0.225177
1   1.824270   3.603676 -0.118321
1   1.545448   2.609061   1.326361
6   -1.620854   2.575217   0.226621
1   -1.823903   3.603834 -0.115749
1   -1.544570   2.607679   1.327805
6   2.752723   1.627450 -0.198672
1   2.924467   1.706956 -1.286341
1   3.719042   1.827434   0.298244
6   -2.752606   1.627731 -0.197630
1   -3.718793   1.827548   0.299605

```
  1 -2.924548  1.707961 -1.285215
 15  2.247748 -0.143991  0.105417
 15  -2.247826 -0.143982  0.10530
 77 -0.000021 -0.472653 -0.185300
  6 -2.781703 -0.403165  1.859015
  1 -3.845068 -0.149518  2.001395
  1 -2.616507 -1.452815  2.145155
  1 -2.161713  0.227617  2.511221
  6 -3.574485 -1.076599 -0.794903
  1 -3.494986 -2.150707 -0.563572
  1 -4.582823 -0.729598 -0.515384
  1 -3.433035 -0.945639 -1.877871
  6  2.781288 -0.401973  1.859412
  1  2.616103 -1.451440  2.146234
  1  3.844613 -0.148176  2.001832
  1  2.161134  0.229211  2.511071
  6  3.574537 -1.077345 -0.793852
  1  4.582848 -0.730262 -0.514337
  1  3 .494858 -2.151282 -0.561787
  1  3.433373 -0.947114 -1.876948
  1  0.003823 -3.107663  0.870571
  1 -0.821343 -3.179530 -0.551108
  1  0.819257 -3.178582 -0.556809
  7  0.000307 -2.780044 -0.097051
 14 -0.000087  1.827682 -0.499462
```

TS (X=SiH)
```
  1  0.000060  2.504209 -1.732431
  6  1.633600  2.520593  0.453494
  1  1.843292  3.584487  0.252240
  1  1.568279  2.402330  1.549262
  6 -1.633413  2.520850  0.453734
  1 -1.843085  3.584632  0.251887
  1 -1.567704  2.403238  1.549544
  6  2.757271  1.635807 -0.110166
  1  2.895895  1.844646 -1.185383
  1  3.736480  1.792049  0.375955
  6 -2.757433  1.635909 -0.109026
  1 -3.736097  1.791769  0.378306
  1 -2.897405  1.845184 -1.183976
 15  2.290370 -0.167221 -0.005299
 15 -2.290343 -0.167204 -0.005297
 77 -0.000011 -0.467021 -0.151698
  6 -3.012640 -0.691647  1.608994
  1 -4.099807 -0.518905  1.645808
  1 -2.806218 -1.760166  1.771514
  1 -2.522779 -0.124521  2.413443
  6 -3.425978 -0.971166 -1.214204
  1 -3.323381 -2.063565 -1.132833
  1 -4.476278 -0.687140 -1.040118
```

```
  1 -3.130819 -0.675125 -2.231439
  6  3.012211 -0.690673  1.609512
  1  2.804517 -1.758761  1.773218
  1  4.099582 -0.519159  1.646070
  1  2.523065 -0.122100  2.413372
  6  3.426497 -0.971770 -1.213355
  1  4.476444 -0.685782 -1.040365
  1  3.325681 -2.064176 -1.129845
  1  3.130325 -0.678135 -2.230989
  1 -0.000123 -1.297292  1.229770
  1 -0.815814 -3.042200  0.707200
  1  0.815933 -3.042102  0.707092
  7  0.000006 -2.591602  0.291543
 14 -0.000024  1.891243 -0.345166
```

P (X=SiH)
```
  1  0.000004  1.909643 -2.122679
  6  1.650500  2.533769 -0.038872
  1  1.865036  3.507331 -0.510202
  1  1.609415  2.696368  1.051657
  6 -1.650504  2.533768 -0.038880
  1 -1.865040  3.507327 -0.510214
  1 -1.609421  2.696372  1.051649
  6  2.756564  1.520087 -0.388103
  1  2.878613  1.465487 -1.483775
  1  3.742341  1.783903  0.033236
  6 -2.756565  1.520082 -0.388109
  1 -3.742343  1.783898  0.033227
  1 -2.878612  1.465479 -1.483782
 15  2.298923 -0.210164  0.145546
 15 -2.298923 -0.210165  0.145547
 77  0.000000 -0.475263  0.039017
  6 -3.018576 -0.348277  1.832757
  1 -4.102165 -0.150245  1.828011
  1 -2.828025 -1.357401  2.226119
  1 -2.511936  0.374529  2.487494
  6 -3.418332 -1.273211 -0.855084
  1 -3.324919 -2.315308 -0.514113
  1 -4.469331 -0.956672 -0.764876
  1 -3.110311 -1.223524 -1.909717
  6  3.018575 -0.348283  1.832755
  1  2.828025 -1.357410  2.226112
  1  4.102165 -0.150251  1.828010
  1  2.511935  0.374519  2.487496
  6  3.418333 -1.273204 -0.855090
  1  4.469332 -0.956666 -0.764880
  1  3.324920 -2.315303 -0.514124
  1  3.110313 -1.223512 -1.909723
  1 -0.000001  0.474279  1.363034
  1 -0.822980 -2.653704 -1.371268
```

```
1    0.822998 -2.653753 -1.371183
7    0.000001 -2.222193 -0.956490
14   0.000000  1.752983 -0.619216
```

F (X=O)
```
6  1.217776  2.253775  0.041318
1  1.113793  3.255592 -0.401479
1  1.261478  2.348714  1.139043
6 -1.217778  2.253772  0.041294
1 -1.113794  3.255584 -0.401513
1 -1.261496  2.348723  1.139018
6  2.414226  1.512678 -0.518798
1  2.399369  1.545619 -1.619081
1  3.344333  1.991786 -0.175180
6 -2.414217  1.512664 -0.518830
1 -3.344330  1.991779 -0.175238
1 -2.399338  1.545584 -1.619113
15 2.318470  -0.268745 -0.000433
15 -2.318477 -0.268751 -0.000434
77 0.000005  -0.505888  0.039052
6 -3.250129  -0.356151  1.577047
1 -4.293048  -0.029547  1.443248
1 -3.242013  -1.393281  1.944133
1 -2.757724   0.273393  2.331953
6 -3.373087  -1.162298 -1.200701
1 -3.419123  -2.225002 -0.919206
1 -4.394541  -0.751712 -1.214182
1 -2.928876  -1.087485 -2.203359
6  3.250151  -0.356186  1.577028
1  3.241952  -1.393303  1.944147
1  4.293094  -0.029674  1.443196
1  2.757818   0.273426  2.331925
6  3.373030  -1.162297 -1.200741
1  4.394498  -0.751746 -1.214237
1  3.419036  -2.225008 -0.919268
1  2.928796  -1.087450 -2.203387
8  0.000003   1.523009 -0.303891
```

R (X=O)
```
6  1.205970  2.436645  0.119933
1  1.136852  3.459895 -0.282566
1  1.260206  2.496280  1.221422
6 -1.211006  2.435713  0.116699
1 -1.142629  3.458298 -0.287619
1 -1.267008  2.497324  1.217993
6  2.394407  1.696104 -0.462998
1  2.374196  1.761339 -1.561921
1  3.334421  2.149587 -0.111304
6 -2.397515  1.692353 -0.466514
1 -3.338690  2.144989 -0.116841
```

```
1 -2.375971  1.755422 -1.565528
15  2.293097 -0.104313 -0.009570
15 -2.293623 -0.106825 -0.009174
77 -0.000193 -0.416025 -0.015694
6 -3.199783 -0.221693  1.586949
1 -4.234039  0.144010  1.491045
1 -3.221037 -1.269705  1.921637
1 -2.669578  0.364796  2.350831
6 -3.430879 -0.924967 -1.197608
1 -3.520108 -1.993288 -0.947056
1 -4.435291 -0.474825 -1.166237
1 -3.019932 -0.838560 -2.213596
6  3.199706 -0.221578  1.586132
1  3.221920 -1.270399  1.918387
1  4.233679  0.145121  1.490985
1  2.669157  0.362808  2.351399
6  3.431697 -0.917568 -1.200102
1  4.434839 -0.464553 -1.169283
1  3.524011 -1.985856 -0.950580
1  3.019599 -0.830927 -2.215630
1  0.097148 -2.789855  1.129150
1 -0.841876 -2.938676 -0.210824
1  0.783631 -2.931611 -0.359406
7  0.008246 -2.498137  0.149535
8 -0.001762  1.735783 -0.248321
```

TS (X=O)
```
6  1.211634  2.435196  0.127116
1  1.156101  3.461499 -0.269190
1  1.247694  2.483559  1.229479
6 -1.211633  2.435195  0.127121
1 -1.156100  3.461499 -0.269183
1 -1.247690  2.483556  1.229484
6  2.405145  1.691108 -0.444032
1  2.401798  1.763858 -1.543099
1  3.340999  2.143767 -0.080375
6 -2.405145  1.691109 -0.444027
1 -3.340998  2.143769 -0.080366
1 -2.401801  1.763863 -1.543093
15  2.310494 -0.114807 -0.007866
15 -2.310495 -0.114806 -0.007867
77  0.000000 -0.414247 -0.022246
6 -3.197152 -0.276759  1.587704
1 -4.244462  0.050953  1.500801
1 -3.175111 -1.329881  1.906164
1 -2.683317  0.319800  2.354908
6 -3.400335 -0.941662 -1.224126
1 -3.449335 -2.015824 -0.991119
1 -4.418223 -0.522973 -1.201820
1 -2.973410 -0.828941 -2.230849
```

```
6    3.197151 -0.276754  1.587706
1    3.175110 -1.329874  1.906169
1    4.244461  0.050959  1.500802
1    2.683316  0.319808  2.354907
6    3.400336 -0.941666 -1.224123
1    4.418224 -0.522977 -1.201816
1    3.449336 -2.015828 -0.991111
1    2.973411 -0.828949 -2.230846
1   -0.000001 -1.472009  1.196865
1   -0.833026 -2.976543  0.296010
1    0.833028 -2.976542  0.296011
7    0.000001 -2.449273  0.048270
8    0.000000  1.745625 -0.260970

P (X=O)
6    1.211163  2.445323 -0.008679
1    1.186862  3.455173 -0.449286
1    1.241754  2.544529  1.091483
6   -1.211159  2.445325 -0.008686
1   -1.186858  3.455172 -0.449297
1   -1.241752  2.544537  1.091475
6    2.397708  1.653746 -0.535024
1    2.385534  1.654565 -1.636296
1    3.338953  2.123859 -0.209252
6   -2.397704  1.653745 -0.535030
1   -3.338950  2.123861 -0.209262
```

```
1   -2.385528  1.654559 -1.636301
15   2.317183 -0.122382  0.013141
15  -2.317183 -0.122381  0.013144
77   0.000000 -0.441934  0.039644
6   -3.213047 -0.185055  1.608006
1   -4.257089  0.144341  1.493786
1   -3.198644 -1.216751  1.989748
1   -2.700371  0.454439  2.340596
6   -3.388216 -1.024153 -1.163384
1   -3.445117 -2.081247 -0.863442
1   -4.405314 -0.603537 -1.180546
1   -2.947548 -0.973503 -2.169247
6    3.213042 -0.185066  1.608004
1    3.198635 -1.216763  1.989742
1    4.257085  0.144328  1.493787
1    2.700367  0.454428  2.340595
6    3.388220 -1.024151 -1.163388
1    4.405318 -0.603533 -1.180550
1    3.445125 -2.081245 -0.863448
1    2.947553 -0.973499 -2.169252
1    0.000004  0.169238  1.489155
1   -0.824738 -2.910783 -0.010481
1    0.824643 -2.910815 -0.010137
7    0.000005 -2.347046 -0.213076
8    0.000003  1.762510 -0.381223
```