

Six-Coordinate High-Spin Iron(II) Complexes with Bidentate PN Ligands based on 2-Aminopyridine – New Fe(II) Spin Crossover Systems

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Supporting Information

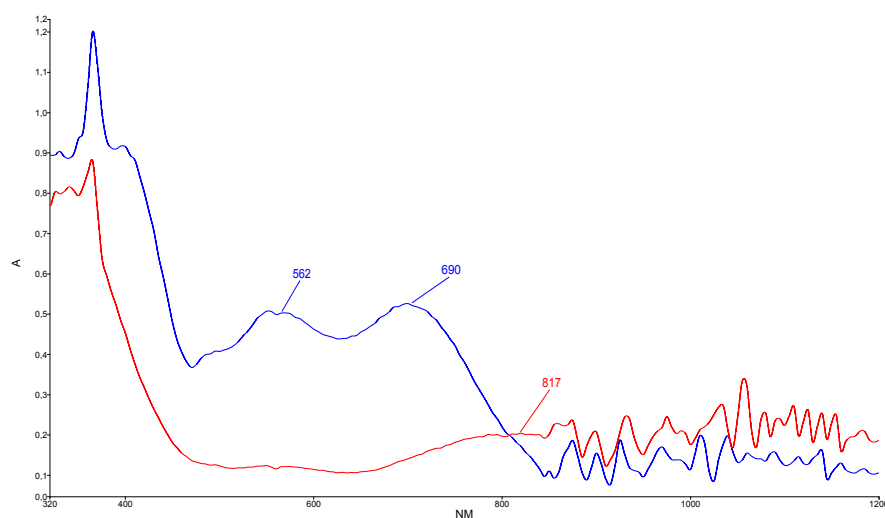


Figure S1. Experimental UV/Vis Spectra of **2a** at 123 K (blue) and 293 K (red).

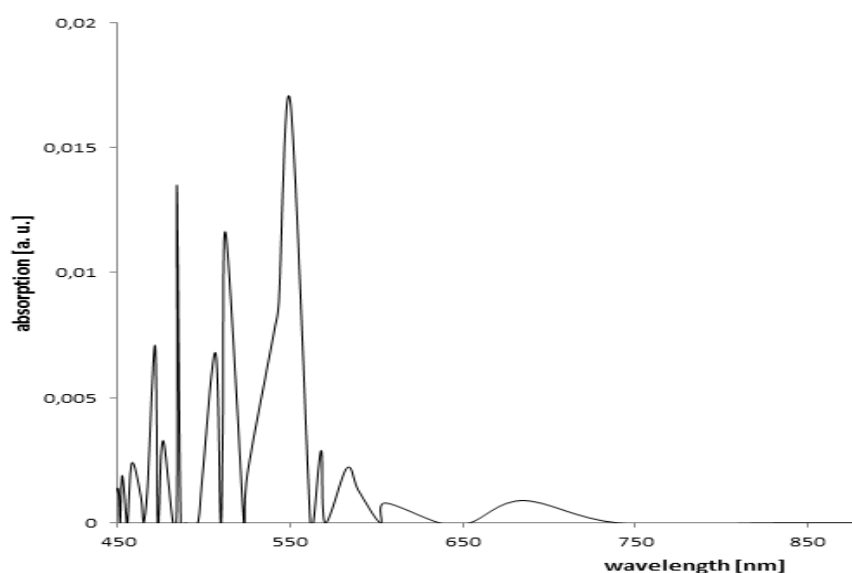


Figure S2. Calculated UV/Vis Spectra of **B^{LS}**.

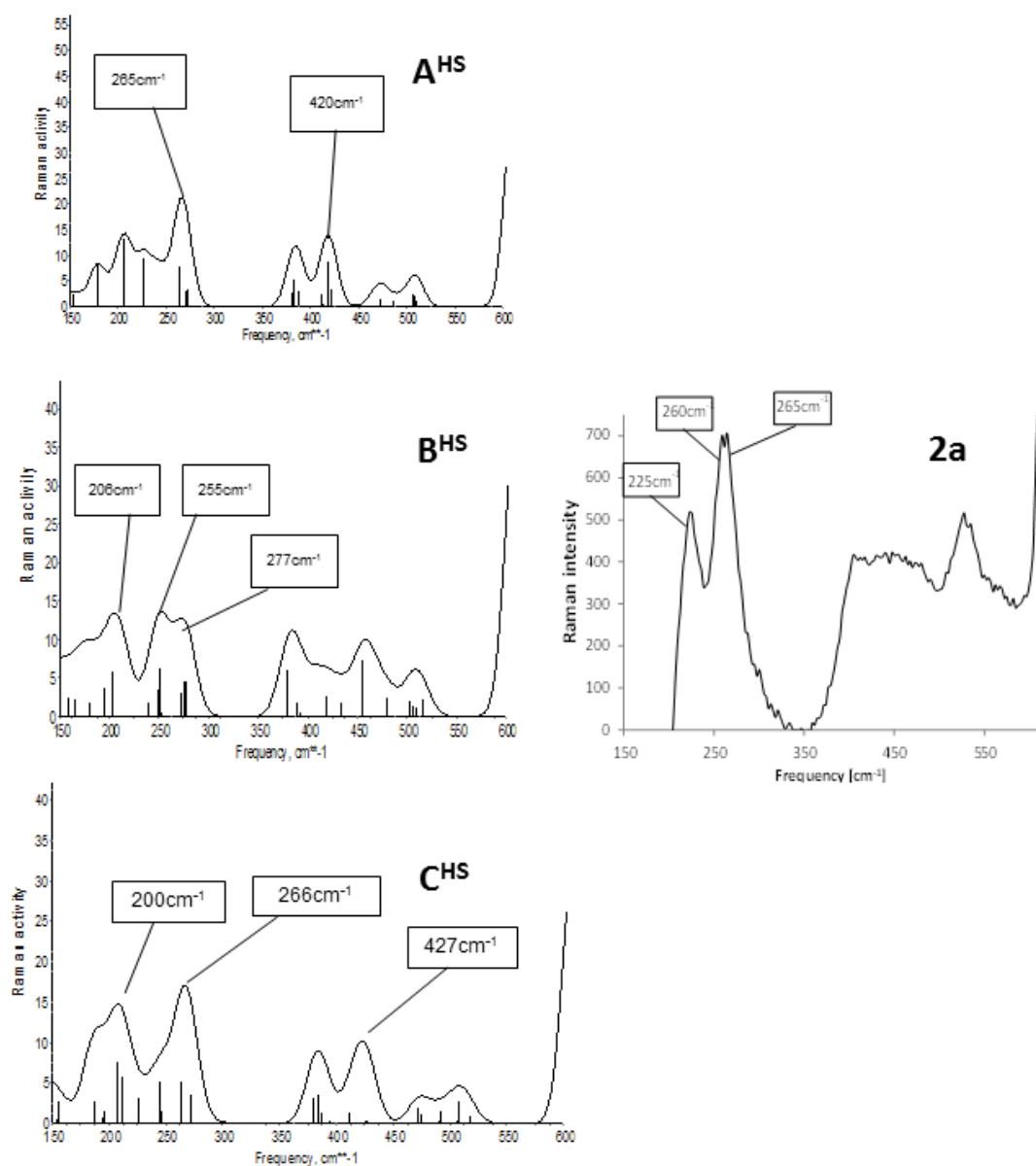


Figure S3. Calculated (left) and experimental (right) Raman spectra in the range of 150 – 600 cm⁻¹.

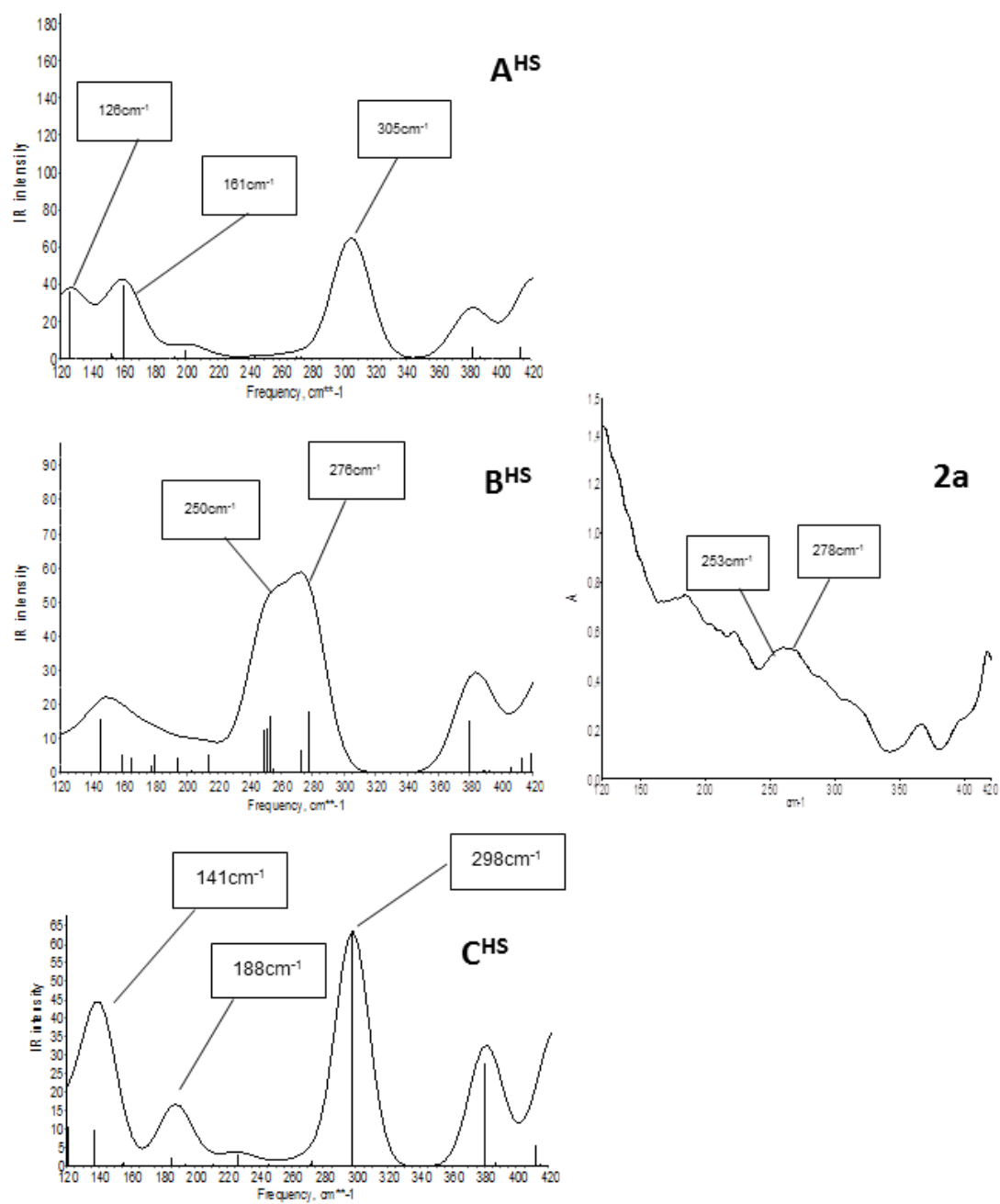


Figure S4. Calculated (left) and experimental (right) FIR spectra in the range of 120 - 420 cm^{-1} .

Table S1. Energies of Isomers **A-E**. All calculations with the OPBE functional, Fe: sdd, other atoms 6-31g** (gas phase). Reference point is *trans*-N,P,Cl-[Fe(PN)₂Cl₂] (**A^{HS}**) set to 0.0 kcal/mol

<i>trans</i> -N,P,Cl-[Fe(PN) ₂ Cl ₂] (A)		energies (hartrees)	ΔE (kcal/mol)	<i>cis</i> -N,P,Cl-[Fe(PN) ₂ Cl ₂] (B)	energies (hartrees)	ΔE (kcal/mol)
A^{LS} S = 0	ΔE	-3259.308981	20.3	B^{LS} S = 0	-3259.322313	11.9
	ΔH	-3258.709465	20.6		-3258.722469	12.5
	ΔG	-3258.827230	26.2		-3258.837084	20.1
A^{HS} S = 2	ΔE	-3259.341276	0.0	B^{HS} S = 2	-3259.337761	2.2
	ΔH	-3258.742316	0.0		-3258.738751	2.2
	ΔG	-3258.869055	0.0		-3258.863464	3.5
<i>cis</i> -N,P, <i>trans</i> -Cl-[Fe(PN) ₂ Cl ₂] (C)				<i>cis</i> -Cl,N, <i>trans</i> -P-[Fe(PN) ₂ Cl ₂] (D)		
C^{LS} S = 0	ΔE	-3259.319097	13.9	D^{LS} S = 0	-3259.311458	18.7
	ΔH	-3258.718977	14.6		-3258.712044	19.0
	ΔG	-3258.832975	22.6		-3258.828212	25.6
C^{HS} S = 2	ΔE	-3259.3424741	-0.8	D^{HS} S = 2	-3259.340594	0.4
	ΔH	-3258.743551	-0.8		-3258.741731	0.4
	ΔG	-3258.868983	0.0		-3258.870643	-1.0
<i>cis</i> -Cl,P, <i>trans</i> -N-[Fe(PN) ₂ Cl ₂] (E)						
E^{LS} S = 0	ΔE	-3259.311946	18.4			
	ΔH	-3258.712250	18.9			
	ΔG	-3258.826297	27.1			
E^{HS} S = 2	ΔE	-3259.323620	11.1			
	ΔH	-3258.724845	11.0			
	ΔG	-3258.853566	9.7			

Isomer A^{HS}

26	-0.028453000	-0.014674000	-0.002558000
15	-1.041115000	2.139273000	1.258983000
17	-0.693849000	-1.572096000	1.601435000
7	1.653801000	0.801932000	1.381931000
6	-1.909631000	2.240672000	2.892923000
6	-1.051865000	4.432219000	-0.422573000
1	0.029324000	4.321289000	-0.465576000
6	1.651821000	2.076084000	1.818795000
6	-2.243728000	1.047294000	3.554882000
1	-2.019134000	0.090576000	3.085329000
6	-1.812351000	3.543445000	0.356973000
6	3.911470000	1.870850000	2.636282000
1	4.790689000	2.299280000	3.118037000
6	-3.215648000	3.668845000	0.354602000
1	-3.826956000	2.991282000	0.950571000
6	3.900024000	0.532353000	2.224198000
1	4.754213000	-0.123424000	2.377908000
6	-2.788689000	3.504009000	4.780570000
1	-3.002371000	4.463452000	5.253165000
6	2.782287000	2.652171000	2.442053000
1	2.756468000	3.690820000	2.770035000
6	-3.837600000	4.671541000	-0.392672000
1	-4.924447000	4.758543000	-0.376100000
6	-3.071807000	5.563081000	-1.150794000
1	-3.557909000	6.347222000	-1.731610000
6	-2.846494000	1.086163000	4.817281000
1	-3.100730000	0.151689000	5.318228000
6	-2.190598000	3.471333000	3.519645000
1	-1.960008000	4.410334000	3.015764000
6	-1.680122000	5.437747000	-1.162897000
1	-1.074251000	6.120138000	-1.759708000
6	-3.118529000	2.309954000	5.432602000
1	-3.587834000	2.337504000	6.416592000
6	2.749632000	0.056981000	1.604634000
1	2.679661000	-0.976548000	1.271821000
7	0.505591000	2.822503000	1.646518000
15	1.012520000	-2.141601000	-1.256476000
17	0.607547000	1.534432000	-1.625597000
7	-1.700320000	-0.812081000	-1.403355000
6	1.984522000	-2.191759000	-2.833698000
6	0.906688000	-4.476874000	0.357509000
1	-0.171364000	-4.332858000	0.369133000
6	-1.666087000	-2.059011000	-1.910054000
6	2.494194000	-0.993133000	-3.359202000
1	2.320881000	-0.057050000	-2.830981000
6	1.720103000	-3.590247000	-0.369607000
6	-3.911968000	-1.848444000	-2.763141000
1	-4.772415000	-2.264046000	-3.288082000
6	3.117492000	-3.762211000	-0.327478000
1	3.769011000	-3.089326000	-0.884606000
6	-3.935832000	-0.537297000	-2.271875000
1	-4.800377000	0.109760000	-2.402857000
6	2.893315000	-3.388304000	-4.750927000
1	3.050007000	-4.324475000	-5.288026000
6	-2.771481000	-2.618391000	-2.590769000
1	-2.718266000	-3.635151000	-2.978598000
6	3.682520000	-4.806476000	0.408390000
1	4.765998000	-4.928638000	0.423332000
6	2.864507000	-5.695198000	1.113101000
1	3.306148000	-6.512436000	1.683747000
6	3.198113000	-0.995754000	-4.569019000
1	3.585968000	-0.056870000	-4.965029000
6	2.197124000	-3.391744000	-3.541264000
1	1.837194000	-4.339565000	-3.139886000
6	1.477817000	-5.524957000	1.084675000
1	0.831268000	-6.205393000	1.639595000
6	3.396367000	-2.188358000	-5.267645000
1	3.942277000	-2.187537000	-6.211641000
6	-2.806742000	-0.077000000	-1.603640000
1	-2.764346000	0.936344000	-1.210645000
7	-0.513184000	-2.798159000	-1.750373000
1	0.524252000	3.733336000	2.088084000
1	-0.517624000	-3.695129000	-2.219138000

Isomer A^{LS}

26	0.000255000	0.000184000	-0.000107000
15	-0.891840000	1.864422000	0.896904000
17	-0.627392000	-1.304652000	1.793759000
7	1.607656000	0.623069000	1.038772000
6	-1.824643000	1.805988000	2.492666000
6	-1.078664000	4.048354000	-0.896678000
1	-0.044624000	3.811723000	-1.135240000
6	1.712331000	1.927153000	1.411157000
6	-2.905345000	0.914144000	2.608350000
1	-3.128637000	0.226280000	1.796052000
6	-1.766143000	3.267648000	0.053330000
6	3.978846000	1.641307000	2.181637000
1	4.902670000	2.046139000	2.594087000
6	-3.117029000	3.560740000	0.319579000
1	-3.667463000	2.983695000	1.059868000
6	3.840202000	0.274906000	1.915706000
1	4.634223000	-0.437345000	2.129060000
6	-2.274998000	2.595409000	4.749743000
1	-2.016835000	3.245908000	5.585955000
6	2.894380000	2.474151000	1.944710000
1	2.932319000	3.535293000	2.186385000
6	-3.762306000	4.606740000	-0.345765000
1	-4.807249000	4.821813000	-0.120212000
6	-3.070833000	5.379534000	-1.282791000
1	-3.574674000	6.197592000	-1.798444000
6	-3.673412000	0.881857000	3.775487000
1	-4.505971000	0.182042000	3.851572000
6	-1.515188000	2.641170000	3.577714000
1	-0.671139000	3.327188000	3.521611000
6	-1.728826000	5.097084000	-1.552544000
1	-1.180402000	5.690425000	-2.284765000
6	-3.360511000	1.720332000	4.848882000
1	-3.953356000	1.685112000	5.763259000
6	2.648503000	-0.176661000	1.362965000
1	2.498884000	-1.232734000	1.173851000
7	0.577706000	2.677717000	1.267189000
15	0.892305000	-1.864094000	-0.897095000
17	0.627895000	1.305062000	-1.793943000
7	-1.607137000	-0.622688000	-1.038997000
6	1.825019000	-1.805715000	-2.492911000
6	1.079208000	-4.048024000	0.896488000
1	0.045166000	-3.811418000	1.135067000
6	-1.711866000	-1.926794000	-1.411298000
6	2.905692000	-0.913849000	-2.608689000
1	3.129007000	-0.225893000	-1.796430000
6	1.766650000	-3.267300000	-0.053531000
6	-3.978345000	-1.640881000	-2.181857000
1	-4.902182000	-2.045694000	-2.594299000
6	3.117534000	-3.560331000	-0.319817000
1	3.667938000	-2.983313000	-1.060120000
6	-3.839630000	-0.274465000	-1.916036000
1	-4.633603000	-0.437813000	-2.129477000
6	2.275278000	-2.595223000	-4.749976000
1	2.017092000	-3.245768000	-5.586145000
6	-2.893932000	-2.473768000	-1.944838000
1	-2.931922000	-3.534926000	-2.186435000
6	3.762850000	-4.606353000	0.345513000
1	4.807792000	-4.821404000	0.119935000
6	3.071416000	-5.379160000	1.282556000
1	3.575286000	-6.197208000	1.798198000
6	3.673696000	-0.881589000	-3.775868000
1	4.506233000	-0.181756000	-3.852027000
6	1.515532000	-2.640955000	-3.577905000
1	0.671509000	-3.327000000	-3.521726000
6	1.729408000	-5.096741000	1.552380000
1	1.181013000	-5.690096000	2.284569000
6	3.360761000	-1.720118000	-4.849210000
1	3.953556000	-1.684920000	-5.763621000
6	-2.647922000	0.177079000	-1.362395000
1	-2.498239000	1.233159000	-1.174268000
7	-0.577271000	-2.677391000	-1.267268000
1	0.614185000	3.657005000	1.510355000
1	-0.613773000	-3.656685000	-1.510406000S

Isomer B^{HS}

26	-0.221509000	0.116599000	0.011838000
15	-1.373177000	2.114377000	1.050467000
17	-0.161343000	1.121371000	-2.078515000
7	-0.263247000	-0.335374000	2.356200000
6	-3.082336000	2.636433000	0.603523000
6	0.085365000	4.104361000	2.486912000
1	0.079904000	3.409772000	3.326326000
6	-1.091028000	0.368799000	3.151028000
6	-3.737873000	1.985999000	-0.454439000
1	-3.230266000	1.188841000	-0.992161000
6	-0.566730000	3.755374000	1.292237000
6	-0.945492000	-1.289610000	4.893558000
1	-1.219007000	-1.655273000	5.883449000
6	-0.549233000	4.666468000	0.218860000
1	-1.043228000	4.414194000	-0.718910000
6	-0.091955000	-2.029933000	4.066614000
1	0.323233000	-2.985694000	4.378263000
6	-5.051514000	4.021044000	0.954978000
1	-5.557241000	4.817980000	1.501243000
6	-1.453343000	-0.081625000	4.439522000
1	-2.128175000	0.511200000	5.056054000
6	0.093268000	5.899215000	0.348256000
1	0.091642000	6.596149000	-0.490358000
6	0.733793000	6.242015000	1.543807000
1	1.233310000	7.205937000	1.642070000
6	-5.041607000	2.355539000	-0.800795000
1	-5.540615000	1.844631000	-1.624356000
6	-3.745791000	3.665840000	1.298851000
1	-3.238747000	4.209688000	2.096698000
6	0.728511000	5.340393000	2.611046000
1	1.221799000	5.599400000	3.548750000
6	-5.701612000	3.365392000	-0.096759000
1	-6.719244000	3.647743000	-0.368563000
6	0.205729000	-1.509050000	2.813229000
1	0.845793000	-2.054561000	2.122831000
7	-1.570941000	1.573824000	2.681617000
15	2.411050000	0.609954000	0.306556000
17	-2.228255000	-1.157139000	0.113265000
7	0.980831000	-1.757735000	-0.899118000
6	3.418753000	2.037219000	-0.296433000
6	3.966279000	-1.020846000	2.066371000
1	4.025305000	-1.737074000	1.247753000
6	2.253955000	-1.623853000	-1.315556000
6	2.841783000	2.936449000	-1.210585000
1	1.809289000	2.795136000	-1.523559000
6	3.286739000	0.194028000	1.880413000
6	2.078004000	-3.558929000	-2.737422000
1	2.510955000	-4.250894000	-3.460432000
6	3.219191000	1.102493000	2.953663000
1	2.698968000	2.051828000	2.831730000
6	0.759972000	-3.715250000	-2.293546000
1	0.127388000	-4.525335000	-2.650102000
6	5.507486000	3.280251000	-0.429329000
1	6.544942000	3.410776000	-0.119563000
6	2.839075000	-2.505988000	-2.250052000
1	3.867486000	-2.355674000	-2.577036000
6	3.830231000	0.806658000	4.173636000
1	3.775853000	1.525414000	4.991869000
6	4.507447000	-0.405280000	4.348497000
1	4.980877000	-0.636227000	5.302906000
6	3.596440000	3.993256000	-1.727056000
1	3.136170000	4.682472000	-2.435403000
6	4.760032000	2.220492000	0.091125000
1	5.221461000	1.542894000	0.807900000
6	4.571743000	-1.317197000	3.292155000
1	5.098065000	-2.264117000	3.417668000
6	4.927524000	4.169545000	-1.339159000
1	5.511531000	4.997499000	-1.742317000
6	0.260514000	-2.785239000	-1.387773000
1	-0.768388000	-2.822972000	-1.029341000
7	3.005145000	-0.598313000	-0.777991000
1	-2.281363000	2.008839000	3.255783000
1	3.929237000	-0.474489000	-1.170363000

BLS

26	-0.035512000	0.165898000	0.260376000
15	-1.011254000	1.903510000	1.070342000
17	-0.154401000	1.028451000	-1.892286000
7	-0.133462000	-0.575961000	2.079364000
6	-2.660762000	2.578275000	0.558399000
6	0.127281000	4.031764000	2.628210000
1	-0.079084000	3.426196000	3.510435000
6	-0.871385000	0.083689000	3.015348000
6	-3.217496000	2.291197000	-0.696696000
1	-2.689385000	1.625274000	-1.373310000
6	-0.180666000	3.534320000	1.351300000
6	-0.669723000	-1.739363000	4.585339000
1	-0.890228000	-2.187728000	5.553612000
6	0.087957000	4.335599000	0.226369000
1	-0.136033000	3.959404000	-0.770640000
6	0.111096000	-2.410285000	3.638298000
1	0.527920000	-3.396369000	3.831080000
6	-4.578787000	3.991924000	1.063627000
1	-5.099223000	4.657983000	1.752556000
6	-1.157726000	-0.478237000	4.273261000
1	-1.758908000	0.084928000	4.985450000
6	0.646190000	5.605368000	0.381741000
1	0.851265000	6.212576000	-0.500063000
6	0.944602000	6.096675000	1.657134000
1	1.376029000	7.091005000	1.775064000
6	-4.443238000	2.854852000	-1.063431000
1	-4.863421000	2.622796000	-2.042381000
6	-3.343175000	3.450777000	1.426717000
1	-2.908617000	3.743543000	2.383142000
6	0.686696000	5.305653000	2.779144000
1	0.914079000	5.680052000	3.778134000
6	-5.132499000	3.694633000	-0.185104000
1	-6.092862000	4.123375000	-0.473240000
6	0.347238000	-1.792519000	2.418219000
1	0.936847000	-2.284109000	1.652390000
7	-1.296861000	1.348452000	2.687931000
15	2.070236000	0.672909000	0.327368000
17	-2.235634000	-0.654714000	0.141793000
7	0.678456000	-1.572266000	-0.672460000
6	3.007935000	2.121520000	-0.357389000
6	4.010468000	-0.608265000	1.992839000
1	4.274692000	-1.194507000	1.114330000
6	1.950568000	-1.568741000	-1.141520000
6	2.959451000	2.360934000	-1.745089000
1	2.326526000	1.738189000	-2.373633000
6	2.994459000	0.358574000	1.909208000
6	1.615441000	-3.631510000	-2.337072000
1	1.981716000	-4.422737000	-2.991427000
6	2.663629000	1.081421000	3.069448000
1	1.874214000	1.827907000	3.037019000
6	0.309367000	-3.655336000	-1.836666000
1	-0.384484000	-4.456629000	-2.081671000
6	4.534151000	4.003251000	-0.124142000
1	5.149111000	4.636466000	0.515959000
6	2.450771000	-2.581147000	-1.983303000
1	3.478245000	-2.529165000	-2.340265000
6	3.341096000	0.856602000	4.270656000
1	3.070995000	1.432053000	5.156723000
6	4.352964000	-0.105290000	4.339897000
1	4.877555000	-0.284984000	5.278500000
6	3.694282000	3.407476000	-2.307540000
1	3.643639000	3.577226000	-3.383576000
6	3.803495000	2.956421000	0.445306000
1	3.870299000	2.789769000	1.517301000
6	4.681830000	-0.839133000	3.197320000
1	5.465372000	-1.596513000	3.239710000
6	4.484475000	4.232107000	-1.501239000
1	5.059542000	5.046130000	-1.943746000
6	-0.109215000	-2.611033000	-1.020623000
1	-1.123789000	-2.552177000	-0.629462000
7	2.736766000	-0.527398000	-0.727391000
1	-2.050710000	1.723123000	3.247950000
1	3.638404000	-0.404025000	-1.166415000

CHS

26	0.106463000	-0.288242000	0.084175000
15	1.958030000	0.529729000	1.673156000
17	-0.840191000	-2.032488000	1.321406000
7	-0.948360000	1.190514000	1.662845000
6	3.517391000	1.242023000	1.014972000
6	3.498737000	0.326648000	4.074979000
1	3.964944000	1.270578000	3.791542000
6	-0.200900000	2.079472000	2.341978000
6	3.581382000	2.551333000	0.509273000
1	2.694564000	3.180721000	0.531712000
6	2.547878000	-0.279184000	3.229580000
6	-2.165949000	3.184140000	3.193971000
1	-2.632832000	3.971706000	3.785963000
6	1.985070000	-1.509892000	3.607828000
1	1.240458000	-1.982982000	2.969143000
6	-2.945970000	2.229730000	2.529216000
1	-4.032222000	2.233185000	2.590537000
6	5.838617000	0.907819000	0.360527000
1	6.714376000	0.260718000	0.303456000
6	-0.782666000	3.110972000	3.112779000
1	-0.151595000	3.826559000	3.639012000
6	2.366856000	-2.119843000	4.808010000
1	1.922400000	-3.075426000	5.087358000
6	3.306611000	-1.510673000	5.642376000
1	3.601784000	-1.987828000	6.577460000
6	4.768754000	3.035267000	-0.047488000
1	4.802901000	4.055149000	-0.431786000
6	4.657724000	0.420955000	0.924847000
1	4.629095000	-0.598747000	1.308133000
6	3.871927000	-0.284388000	5.273317000
1	4.609679000	0.194969000	5.917877000
6	5.900225000	2.218641000	-0.123030000
1	6.823776000	2.598943000	-0.560103000
6	-2.282834000	1.259539000	1.784024000
1	-2.832643000	0.477344000	1.262684000
7	1.172624000	1.952541000	2.274084000
15	1.099488000	-2.133408000	-1.400172000
17	0.586268000	1.629524000	-1.171656000
7	-1.547743000	-0.770636000	-1.581944000
6	2.178850000	-1.923381000	-2.887639000
6	0.956029000	-4.701928000	-0.189729000
1	-0.123610000	-4.617079000	-0.292048000
6	-1.501953000	-1.940116000	-2.245601000
6	2.543561000	-0.622704000	-3.274100000
1	2.216359000	0.228123000	-2.677872000
6	1.783684000	-3.668660000	-0.660491000
6	-3.661676000	-1.539870000	-3.237729000
1	-4.486555000	-1.852851000	-3.878285000
3	3.174829000	-3.769693000	-0.467277000
1	3.835569000	-2.979882000	-0.823664000
6	-3.690379000	-0.300394000	-2.586659000
1	-4.521752000	0.391105000	-2.706287000
6	3.357930000	-2.805158000	-4.826425000
1	3.676403000	-3.658165000	-5.426822000
6	-2.559698000	-2.368106000	-3.079212000
1	-2.501285000	-3.327596000	-3.592209000
6	3.723500000	-4.887363000	0.164961000
1	4.803389000	-4.951948000	0.301612000
6	2.894605000	-5.920431000	0.614098000
1	3.324191000	-6.794226000	1.104517000
6	3.310508000	-0.419630000	-4.426560000
1	3.587497000	0.595237000	-4.712968000
6	2.596245000	-3.014595000	-3.675408000
1	2.343060000	-4.033627000	-3.381985000
6	1.512202000	-5.822061000	0.434948000
1	0.856145000	-6.616904000	0.791049000
6	3.717400000	-1.506048000	-5.204238000
1	4.315037000	-1.345120000	-6.102130000
6	-2.607629000	0.028874000	-1.777260000
1	-2.562527000	0.987550000	-1.262842000
7	-0.374110000	-2.722975000	-2.097025000
1	-0.330319000	-3.528852000	-2.708103000
1	1.688558000	2.561712000	2.896473000

CLS

26	0.180066000	-0.186030000	0.222336000
15	1.995186000	0.303025000	1.333593000
17	-0.475105000	-1.329971000	2.134009000
7	-0.498081000	1.523025000	1.113628000
6	3.428226000	1.339613000	0.758241000
6	2.457726000	-1.247776000	3.677025000
1	1.529750000	-0.819325000	4.047172000
6	0.149071000	1.988838000	2.212569000
6	3.581823000	1.672321000	-0.595629000
1	2.851566000	1.315984000	-1.317404000
6	2.915722000	-0.897499000	2.395156000
6	-1.417397000	3.803730000	2.464557000
1	-1.785152000	4.674117000	3.007863000
6	4.104059000	-1.477897000	1.916416000
1	4.493221000	-1.198393000	0.939078000
6	-2.019053000	3.393235000	1.269473000
1	-2.853271000	3.935456000	0.829828000
6	5.417070000	2.651154000	1.276557000
1	6.131367000	3.025100000	2.010963000
6	-0.313319000	3.107075000	2.935194000
1	0.213369000	3.423470000	3.834073000
6	4.812904000	-2.394479000	2.697010000
1	5.733108000	-2.833396000	2.310325000
6	4.352601000	-2.735329000	3.972214000
1	4.909462000	-3.445194000	4.584538000
6	4.645410000	2.483851000	-1.007279000
1	4.749037000	2.731453000	-2.064082000
6	4.364860000	1.833028000	1.689720000
1	4.293842000	1.561873000	2.743700000
6	3.177589000	-2.155873000	4.459388000
1	2.811088000	-2.413962000	5.453496000
6	5.560815000	2.978579000	-0.076835000
1	6.385529000	3.614539000	-0.400383000
6	-1.519590000	2.262438000	0.634494000
1	-1.928342000	1.921342000	-0.311607000
7	1.298776000	1.329308000	2.554893000
15	0.845656000	-1.823887000	-1.059375000
17	0.408336000	1.151067000	-1.662620000
7	-1.652513000	-0.732858000	-0.493797000
6	2.220814000	-1.686719000	-2.287142000
6	1.166730000	-4.596413000	-1.594048000
1	1.198897000	-4.312592000	-2.646588000
6	-1.718363000	-1.471307000	-1.631034000
6	2.039613000	-1.048813000	-3.526635000
1	1.075526000	-0.605785000	-3.763693000
6	1.052152000	-3.611846000	-0.591223000
6	-4.128074000	-1.442576000	-1.606488000
1	-5.086986000	-1.699045000	-2.056739000
6	1.063067000	-4.011352000	0.753101000
1	0.954262000	-3.262040000	1.532719000
6	-4.064742000	-0.780641000	-0.375066000
1	-4.960470000	-0.520770000	0.184693000
6	4.538194000	-2.131574000	-2.890155000
1	5.508131000	-2.560593000	-2.636907000
6	-2.946286000	-1.806921000	-2.235631000
1	-2.951922000	-2.367157000	-3.169201000
6	1.179177000	-5.366014000	1.086055000
1	1.185726000	-5.658186000	2.136527000
6	1.278711000	-6.335502000	0.086752000
1	1.364089000	-7.390403000	0.349782000
6	3.096853000	-0.963599000	-4.437514000
1	2.938367000	-0.469368000	-5.396592000
6	3.481197000	-2.231279000	-1.981985000
1	3.635982000	-2.756005000	-1.041054000
6	1.271823000	-5.946672000	-1.257927000
1	1.357734000	-6.695083000	-2.046534000
6	4.348944000	-1.498727000	-4.122219000
1	5.171776000	-1.427500000	-4.834118000
6	-2.813351000	-0.459849000	0.137366000
1	-2.707382000	0.023060000	1.103927000
7	-0.520698000	-1.902445000	-2.134266000
1	-0.564788000	-2.590800000	-2.873983000
1	1.878063000	1.770987000	3.256449000

DHS

26	-0.100951000	-0.449981000	0.160593000
15	-1.180471000	2.262970000	1.194387000
17	0.465241000	-2.623219000	-0.413582000
7	-0.341249000	-0.476733000	2.401415000
6	-2.812824000	3.044101000	0.793857000
6	0.093546000	4.026849000	3.087238000
1	-0.118157000	3.281581000	3.853064000
6	-1.178746000	0.272060000	3.151272000
6	-3.544274000	2.601593000	-0.321033000
1	-3.160890000	1.781574000	-0.922987000
6	-0.292663000	3.788843000	1.758999000
6	-1.209851000	-1.391650000	4.905073000
1	-1.564020000	-1.742339000	5.874625000
6	0.025683000	4.752321000	0.781776000
1	-0.257317000	4.587388000	-0.258930000
6	-0.319793000	-2.158117000	4.143012000
1	0.046759000	-3.123981000	4.483061000
6	-4.584330000	4.644307000	1.284132000
1	-4.982249000	5.443211000	1.910791000
6	-1.640612000	-0.170643000	4.413081000
1	-2.328882000	0.451054000	4.984758000
6	0.681387000	5.933780000	1.132260000
1	0.907291000	6.674287000	0.364068000
6	1.038904000	6.172480000	2.464427000
1	1.543067000	7.099193000	2.739641000
6	-4.780746000	3.178715000	-0.627969000
1	-5.337581000	2.821282000	-1.494485000
6	-3.343138000	4.080459000	1.587329000
1	-2.778043000	4.468537000	2.434582000
6	0.748347000	5.213013000	3.437307000
1	1.031010000	5.384634000	4.476590000
6	-5.305852000	4.195539000	0.173172000
1	-6.272216000	4.639855000	-0.067233000
6	0.072795000	-1.658916000	2.908866000
1	0.726566000	-2.233870000	2.254568000
7	-1.576995000	1.511481000	2.703209000
15	2.588773000	0.233637000	0.374491000
17	-2.421934000	-0.670916000	-0.141822000
7	0.440433000	0.672115000	-1.672850000
6	3.319296000	1.171433000	1.775143000
6	3.842668000	-1.896480000	-0.965056000
1	2.824883000	-2.239473000	-1.148625000
6	1.571871000	1.376444000	-1.890386000
6	3.629733000	0.432945000	2.934582000
1	3.434166000	-0.638909000	2.968215000
6	4.058659000	-0.746440000	-0.184694000
6	0.867912000	1.943891000	-4.127780000
1	1.041395000	2.448257000	-5.078502000
6	5.380391000	-0.331609000	0.071836000
1	5.571987000	0.548645000	0.683614000
6	-0.285903000	1.179433000	-3.918656000
1	-1.041264000	1.056798000	-4.691744000
6	4.154662000	3.172277000	2.876535000
1	4.348055000	4.244502000	2.849932000
6	1.808081000	2.043364000	-3.110871000
1	2.725487000	2.614465000	-3.249609000
6	6.460005000	-1.052482000	-0.444252000
1	7.477761000	-0.721535000	-0.234203000
6	6.237614000	-2.194380000	-1.220780000
1	7.082154000	-2.758079000	-1.618449000
6	4.203745000	1.057053000	4.042721000
1	4.441236000	0.468405000	4.929114000
6	3.575642000	2.551368000	1.764698000
1	3.308445000	3.150358000	0.896455000
6	4.929144000	-2.611824000	-1.477818000
1	4.745305000	-3.505790000	-2.074337000
6	4.474237000	2.429569000	4.015178000
1	4.925740000	2.916961000	4.879493000
6	-0.453208000	0.571985000	-2.680253000
1	-1.336528000	-0.020981000	-2.444100000
7	2.510353000	1.443950000	-0.873486000
1	-2.304193000	1.939980000	3.261608000
1	3.392418000	1.844925000	-1.172364000

DLS

26	0.063134000	0.113429000	0.272110000
15	-0.812029000	1.904372000	1.156395000
17	0.602830000	-1.936953000	-0.690524000
7	-0.121452000	-0.674875000	2.106371000
6	-2.443960000	2.685127000	0.706471000
6	0.403958000	3.962147000	2.760850000
1	0.273049000	3.299773000	3.614385000
6	-0.781169000	0.029975000	3.061800000
6	-2.991096000	2.574740000	-0.579549000
1	-2.502191000	1.949503000	-1.317387000
6	0.040776000	3.526284000	1.477699000
6	-0.692181000	-1.819260000	4.607536000
1	-0.925235000	-2.259747000	5.576904000
6	0.244097000	4.395095000	0.389138000
1	-0.044868000	4.090752000	-0.615965000
6	0.002668000	-2.542087000	3.632175000
1	0.331264000	-3.565446000	3.800293000
6	-4.305161000	4.133276000	1.328629000
1	-4.807509000	4.743036000	2.080111000
6	-1.085155000	-0.519125000	4.322263000
1	-1.622955000	0.081744000	5.054107000
6	0.791978000	5.664219000	0.582300000
1	0.936424000	6.324579000	-0.273512000
6	1.137290000	6.094310000	1.867963000
1	1.553433000	7.090420000	2.020636000
6	-4.177344000	3.236854000	-0.908034000
1	-4.587132000	3.132982000	-1.913053000
6	-3.106034000	3.492431000	1.649412000
1	-2.682186000	3.661638000	2.639509000
6	0.942730000	5.238558000	2.954191000
1	1.213536000	5.560648000	3.960221000
6	-4.845763000	4.007540000	0.046140000
1	-5.778152000	4.512027000	-0.208161000
6	0.256348000	-1.937019000	2.407640000
1	0.750275000	-2.459322000	1.590329000
7	-1.107256000	1.328941000	2.758670000
15	2.160234000	0.598633000	0.402841000
17	-2.196309000	-0.501819000	0.090754000
7	0.221092000	0.811202000	-1.579637000
6	2.952023000	1.587101000	1.748907000
6	3.734078000	-1.126118000	-1.196463000
1	3.060615000	-0.842836000	-2.001108000
6	1.338742000	1.491001000	-1.949365000
6	2.788781000	1.160202000	3.079216000
1	2.128914000	0.326141000	3.305075000
6	3.540676000	-0.616882000	0.101726000
6	0.527718000	1.762290000	-4.203782000
1	0.643139000	2.151957000	-5.215043000
6	4.396698000	-1.052846000	1.126735000
1	4.282722000	-0.673998000	2.139557000
6	-0.579463000	0.984042000	-3.850555000
1	-1.350268000	0.722065000	-4.572263000
6	4.482104000	3.308885000	2.537707000
1	5.133958000	4.154932000	2.318593000
6	1.503698000	2.010949000	-3.246686000
1	2.399708000	2.581109000	-3.487630000
6	5.422270000	-1.965632000	0.861174000
1	6.075640000	-2.288131000	1.672414000
6	5.616672000	-2.450298000	-0.433798000
1	6.420332000	-3.157163000	-0.641647000
6	3.475279000	1.790546000	4.121476000
1	3.340066000	1.438340000	5.144637000
6	3.803289000	2.675071000	1.494367000
1	3.932224000	3.051174000	0.481746000
6	4.769256000	-2.024993000	-1.460979000
1	4.900330000	-2.406613000	-2.473815000
6	4.328190000	2.864249000	3.853822000
1	4.865542000	3.355402000	4.665324000
6	-0.685264000	0.527634000	-2.542137000
1	-1.513696000	-0.090072000	-2.200252000
7	2.316289000	1.629518000	-0.986617000
1	-1.794764000	1.764516000	3.357612000
1	3.233315000	1.868617000	-1.343554000

EHS

26	-0.374441000	0.189600000	0.398614000
15	-1.198304000	-1.161022000	2.410064000
17	1.317179000	-1.280515000	-0.028616000
7	-0.696073000	1.731888000	2.033510000
6	0.043986000	-1.788749000	3.615879000
6	-3.367905000	-2.623039000	1.413166000
1	-3.192311000	-2.057123000	0.500008000
6	-1.619973000	1.480424000	2.988462000
6	0.779936000	-2.938249000	3.272734000
1	0.593913000	-3.443786000	2.326367000
6	-2.549870000	-2.404260000	2.536299000
6	-1.824749000	3.825289000	3.506168000
1	-2.281873000	4.637172000	4.072399000
6	-2.785745000	-3.137740000	3.714312000
1	-2.143938000	-2.997987000	4.583474000
6	-0.828854000	4.085084000	2.556187000
1	-0.474724000	5.093496000	2.355023000
6	1.325954000	-1.618538000	5.675942000
1	1.539031000	-1.095674000	6.608930000
6	-2.224445000	2.517142000	3.733344000
1	-2.985970000	2.281453000	4.475706000
6	-3.830355000	-4.063927000	3.769345000
1	-4.003521000	-4.628188000	4.686271000
6	-4.643629000	-4.273195000	2.650820000
1	-5.454140000	-5.001316000	2.694232000
6	1.764673000	-3.426700000	4.132925000
1	2.326688000	-4.318200000	3.854018000
6	0.333570000	-1.128842000	4.820961000
1	-0.214025000	-0.227881000	5.093607000
6	-4.409714000	-3.552661000	1.476063000
1	-5.037091000	-3.714632000	0.599329000
6	2.040865000	-2.769905000	5.336893000
1	2.815698000	-3.149963000	6.002987000
6	-0.309361000	3.009830000	1.845744000
1	0.462706000	3.148994000	1.092752000
7	-1.937122000	0.166677000	3.241298000
15	0.646510000	1.718868000	-1.637496000
17	-2.476461000	0.416404000	-0.514047000
7	2.783374000	2.411361000	0.369267000
6	0.296403000	1.010472000	-3.308402000
6	1.093054000	4.517869000	-2.022938000
1	2.155006000	4.280993000	-2.045493000
6	3.269446000	1.886319000	-0.765884000
6	-0.062111000	-0.344026000	-3.417942000
1	-0.166261000	-0.950708000	-2.521370000
6	0.154014000	3.485298000	-1.866820000
6	5.481699000	1.703584000	0.158745000
1	6.531457000	1.421958000	0.071038000
6	-1.216625000	3.804903000	-1.830333000
1	-1.955102000	3.016509000	-1.689132000
6	4.984239000	2.242453000	1.353030000
1	5.623464000	2.398892000	2.219742000
6	0.205154000	1.205730000	-5.732222000
1	0.304527000	1.815473000	-6.630891000
6	4.625282000	1.515016000	-0.917213000
1	4.983325000	1.081361000	-1.850446000
6	-1.632689000	5.131152000	-1.969004000
1	-2.697813000	5.363975000	-1.946774000
6	-0.692749000	6.154976000	-2.129225000
1	-1.021073000	7.189693000	-2.232422000
6	-0.279676000	-0.914898000	-4.675238000
1	-0.559232000	-1.966326000	-4.745071000
6	0.423225000	1.782169000	-4.478364000
1	0.682351000	2.837595000	-4.409606000
6	0.669861000	5.844487000	-2.152702000
1	1.410122000	6.636306000	-2.274430000
6	-0.146246000	-0.144084000	-5.833278000
1	-0.320709000	-0.591572000	-6.812306000
6	3.630122000	2.567623000	1.395479000
1	3.191027000	2.985096000	2.305290000
7	2.381692000	1.764783000	-1.817153000
1	-2.667040000	-0.002777000	3.920248000
1	2.735275000	1.299123000	-2.642281000

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26	-0.084270000	0.684453000	0.570937000
15	-0.654327000	-0.604499000	2.251979000
17	0.610538000	-1.345376000	-0.384353000
7	-0.665622000	2.176794000	1.728281000
6	0.546620000	-1.415196000	3.416962000
6	-3.304013000	-1.595048000	2.247080000
1	-3.609336000	-0.557208000	2.355495000
6	-1.321836000	1.897672000	2.893244000
6	1.649985000	-2.111349000	2.890504000
1	1.795271000	-2.137399000	1.811147000
6	-1.940676000	-1.917792000	2.137131000
6	-1.636416000	4.240616000	3.392606000
1	-2.026872000	5.031261000	4.032650000
6	-1.571474000	-3.257998000	1.933365000
1	-0.523924000	-3.528520000	1.830815000
6	-0.921775000	4.536304000	2.227560000
1	-0.727741000	5.559405000	1.913342000
6	1.299261000	-1.993023000	5.661107000
1	1.157788000	-1.939371000	6.741132000
6	-1.830661000	2.908200000	3.730414000
1	-2.358315000	2.630067000	4.641601000
6	-2.546710000	-4.254403000	1.854087000
1	-2.243524000	-5.289092000	1.692669000
6	-3.900161000	-3.929846000	1.983034000
1	-4.659345000	-4.710419000	1.925841000
6	2.556155000	-2.749899000	3.742629000
1	3.404456000	-3.286488000	3.316369000
6	0.385655000	-1.361536000	4.812976000
1	-0.451006000	-0.823553000	5.256588000
6	-4.274461000	-2.598127000	2.178407000
1	-5.328064000	-2.330828000	2.264011000
6	2.385199000	-2.694409000	5.128351000
1	3.094958000	-3.190355000	5.791043000
6	-0.468286000	3.483904000	1.443510000
1	0.067014000	3.678870000	0.522586000
7	-1.441805000	0.573391000	3.234252000
15	0.340754000	1.550451000	-1.417039000
17	-2.305524000	0.543686000	-0.134460000
7	1.817373000	1.087560000	0.939390000
6	0.009344000	0.718259000	-3.033863000
6	0.977274000	4.296218000	-1.972984000
1	2.008952000	4.050231000	-1.722703000
6	2.656010000	1.335814000	-0.110996000
6	-0.866175000	-0.371754000	-3.146326000
1	-1.369656000	-0.745000000	-2.259377000
6	-0.011123000	3.297673000	-1.929917000
6	4.588214000	1.437620000	1.335309000
1	5.663263000	1.542859000	1.478398000
6	-1.341798000	3.643937000	-2.235237000
1	-2.122581000	2.886293000	-2.185769000
6	3.721990000	1.299556000	2.425510000
1	4.082344000	1.297582000	3.451713000
6	0.436374000	0.601905000	-5.428871000
1	0.940584000	0.991499000	-6.313757000
6	4.047411000	1.467379000	0.056887000
1	4.677484000	1.621417000	-0.817865000
6	-1.665783000	4.955007000	-2.588630000
1	-2.700204000	5.207451000	-2.823714000
6	-0.673592000	5.940591000	-2.642335000
1	-0.930069000	6.962587000	-2.922495000
6	-1.084755000	-0.964867000	-4.393612000
1	-1.769517000	-1.810005000	-4.467618000
6	0.645052000	1.211044000	-4.189551000
1	1.288431000	2.090198000	-4.138892000
6	0.647355000	5.608042000	-2.331344000
1	1.427644000	6.369315000	-2.638622000
6	-0.430895000	-0.489914000	-5.533081000
1	-0.601678000	-0.961351000	-6.501509000
6	2.367361000	1.125983000	2.175379000
1	1.671918000	0.983849000	2.995471000
7	2.067222000	1.513555000	-1.335279000
1	-2.012414000	0.352776000	4.038401000
1	2.664033000	1.514359000	-2.150395000

