

Supporting Information

Hydrogenation of Carbon Dioxide Catalyzed by PNP Pincer Iridium, Iron and Cobalt Complexes: A Computational Design of Base Metal Catalysts

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1. Complete citation for reference 30

Gaussian 09, Revision A.02, suite of programs for *ab initio* calculation; Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian, Inc.*, Wallingford CT, **2009**.

2. Evaluation of the solvent corrections for the reaction $\text{CO}_2 + \text{H}_2 + \text{OH}^- \rightarrow \text{HCOO}^- + \text{H}_2\text{O}$

Table S1. Experimental and calculated enthalpies and free energies at 298.15 K in kcal mol⁻¹.

	Reactants			Products		$\Delta H^\circ_{\text{Rxn}} / \Delta G^\circ_{\text{Rxn}}$
	H ₂ (1atm)	CO ₂ (1atm)	OH ⁻ (1M)	H ₂ O (Liq.)	HCOO ⁻ (1M)	
ΔH°_f	0.0	-94.1	-55.0	-68.3	-100.7	-19.9
$\Delta H^\circ_{\text{Bondi}}$						-35.2
$\Delta H^\circ_{\text{UAKS}}$						-18.9
ΔG°_f	0.0	-94.3	-37.6	-56.7	-83.9	-8.7
$\Delta G^\circ_{\text{Bondi}}$						-29.2
$\Delta G^\circ_{\text{UAKS}}$						-12.8

ΔH°_f : Standard molar enthalpy of formation, values from the NBS tables of chemical thermodynamic properties.

ΔG°_f : Standard molar Gibbs energy of formation, values from the NBS tables of chemical thermodynamic properties.

$\Delta H^\circ_{\text{Bondi}}$: Calculated enthalpy of reaction with solvent (water) effect correction using the IEFPCM and the Bondi atomic radii.

$\Delta H^\circ_{\text{UAKS}}$: Calculated enthalpy of reaction with solvent (water) effect correction using the IEFPCM and the UAKS radii.

$\Delta G^\circ_{\text{Bondi}}$: Calculated free energy of reaction with solvent (water) effect correction using the IEFPCM and the Bondi atomic radii.

$\Delta G^\circ_{\text{UAKS}}$: Calculated free energy of reaction with solvent (water) effect correction using the IEFPCM and the UAKS radii.

Comparing the values of experimental and calculated $\Delta H^\circ_{\text{Rxn}}$ and $\Delta G^\circ_{\text{Rxn}}$ listed in Table S1, the UAKS radii have much better description for the solvation of the ions than the Bondi atomic radii. The calculated $\Delta H^\circ_{\text{Rxn}}$ using the UAKS radii is only 1.0 kcal mol⁻¹ higher than the experimental $\Delta H^\circ_{\text{Rxn}}$ of the reaction obtained from the NBS tables of chemical thermodynamic properties. Therefore, the catalytic mechanisms were analyzed based on the relative enthalpies with solvent effect corrections using the UAKS radii.

3. Cartesian coordinates (angstrom) of all optimized intermediate and transition state structures.

1-Ir

Ir	0.00000000	0.56061500	-0.00000100
P	2.28164900	0.24823600	-0.12182200
N	0.00000000	-1.62562300	0.00000000
C	2.33927300	-1.50532800	-0.72465500
C	1.12695800	-2.30241500	-0.31460900
C	1.15714700	-3.69441100	-0.30933900
C	0.00000100	-4.39881600	0.00000000
C	3.27014700	1.13286700	-1.42496900
C	3.05965600	2.65000800	-1.41650000
C	4.75976700	0.77880000	-1.42397700
C	3.33546500	0.20086300	1.40724700
C	3.44743100	1.57672800	2.06961000
C	2.82002100	-0.83910700	2.40724400
H	3.56374100	3.09060000	-2.28422200
H	2.34848800	-1.44993600	-1.82117000
H	0.00000100	-5.48515700	0.00000100
H	2.07923000	-4.21008900	-0.55901400
H	4.93144600	-0.30323700	-1.42221600
H	3.48045800	3.11488400	-0.51866900
H	3.25679200	-2.02207200	-0.42493500
H	2.82149400	0.74713200	-2.35063700
H	4.33139200	-0.11518300	1.07136100
H	5.26844000	1.20792100	-0.55315300
H	5.23424800	1.19209300	-2.32104400
H	1.99798300	2.90837100	-1.47000500
H	3.93825200	2.30992400	1.42248400
H	1.81638300	-0.58094400	2.76269100
H	2.45691900	1.96397700	2.33763200
H	3.48853000	-0.86916300	3.27494200
H	4.03758900	1.49601100	2.98947000
H	2.78405300	-1.84767900	1.98141400
H	0.03458900	0.61834100	-1.67636100
H	0.00000000	2.16507000	-0.00000100
P	-2.28164900	0.24823500	0.12182200
C	-2.33927200	-1.50532900	0.72465400
C	-1.12695800	-2.30241500	0.31460900
C	-1.15714600	-3.69441200	0.30933900
C	-3.27014600	1.13286600	1.42497000
C	-3.05965400	2.65000800	1.41650100
C	-4.75976600	0.77879900	1.42398000
C	-3.33546700	0.20086300	-1.40724600
C	-3.44743500	1.57672900	-2.06960700
C	-2.82002300	-0.83910600	-2.40724400
H	-3.56373900	3.09059900	2.28422400
H	-2.34848800	-1.44993700	1.82117000
H	-2.07922900	-4.21008900	0.55901400
H	-4.93144500	-0.30323800	1.42221800
H	-3.48045500	3.11488400	0.51867000
H	-3.25679100	-2.02207300	0.42493400
H	-2.82149200	0.74713000	2.35063800
H	-4.33139400	-0.11518400	-1.07135800
H	-5.26843900	1.20792100	0.55315600
H	-5.23424500	1.19209200	2.32104700
H	-1.99798100	2.90837000	1.47000800
H	-3.93825600	2.30992300	-1.42248200
H	-1.81638700	-0.58094200	-2.76269300
H	-2.45692300	1.96397800	-2.33763000
H	-3.48853400	-0.86916300	-3.27494000

H	-4.03759200	1.49601100	-2.98946800
H	-2.78405300	-1.84767800	-1.98141500
H	-0.03458900	0.61834200	1.67635900

1-Fe

Fe	-0.00002400	-0.45628300	0.00002000
P	2.20494200	-0.19899800	0.11336100
N	0.00000600	1.65175400	-0.00000600
C	2.33636800	1.54784600	0.69944400
C	1.12116300	2.34047600	0.30695900
C	1.15521000	3.73285500	0.30399800
C	0.00005500	4.44108100	-0.00006600
C	3.20458500	-1.07190300	1.42497000
C	2.98388600	-2.58603700	1.48447600
C	4.69939400	-0.73993800	1.38452000
C	3.26477000	-0.20252300	-1.41687400
C	3.32469200	-1.59244400	-2.05692000
C	2.78358200	0.83727500	-2.43422600
H	3.58014000	-3.00478500	2.30357300
H	2.38118600	1.51153000	1.79548600
H	0.00007500	5.52749600	-0.00008900
H	2.08116600	4.24367400	0.55001900
H	4.88833300	0.33779100	1.32988900
H	3.29514400	-3.08552300	0.56081100
H	3.25061300	2.04498700	0.35922500
H	2.78445600	-0.64910500	2.34766100
H	4.27332000	0.08367600	-1.09307500
H	5.18844700	-1.21666000	0.52714700
H	5.18193500	-1.11917500	2.29241200
H	1.93683500	-2.83597300	1.67191900
H	3.78791500	-2.33270200	-1.39720200
H	1.77726800	0.59947100	-2.79627500
H	2.31978200	-1.94723000	-2.31747700
H	3.46019100	0.84209100	-3.29648000
H	3.91561800	-1.55186200	-2.97921500
H	2.76706300	1.85154000	-2.02037400
H	0.06657400	-0.40336400	1.57021000
P	-2.20495600	-0.19892500	-0.11333400
C	-2.33634300	1.54789600	-0.69948900
C	-1.12112300	2.34050500	-0.30701000
C	-1.15512300	3.73288400	-0.30410800
C	-3.20453100	-1.07193000	-1.42491700
C	-2.98375200	-2.58606000	-1.48424700
C	-4.69935700	-0.74001200	-1.38458200
C	-3.26479400	-0.20239000	1.41689600
C	-3.32478600	-1.59231400	2.05692700
C	-2.78355300	0.83737200	2.43426000
H	-3.57983700	-3.00491800	-2.30341000
H	-2.38114400	1.51154000	-1.79553000
H	-2.08105900	4.24372600	-0.55015800
H	-4.88833700	0.33771300	-1.33002400
H	-3.29514700	-3.08547200	-0.56058600
H	-3.25058000	2.04507200	-0.35930200
H	-2.78435600	-0.64920300	-2.34762000
H	-4.27332800	0.08386200	1.09309900
H	-5.18845300	-1.21670600	-0.52721900
H	-5.18182300	-1.11931500	-2.29248500
H	-1.93664600	-2.83595600	-1.67147000
H	-3.78801600	-2.33254800	1.39718500

H	-1.77725300	0.59951200	2.79630900
H	-2.31989600	-1.94713900	2.31750700
H	-3.46016300	0.84221400	3.29651200
H	-3.91573700	-1.55172000	2.97920600
H	-2.76698000	1.85164100	2.02042000
H	-0.06662500	-0.40341000	-1.57017400
C	-0.00014900	-2.17677200	0.00010600
O	-0.00013000	-3.34625800	-0.00025300

1-Co

Co	0.00000000	0.53607800	0.00000000
P	2.16624300	0.37141500	-0.13048900
N	0.00000100	-1.49966500	0.00000000
C	2.31228900	-1.36446200	-0.75818800
C	1.11563600	-2.17874900	-0.34122300
C	1.14817700	-3.57076500	-0.34158000
C	0.00000100	-4.27560400	-0.00000300
C	3.10000100	1.32887300	-1.42288700
C	2.82516400	2.83532200	-1.38596600
C	4.60381200	1.04136200	-1.44073600
C	3.24175200	0.35161500	1.38654300
C	3.30110200	1.72392200	2.06319000
C	2.77763800	-0.71704400	2.38169000
H	3.30294600	3.31262900	-2.24925700
H	2.32186600	-1.30382700	-1.85419000
H	0.00000100	-5.36206300	-0.00000400
H	2.06431000	-4.08485700	-0.61571700
H	4.82197200	-0.03209800	-1.46117400
H	3.23338200	3.30193300	-0.48319200
H	3.24289700	-1.85545300	-0.45530600
H	2.66207600	0.94022900	-2.35234200
H	4.24792300	0.08070900	1.04156100
H	5.10115200	1.47485700	-0.56549500
H	5.05278400	1.49228700	-2.33298000
H	1.75343500	3.05063500	-1.42596300
H	3.75906800	2.48316300	1.42200900
H	1.76979700	-0.49847900	2.75213600
H	2.29694900	2.06846600	2.33910700
H	3.45723300	-0.73259800	3.24131100
H	3.89763200	1.65864300	2.98034800
H	2.77193300	-1.72188100	1.94557200
H	0.05041500	0.60474800	-1.53479700
H	0.00000000	2.01781100	0.00000100
P	-2.16624300	0.37141300	0.13049000
C	-2.31228700	-1.36446400	0.75818700
C	-1.11563400	-2.17875000	0.34122100
C	-1.14817500	-3.57076600	0.34157600
C	-3.10000100	1.32887000	1.42288800
C	-2.82516900	2.83532000	1.38596400
C	-4.60381100	1.04135400	1.44074000
C	-3.24175200	0.35161500	-1.38654200
C	-3.30110500	1.72392400	-2.06318500
C	-2.77763500	-0.71704000	-2.38169300
H	-3.30295300	3.31262700	2.24925500
H	-2.32186500	-1.30383000	1.85418900
H	-2.06430700	-4.08485800	0.61571100
H	-4.82196800	-0.03210600	1.46118000
H	-3.23339000	3.30192800	0.48319000
H	-3.24289600	-1.85545500	0.45530400
H	-2.66207500	0.94022800	2.35234300
H	-4.24792200	0.08070600	-1.04156100
H	-5.10115400	1.47484700	0.56549800

H	-5.05278400	1.49227900	2.33298300
H	-1.75344100	3.05063600	1.42596000
H	-3.75907100	2.48316200	-1.42200100
H	-1.76979500	-0.49847200	-2.75213700
H	-2.29695300	2.06847100	-2.33910200
H	-3.45723000	-0.73259200	-3.24131400
H	-3.89763600	1.65864800	-2.98034200
H	-2.77192800	-1.72187800	-1.94557800
H	-0.05041500	0.60474700	1.53479800

2-Ir

Ir	-0.03226800	-0.49310000	-0.24100300
P	2.26629200	-0.11755100	-0.28508500
N	-0.06010000	1.66908600	0.05593400
C	2.32576300	1.49877000	0.62104700
C	1.06454400	2.30898200	0.44784000
C	1.05569600	3.67574000	0.71308000
C	-0.13215500	4.38464600	0.58517100
C	3.44122000	-1.16991100	0.69336400
C	3.25625600	-2.66911800	0.43838500
C	4.90679700	-0.75223100	0.54268000
C	3.05542600	0.25274000	-1.91896200
C	3.12388900	-0.98544400	-2.81722100
C	2.33829600	1.40296000	-2.63322200
H	3.89194900	-3.23314500	1.13006400
H	2.42228600	1.24416300	1.68444500
H	-0.16225100	5.44895100	0.80069700
H	1.97229500	4.16641700	1.02477700
H	5.05560800	0.31897000	0.71642500
H	3.54557500	-2.94745100	-0.58042600
H	3.20156700	2.09732700	0.34962300
H	3.12793000	-0.97175900	1.72765300
H	4.07626200	0.58027200	-1.68368700
H	5.28564600	-0.99391800	-0.45697600
H	5.51728300	-1.29862000	1.26993100
H	2.21929400	-2.97940300	0.59782800
H	3.73804700	-1.77980600	-2.38286200
H	1.30568000	1.13284500	-2.88074600
H	2.12215900	-1.38916000	-3.00615900
H	2.86272200	1.62706200	-3.56852600
H	3.56528900	-0.71197900	-3.78203800
H	2.31953700	2.32048500	-2.03566700
H	-0.19963500	-0.86849800	1.87196800
H	-0.01208500	-2.08377300	-0.43932800
P	-2.33116700	-0.20427600	-0.36009300
C	-2.40230700	1.62099700	-0.67032800
C	-1.21303000	2.35808600	-0.10843000
C	-1.27984800	3.71965600	0.16805300
C	-3.24100300	-0.88269900	-1.82626000
C	-3.07973400	-2.39528900	-2.00041100
C	-4.71488900	-0.47033700	-1.87189300
C	-3.38886500	-0.44803100	1.14303600
C	-3.33004600	-1.89341600	1.64733500
C	-3.00061200	0.53154400	2.25656600
H	-3.50564400	-2.69394500	-2.96470100
H	-2.38124000	1.74413800	-1.76114200
H	-2.21999900	4.24694200	0.04086200
H	-4.85126800	0.60792600	-1.73565200
H	-3.61001000	-2.94998800	-1.21923800
H	-3.33657300	2.06948300	-0.31949300
H	-2.71671600	-0.39620400	-2.66033100

H	-4.41573800	-0.21994900	0.83043900
H	-5.29480400	-0.98955700	-1.10065900
H	-5.13934100	-0.74231300	-2.84452200
H	-2.02797600	-2.69615300	-1.98277900
H	-3.67697700	-2.61085700	0.89801800
H	-1.95865900	0.39733100	2.56661500
H	-2.30763800	-2.16669700	1.93408500
H	-3.63447100	0.35002200	3.13153100
H	-3.96804500	-1.99838000	2.53184700
H	-3.13751200	1.57614100	1.95989500
H	-0.06632400	-0.41855800	-1.78229100
C	0.41797600	-0.97085300	2.82862600
O	0.68495700	0.09902500	3.41732200
O	0.69654400	-2.14610200	3.14932100

2-Fe

Fe	-0.02113200	-0.42651900	-0.16045900
P	-2.25725600	-0.23489100	-0.33451200
N	-0.05450600	1.64098400	-0.11268700
C	-2.34849800	1.50434500	-0.93237700
C	-1.19680900	2.30938500	-0.40200200
C	-1.28775100	3.69145200	-0.28293300
C	-0.16759700	4.41422600	0.10990400
C	-3.16219200	-1.15700100	-1.66939100
C	-3.36530900	-2.64447100	-1.36099700
C	-4.49702100	-0.51379300	-2.06067500
C	-3.33700100	-0.28075900	1.17818200
C	-3.14493500	-1.58117100	1.96882600
C	-3.08747000	0.93217800	2.08280700
H	-3.69492200	-3.15665100	-2.27147700
H	-2.24448600	1.45676200	-2.02455500
H	-0.21463100	5.49508500	0.20784900
H	-2.22622700	4.18639700	-0.51163500
H	-4.38645800	0.52569300	-2.38261600
H	-4.14584400	-2.78519700	-0.60557600
H	-3.30525300	1.98903100	-0.71910500
H	-2.47318200	-1.07428700	-2.52061100
H	-4.37311500	-0.23511400	0.81789200
H	-5.21356700	-0.54337600	-1.23209400
H	-4.93463600	-1.07503700	-2.89400300
H	-2.45334200	-3.13553700	-1.01007400
H	-3.31984800	-2.47479600	1.36422900
H	-2.04090500	0.98480800	2.40540000
H	-2.13118300	-1.64545300	2.37872600
H	-3.70780300	0.84505800	2.98178700
H	-3.84743200	-1.60200300	2.80954600
H	-3.34308500	1.87750000	1.59452200
H	-0.06277700	-0.42248000	-1.64760100
P	2.20987400	-0.10208600	-0.24269400
C	2.31853300	1.58677400	0.48938800
C	1.04604400	2.34731000	0.23496100
C	1.01731800	3.73430100	0.35478900
C	3.41380300	-1.05165000	0.81127300
C	3.24644100	-2.57219900	0.73333700
C	4.87161400	-0.64432000	0.57522400
C	2.97953700	0.08320500	-1.92034700
C	2.97235000	-1.23682000	-2.69681400
C	2.30292000	1.19267100	-2.73223400
H	3.95705000	-3.04578900	1.42013200
H	2.43951200	1.45776100	1.57153900
H	1.92196900	4.26268200	0.63870500

H	5.01492000	0.44093200	0.61399100
H	3.45016000	-2.95681900	-0.27154800
H	3.18208500	2.15236400	0.12479900
H	3.13275000	-0.74350000	1.82748200
H	4.01899400	0.38317300	-1.73741000
H	5.22982800	-1.00363700	-0.39617400
H	5.50329700	-1.09443500	1.34888600
H	2.24099000	-2.88616300	1.02546300
H	3.55518800	-2.01557800	-2.19604900
H	1.25136800	0.95562700	-2.92732100
H	1.94914000	-1.60648700	-2.83332900
H	2.81300300	1.29154100	-3.69685400
H	3.40914000	-1.07923500	-3.68924500
H	2.34983600	2.16562000	-2.23185100
H	-0.24925100	-0.46228200	1.71925500
C	0.03147500	-2.15674100	-0.35053000
O	0.07147200	-3.29587600	-0.56407500
C	0.37370200	-0.52837500	2.68038200
O	0.66960200	0.56772000	3.19788900
O	0.59836400	-1.68936800	3.07907700

2-Co

Co	-0.03718100	-0.45083200	-0.17051900
P	2.16007200	-0.24449000	-0.27316300
N	-0.04619600	1.55955500	-0.02285400
C	2.32763600	1.40400100	0.54901200
C	1.07516500	2.21840800	0.34552300
C	1.07487300	3.59795600	0.53079300
C	-0.10227400	4.30806000	0.33023100
C	3.29013700	-1.32533200	0.72566200
C	3.05557900	-2.82241200	0.49980700
C	4.76977000	-0.96305900	0.56975900
C	2.92682100	-0.00172000	-1.94222800
C	2.86850700	-1.27664100	-2.78878400
C	2.27968100	1.17076400	-2.68683000
H	3.63859500	-3.39199800	1.23215500
H	2.45029600	1.21168900	1.62204300
H	-0.12706000	5.38390500	0.47893200
H	1.99071900	4.09838800	0.82901200
H	4.95588900	0.10481200	0.72694500
H	3.37959900	-3.13671100	-0.49754900
H	3.20768000	1.96126200	0.21148400
H	2.98508500	-1.09572400	1.75550300
H	3.97722400	0.25315000	-1.75131600
H	5.14003200	-1.23402200	-0.42545000
H	5.35993800	-1.51932500	1.30631900
H	2.00189900	-3.09117700	0.61919200
H	3.42910500	-2.10085100	-2.33872200
H	1.21932600	0.97723100	-2.88443300
H	1.83209800	-1.60369900	-2.93379600
H	2.78420800	1.30522300	-3.64987000
H	3.30110900	-1.07807900	-3.77559600
H	2.36046500	2.11338800	-2.13562700
H	-0.25154400	-0.79545700	1.67406600
H	-0.02348300	-1.91882200	-0.31845200
P	-2.21622100	-0.31062200	-0.39359300
C	-2.35359700	1.48189100	-0.81963800
C	-1.18234800	2.25230700	-0.26758600
C	-1.24366900	3.62907100	-0.08202200
C	-3.01363600	-1.14594400	-1.84402700
C	-2.73370500	-2.64994800	-1.91715900

C	-4.51176500	-0.85322500	-1.96355700
C	-3.34084500	-0.50612200	1.06960300
C	-3.27859700	-1.92283400	1.64916100
C	-3.03835000	0.53952300	2.14934600
H	-3.11218700	-3.04000800	-2.86857100
H	-2.31254200	1.55025500	-1.91450100
H	-2.17332200	4.15527500	-0.27434000
H	-4.73417800	0.21760700	-1.90222000
H	-3.23860000	-3.19477000	-1.11279800
H	-3.30344900	1.92596500	-0.50743900
H	-2.49709000	-0.67207500	-2.68971400
H	-4.35479900	-0.32017600	0.69304800
H	-5.07857100	-1.36692300	-1.17897300
H	-4.87811100	-1.21775400	-2.92955600
H	-1.66311100	-2.86657200	-1.85940100
H	-3.58742500	-2.68125200	0.92391200
H	-2.01713800	0.44323600	2.53296200
H	-2.26482900	-2.16655100	1.98808000
H	-3.72547100	0.39458200	2.99032100
H	-3.94878100	-1.99392300	2.51303900
H	-3.17168700	1.56397600	1.78759200
H	-0.06654300	-0.45839800	-1.60349200
C	0.33868200	-0.87399800	2.65402200
O	0.60543900	0.20753600	3.21667200
O	0.57428300	-2.04477100	3.01657900

3-Ir

Ir	0.01706500	-0.53457800	-0.03666600
P	-2.29431900	-0.25637800	-0.09596800
N	-0.00924400	1.64016900	-0.02543400
C	-2.38624600	1.50905800	-0.65315200
C	-1.15610300	2.30696400	-0.29611000
C	-1.19843000	3.69795300	-0.28936000
C	-0.03702200	4.41258700	-0.02368700
C	-3.30356300	-1.12790700	-1.38698000
C	-3.07250100	-2.64204300	-1.41507400
C	-4.79561400	-0.78873100	-1.32441500
C	-3.24240200	-0.27316200	1.49342800
C	-3.31915100	-1.67657300	2.10072100
C	-2.64556300	0.72105700	2.49490200
H	-3.59528400	-3.07007900	-2.27772800
H	-2.46817500	1.48479200	-1.74725900
H	-0.04779700	5.49878300	-0.02349600
H	-2.13387700	4.20549900	-0.50262700
H	-4.97676600	0.29144000	-1.30529100
H	-3.46219900	-3.13070400	-0.51620900
H	-3.28506500	2.01260800	-0.28272600
H	-2.89223200	-0.71645300	-2.31903700
H	-4.25567700	0.06227900	1.23715500
H	-5.26341200	-1.23126600	-0.43761200
H	-5.30060800	-1.19853200	-2.20600800
H	-2.00983900	-2.88671000	-1.50348900
H	-3.86068900	-2.37678100	1.45808000
H	-1.62842100	0.43041100	2.78030300
H	-2.31643100	-2.08096400	2.28304800
H	-3.26119200	0.73248600	3.40097000
H	-3.84461100	-1.63019700	3.06097100
H	-2.61312000	1.74336100	2.10307600
H	0.03626300	-2.13813900	-0.06828500
P	2.30002900	-0.22277400	0.11863400
C	2.36400700	1.55758300	0.62666900

C	1.12265400	2.32934300	0.25197800
C	1.13764300	3.72088900	0.24461500
C	3.30401500	-1.05654800	1.43164300
C	3.10411700	-2.57458100	1.47195000
C	4.78782700	-0.68030500	1.38126900
C	3.23532800	-0.25930200	-1.47794500
C	3.43702700	-1.68514200	-1.99862900
C	2.48946300	0.59338600	-2.51150200
H	3.62796700	-2.98306700	2.34330000
H	2.44794200	1.56830200	1.72098900
H	2.06181600	4.24677700	0.46261000
H	4.94045100	0.40429000	1.36681900
H	3.51057600	-3.06399200	0.58107500
H	3.25502600	2.06180100	0.23840800
H	2.87062300	-0.64315000	2.35271100
H	4.21555400	0.19547200	-1.28425900
H	5.27524700	-1.10698000	0.49744200
H	5.29589600	-1.07894300	2.26612800
H	2.04564000	-2.83880200	1.55477400
H	4.08685000	-2.27620800	-1.34689900
H	1.48942900	0.18467100	-2.70518400
H	2.47863100	-2.20925000	-2.09610400
H	3.04347700	0.59331100	-3.45647800
H	3.90346800	-1.64831200	-2.98936100
H	2.37616600	1.63481700	-2.19134800
H	-0.03347400	-0.68111000	1.49089500

3-Fe

Fe	-0.02469600	-0.39533500	0.00417400
P	-2.24463800	-0.15907700	-0.10600700
N	-0.00177900	1.67368000	0.01244000
C	-2.39111000	1.61736600	-0.56697600
C	-1.13412000	2.37656000	-0.23948500
C	-1.15134000	3.76756200	-0.24041800
C	0.02523600	4.46428500	-0.00154700
C	-3.31143100	-0.98213800	-1.37938400
C	-3.07647200	-2.48920600	-1.51388200
C	-4.79738200	-0.65705700	-1.19669600
C	-3.08251800	-0.26117700	1.54223900
C	-3.22331400	-1.70616300	2.02960700
C	-2.27891000	0.57069200	2.54982800
H	-3.72320800	-2.88184100	-2.30645800
H	-2.54551700	1.66129600	-1.65219400
H	0.03607500	5.55042500	-0.00815200
H	-2.08292300	4.28741300	-0.44071800
H	-4.97909700	0.41942700	-1.10693300
H	-3.31584700	-3.02918100	-0.59203000
H	-3.25942300	2.09747200	-0.10384400
H	-2.96654500	-0.51395700	-2.31132600
H	-4.08107400	0.18091800	1.43130100
H	-5.20433500	-1.14841100	-0.30565500
H	-5.35916200	-1.02195500	-2.06342400
H	-2.04150300	-2.71390100	-1.78485400
H	-3.88683300	-2.29721300	1.39156500
H	-1.25652200	0.18182000	2.64826400
H	-2.24867500	-2.20763800	2.06880100
H	-2.75618800	0.52017000	3.53459000
H	-3.64350500	-1.70980100	3.04152100
H	-2.21489700	1.62612800	2.26382300
H	0.00563200	-0.50752200	-1.47655100
P	2.21937700	-0.19283600	0.09509300

C	2.38824800	1.57588800	0.58440100
C	1.14460400	2.35666100	0.25568300
C	1.18808100	3.74731600	0.24393600
C	3.19597400	-1.04136900	1.43220600
C	2.89908400	-2.53724300	1.57339500
C	4.70186600	-0.77940200	1.33274400
C	3.18762500	-0.31994900	-1.47935100
C	3.19632900	-1.75017400	-2.02643900
C	2.66280800	0.66071100	-2.53303800
H	3.48620100	-2.94136900	2.40575000
H	2.53183500	1.60169700	1.67156400
H	2.13009600	4.25111600	0.43616800
H	4.93378400	0.28581700	1.22491400
H	3.16926500	-3.09895000	0.67319900
H	3.26855200	2.05155000	0.14034000
H	2.82053300	-0.54956700	2.33972000
H	4.21382500	-0.02944700	-1.22069900
H	5.13994300	-1.31374600	0.48210300
H	5.19516500	-1.14061700	2.24173600
H	1.84330200	-2.72210300	1.78972700
H	3.67060000	-2.45512200	-1.33691700
H	1.64133400	0.40445900	-2.83382500
H	2.17677400	-2.09926500	-2.22884900
H	3.30206100	0.60971600	-3.42131300
H	3.75497900	-1.77748200	-2.96858100
H	2.66647000	1.69787100	-2.18079700
C	-0.02463500	-2.13348100	-0.05365000
O	-0.01243100	-3.28808300	-0.16911300

3-Co

Co	0.02919500	-0.48411600	-0.05903400
P	-2.17803400	-0.37227200	-0.10371200
N	-0.00347100	1.52800400	-0.03472900
C	-2.36967000	1.38157800	-0.65925800
C	-1.14890800	2.19492300	-0.30986200
C	-1.19742000	3.58526300	-0.30024200
C	-0.04127800	4.30228800	-0.01763200
C	-3.12500100	-1.31130800	-1.39281700
C	-2.80823100	-2.80980800	-1.41324800
C	-4.63392000	-1.05700100	-1.33628400
C	-3.11440200	-0.44605700	1.49070000
C	-3.10441700	-1.85252800	2.09596800
C	-2.56843700	0.57974600	2.48969300
H	-3.29833700	-3.26900200	-2.27902300
H	-2.47268200	1.36315100	-1.75136000
H	-0.05601000	5.38846000	-0.01117400
H	-2.13332900	4.08945600	-0.51918900
H	-4.87509700	0.01148200	-1.32607800
H	-3.17830700	-3.31671400	-0.51626900
H	-3.27421300	1.85506200	-0.26392200
H	-2.73469500	-0.88035100	-2.32499100
H	-4.14750600	-0.16995200	1.24259400
H	-5.07785000	-1.51774400	-0.44649200
H	-5.11301300	-1.50185000	-2.21536200
H	-1.73278400	-2.99453600	-1.49080000
H	-3.60747100	-2.58237600	1.45508600
H	-1.53342200	0.34856700	2.76507800
H	-2.07863800	-2.19732400	2.27242700
H	-3.17587000	0.55269900	3.40093400
H	-3.62649800	-1.83839600	3.05906100
H	-2.59973700	1.60310200	2.10072300
H	0.06173300	-1.96042100	-0.12025300

P	2.19997600	-0.32857900	0.11947700
C	2.35784300	1.44086600	0.62403000
C	1.12142300	2.22255600	0.25725600
C	1.13303500	3.61347100	0.26113300
C	3.14733600	-1.23619800	1.42174400
C	2.84492500	-2.73726400	1.45510000
C	4.65246000	-0.95921200	1.36216800
C	3.10531800	-0.42030500	-1.49182900
C	3.22990300	-1.85678500	-2.00763600
C	2.37305400	0.45847200	-2.51391100
H	3.35202500	-3.18680200	2.31604400
H	2.46477500	1.45873400	1.71589800
H	2.05336900	4.14023300	0.49285800
H	4.87515500	0.11324200	1.35414800
H	3.20401600	-3.24666500	0.55518400
H	3.25241700	1.91696700	0.20926800
H	2.74914500	-0.79812500	2.34706000
H	4.10942700	-0.00986300	-1.32286300
H	5.10432100	-1.40978500	0.47129900
H	5.13956000	-1.39736000	2.24007400
H	1.77226200	-2.92923400	1.55168800
H	3.85948600	-2.47574300	-1.36198400
H	1.34982700	0.09524200	-2.67640300
H	2.24644200	-2.33474100	-2.09036900
H	2.90042100	0.42414200	-3.47340300
H	3.68427100	-1.84577400	-3.00457900
H	2.31739300	1.50675200	-2.20133000
H	0.00464600	-0.67285300	1.35651200

4-Ir

Ir	0.00282200	-0.54337400	-0.07454300
P	-2.30798900	-0.24359900	-0.09977000
N	-0.01520300	1.64358700	-0.04100200
C	-2.37699000	1.50753100	-0.70310500
C	-1.15853600	2.30972100	-0.31829400
C	-1.20182000	3.70005100	-0.28939600
C	-0.04501100	4.40929100	0.01077700
C	-3.32437100	-1.14926000	-1.35809600
C	-3.09120800	-2.66330600	-1.34414800
C	-4.81629900	-0.81081000	-1.29334000
C	-3.24230700	-0.21812500	1.49672200
C	-3.28182900	-1.59864900	2.15796900
C	-2.67139700	0.82979300	2.45736900
H	-3.61588500	-3.11522100	-2.19318900
H	-2.41356600	1.45062700	-1.79890300
H	-0.05550700	5.49532300	0.02717000
H	-2.13308900	4.21139400	-0.51126000
H	-4.99954400	0.26907500	-1.30122500
H	-3.47895000	-3.12646800	-0.43105900
H	-3.28855300	2.02070300	-0.38095500
H	-2.91843600	-0.76321600	-2.30341800
H	-4.26417200	0.08142200	1.23081300
H	-5.27724000	-1.23145600	-0.39248900
H	-5.32578400	-1.24452400	-2.16062600
H	-2.02857400	-2.90955400	-1.42866400
H	-3.80240600	-2.33837800	1.54278400
H	-1.63999000	0.58902000	2.73748500
H	-2.26853500	-1.96682000	2.35736700
H	-3.27516200	0.84436100	3.37125000
H	-3.81035400	-1.52881900	3.11497600

H	-2.68715300	1.83951500	2.03382800
H	0.05036800	-1.18002000	-1.72918700
H	-0.00024600	-2.13173600	0.10143700
P	2.29661300	-0.22849000	0.13718600
C	2.33063800	1.53833000	0.69137100
C	1.10810400	2.32190200	0.28132000
C	1.12286200	3.71373000	0.29761100
C	3.20853400	-1.09677200	1.49718600
C	2.98613800	-2.61200200	1.50978100
C	4.69898400	-0.74830000	1.54166100
C	3.36438600	-0.24173400	-1.37594000
C	3.49070900	-1.64465600	-1.97592300
C	2.85497900	0.75203500	-2.42521600
H	3.45274400	-3.03514100	2.40627100
H	2.35725800	1.51705700	1.78848700
H	2.04064200	4.23574600	0.54902800
H	4.87483900	0.33286700	1.52855300
H	3.43964800	-3.09795800	0.63984400
H	3.24098400	2.05142600	0.36523600
H	2.72550500	-0.68622400	2.39422500
H	4.35303800	0.09469300	-1.03793800
H	5.23407200	-1.19399200	0.69545800
H	5.13902100	-1.14904200	2.46125500
H	1.92175100	-2.86318300	1.52712200
H	3.98202700	-2.34420300	-1.29336500
H	1.87791100	0.45020100	-2.81772200
H	2.50575300	-2.05099100	-2.23560300
H	3.55747400	0.77730900	-3.26525900
H	4.08810700	-1.59735400	-2.89300700
H	2.76839700	1.77145800	-2.03445500
H	-0.01869800	-0.50372200	1.52014400
H	0.01871600	-0.35075700	-1.86867500

4-Fe

Fe	-0.02809700	-0.46725600	-0.18378300
P	-2.24745600	-0.15266700	-0.13852400
N	0.00004700	1.60366600	-0.05791400
C	-2.33527300	1.57876800	-0.76870000
C	-1.09131600	2.33150200	-0.38342100
C	-1.07588300	3.72310900	-0.36457700
C	0.08971800	4.38410200	-0.00060800
C	-3.37017000	-1.04757500	-1.32021400
C	-3.13733300	-2.56033700	-1.37436200
C	-4.85134300	-0.71963900	-1.10955900
C	-3.09955600	-0.09500300	1.50551700
C	-3.10926200	-1.46838500	2.18282300
C	-2.47813100	0.96109400	2.42484700
H	-3.81595100	-3.00043800	-2.11354800
H	-2.39240800	1.51759200	-1.86280300
H	0.12858700	5.46957400	0.01077300
H	-1.97373000	4.26990100	-0.63492400
H	-5.03678100	0.35866100	-1.05622200
H	-3.33603200	-3.04360400	-0.41200500
H	-3.22907000	2.11017000	-0.42682600
H	-3.06059800	-0.63604600	-2.29059800
H	-4.13295400	0.20543700	1.29187000
H	-5.23115600	-1.17980600	-0.19039500
H	-5.43364300	-1.12010300	-1.94646500
H	-2.11463200	-2.80209500	-1.67672200
H	-3.65098200	-2.21703800	1.59653000
H	-1.42988800	0.72870400	2.64274300
H	-2.08796200	-1.83179900	2.34754800

H	-3.02602100	0.97679900	3.37343000
H	-3.60023100	-1.39021100	3.15909900
H	-2.52721300	1.96816000	1.99749100
H	0.40608400	-0.36570800	-1.79178500
P	2.18623500	-0.28155200	0.11073900
C	2.24861600	1.39780500	0.85767700
C	1.11819600	2.24585500	0.34980400
C	1.19899600	3.63420600	0.37024600
C	3.05199000	-1.32927900	1.37532000
C	3.33568900	-2.75474500	0.88911100
C	4.33915200	-0.69256900	1.91118500
C	3.31180300	-0.20944300	-1.36805600
C	3.08904800	-1.40135300	-2.80767500
C	3.14643000	1.10328300	-2.14286100
H	3.66059100	-3.36343600	1.73977400
H	2.09549600	1.25460500	1.93556700
H	2.12025100	4.11066000	0.69017200
H	4.16539100	0.28190400	2.37601300
H	4.14541800	-2.76261300	0.15122000
H	3.21345700	1.89631700	0.73073500
H	2.31975300	-1.37995900	2.19188600
H	4.33583100	-0.25509800	-0.97502400
H	5.08549000	-0.56845000	1.11832200
H	4.77349000	-1.35070200	2.67196500
H	2.46022300	-3.23759500	0.44562500
H	3.14979800	-2.36608100	-1.79727100
H	2.11219400	1.23806900	-2.48374900
H	2.10857600	-1.33809700	-2.79350600
H	3.78651600	1.08058100	-3.03158500
H	3.84938500	-1.38809700	-3.09630800
H	3.42923200	1.97914900	-1.55155800
H	-0.03325500	-0.50925500	1.32175800
C	-0.08120100	-2.20625900	-0.01868600
O	-0.12221600	-3.34411300	0.18794800
H	-0.40806400	-0.40168800	-1.81117200

4-Co

Co	0.00619000	-0.49224900	-0.18055100
P	-2.18825000	-0.35616300	-0.13784800
N	-0.02596400	1.52717100	-0.06371600
C	-2.37786500	1.39095600	-0.71252800
C	-1.16588100	2.20271000	-0.33211700
C	-1.21538200	3.59146800	-0.27207300
C	-0.06599000	4.29624500	0.06550100
C	-3.18101400	-1.31249300	-1.37750100
C	-2.84673500	-2.80734400	-1.39762600
C	-4.68905700	-1.07624000	-1.25768600
C	-3.07683800	-0.40544900	1.48405300
C	-3.03080800	-1.79798300	2.11919200
C	-2.52347900	0.64981100	2.44728900
H	-3.37346600	-3.28266200	-2.23261400
H	-2.44943900	1.35650700	-1.80716900
H	-0.07950000	5.38153800	0.10966100
H	-2.14679900	4.10365100	-0.49170600
H	-4.94297800	-0.01077100	-1.24301800
H	-3.16493700	-3.30802400	-0.47743700
H	-3.29343600	1.86540600	-0.34503200
H	-2.83541700	-0.88524500	-2.32901100
H	-4.11992200	-0.14985300	1.25710300
H	-5.08933900	-1.53747100	-0.34768400
H	-5.19913500	-1.53227700	-2.11322100
H	-1.77415800	-2.97955100	-1.52700600

H	-3.53552000	-2.55022800	1.50588600
H	-1.47131700	0.45511800	2.68382900
H	-1.99583800	-2.12211500	2.28068900
H	-3.09229000	0.61578500	3.38288100
H	-3.53159200	-1.77104000	3.09322400
H	-2.60426400	1.66603400	2.04726900
H	0.00742800	-1.95598200	-0.09462600
P	2.16967200	-0.34292300	0.11810200
C	2.28889200	1.39962300	0.71804900
C	1.08378800	2.20414200	0.30418400
C	1.09629200	3.59470800	0.36108700
C	2.96777600	-1.31318500	1.47999400
C	2.65459100	-2.81154500	1.42988100
C	4.47300200	-1.05874900	1.59820800
C	3.30005600	-0.37937200	-1.35102300
C	3.38071600	-1.77339400	-1.97911200
C	2.88204900	0.66079300	-2.39604000
H	3.05651300	-3.29240000	2.32857400
H	2.30688600	1.36114900	1.81470600
H	2.00725600	4.10960600	0.64956700
H	4.71300600	0.00957800	1.63289700
H	3.11430400	-3.29534100	0.56194300
H	3.21518000	1.89038800	0.40308500
H	2.47357200	-0.90365400	2.37139500
H	4.29088500	-0.10084900	-0.96910500
H	5.01705300	-1.50574400	0.75840000
H	4.84884100	-1.51786800	2.51911300
H	1.57731400	-2.99754500	1.39491600
H	3.81362500	-2.51061200	-1.29669400
H	1.91250000	0.41103100	-2.84002700
H	2.38800700	-2.12692900	-2.28310900
H	3.62291500	0.67689500	-3.20278500
H	4.01211600	-1.73546300	-2.87373000
H	2.82010000	1.67318800	-1.98298200
H	-0.00428900	-0.61493000	1.26880500
H	0.11125300	-1.05613400	-1.72773900
H	-0.03650800	-0.27457700	-1.85253700

5-Ir

Ir	-0.02897500	-0.59791500	-0.01000300
P	-2.31205200	-0.29128800	-0.15686400
N	-0.00093700	1.56039300	-0.35848300
C	-2.36612400	1.36799900	-0.98538900
C	-1.13436500	2.19882500	-0.72693000
C	-1.15437200	3.57704000	-0.92203400
C	0.02005800	4.30356100	-0.76657800
C	-3.30191000	-1.33836300	-1.33263900
C	-3.10665900	-2.84245100	-1.11813000
C	-4.78799600	-0.97419200	-1.38685400
C	-3.37221900	-0.04189400	1.34778600
C	-3.50856400	-1.32157000	2.17701200
C	-2.85106900	1.10606100	2.21703000
H	-3.60559800	-3.39035600	-1.92556100
H	-2.40969000	1.16800100	-2.06422500
H	0.02763000	5.37851800	-0.92340300
H	-2.08231800	4.06327000	-1.20643600
H	-4.94897900	0.09940800	-1.53399700
H	-3.54325700	-3.17922300	-0.17215400
H	-3.26940700	1.93238400	-0.73207300
H	-2.84648100	-1.08530800	-2.29977700

H	-4.36086800	0.24341600	0.96615600
H	-5.30354400	-1.27538700	-0.46777800
H	-5.26345000	-1.50214200	-2.22112100
H	-2.04765500	-3.11662200	-1.12289400
H	-4.02253300	-2.11802300	1.63089500
H	-1.87592100	0.85908500	2.64958200
H	-2.52420000	-1.69532700	2.48437700
H	-3.55045200	1.28100200	3.04221600
H	-4.08706500	-1.11252000	3.08401000
H	-2.75133800	2.04480300	1.66124000
H	-0.08302800	-0.90420900	-1.64837100
H	-0.04481800	-2.18379200	0.23031800
P	2.26046800	-0.31328200	-0.01455700
C	2.37785800	1.51819600	0.25344700
C	1.14575200	2.25891700	-0.20254200
C	1.18537000	3.63494600	-0.41311200
C	3.27883300	-0.97441900	1.39306800
C	3.04438700	-2.46420000	1.66084900
C	4.77276700	-0.65921900	1.28036900
C	3.25459100	-0.56797400	-1.56288200
C	3.32572400	-2.04288500	-1.96659600
C	2.71448200	0.28149400	-2.71753900
H	3.57229400	-2.75503500	2.57613600
H	2.47662300	1.66867500	1.33614200
H	2.12280600	4.16756600	-0.28600200
H	4.96136900	0.40106800	1.07905700
H	3.42596800	-3.08887200	0.84627500
H	3.27254400	1.94791900	-0.20873400
H	2.86955700	-0.41971700	2.24888500
H	4.26600800	-0.21376100	-1.32562000
H	5.24243200	-1.24805700	0.48411000
H	5.27272500	-0.91643000	2.22086200
H	1.98155600	-2.68726600	1.79363800
H	3.83815800	-2.65394600	-1.21741400
H	1.69964600	-0.02654300	-2.99188500
H	2.32104000	-2.45590100	-2.11781000
H	3.35746700	0.14944200	-3.59489200
H	3.87542000	-2.14080000	-2.90958000
H	2.69516900	1.35034600	-2.47856700
H	0.01207000	-0.40824900	1.66348200
O	0.79212400	1.67307500	3.17151700
H	0.50344800	0.95326400	2.57928100
H	0.28180100	1.55073100	3.98039300

5-Fe

P	2.18081300	-0.28504900	-0.05572100
N	0.01062200	1.59284900	-0.32216000
C	2.39331600	1.52707900	0.22974300
C	1.15841000	2.28868500	-0.16541200
C	1.21006400	3.67168600	-0.32384700
C	0.04776000	4.36592400	-0.63092200
C	3.22116600	-0.97412200	1.33059100
C	2.95763400	-2.45030800	1.64100500
C	4.72056900	-0.70857400	1.16664700
C	3.15239800	-0.57005200	-1.61666000
C	3.14507300	-2.04510900	-2.02700900
C	2.64130000	0.30960500	-2.76215400
H	3.58157900	-2.75735600	2.48837800
H	2.55232100	1.66976300	1.30594400
H	0.06137000	5.44598400	-0.74749700

H	2.15688900	4.18679500	-0.19293500
H	4.93682000	0.33952400	0.93202100
H	3.20562300	-3.10058100	0.79514300
H	3.27464000	1.93315300	-0.27747200
H	2.86211100	-0.39421600	2.19205500
H	4.18351900	-0.26778600	-1.39414400
H	5.14897600	-1.33211900	0.37342500
H	5.23974900	-0.95748100	2.09907700
H	1.91398900	-2.62664600	1.91330700
H	3.62721600	-2.68501200	-1.28141400
H	1.61359300	0.04504900	-3.03350000
H	2.11950500	-2.40503900	-2.17608400
H	3.27429000	0.16058300	-3.64434800
H	3.68482400	-2.17010000	-2.97278200
H	2.66496000	1.37625000	-2.51327000
H	0.03642600	-0.25104400	1.52397100
P	-2.23623300	-0.22957000	-0.17733200
C	-2.35913100	1.46210200	-0.90918000
C	-1.11586000	2.26583900	-0.64694800
C	-1.13171000	3.65069100	-0.79218700
C	-3.21574800	-1.21548200	-1.42280400
C	-2.98435000	-2.72767000	-1.35212700
C	-4.71218800	-0.88926900	-1.42846200
C	-3.32286700	-0.10584200	1.32852300
C	-3.42074800	-1.44268200	2.06895400
C	-2.84572800	0.99708800	2.27820100
H	-3.56939000	-3.21856600	-2.13851300
H	-2.45374400	1.33400600	-1.99512500
H	-2.06311300	4.14927200	-1.04258500
H	-4.90477600	0.18842600	-1.47066500
H	-3.30022700	-3.15049600	-0.39240100
H	-3.25007900	2.00453100	-0.57653400
H	-2.78661600	-0.86935200	-2.37297200
H	-4.31908300	0.17209800	0.96202300
H	-5.21043100	-1.29080000	-0.53862800
H	-5.18233700	-1.34840500	-2.30544700
H	-1.93329400	-2.98326300	-1.50876800
H	-3.89925000	-2.21870100	1.46358700
H	-1.87460400	0.74475500	2.71640000
H	-2.42642400	-1.80145900	2.36274000
H	-3.56581800	1.10814800	3.09694700
H	-4.01507800	-1.31884000	2.98160800
H	-2.75310300	1.96983700	1.78240200
H	-0.11557900	-0.66666600	-1.58768900
O	0.79268300	1.68281700	3.14676100
H	0.27245900	1.53515600	3.94498500
Fe	-0.03417900	-0.49503500	-0.03407500
C	-0.07122500	-2.19792700	0.21374900
O	-0.09975500	-3.35327600	0.38607900
H	0.50545700	0.98453500	2.52469000

5-Co

Co	-0.02783900	-0.57053300	-0.00404800
P	2.14521100	-0.43145000	-0.00229000
N	-0.00187600	1.43275000	-0.35949100
C	2.36034600	1.38879100	0.26145900
C	1.13494800	2.14118500	-0.19024000
C	1.17148900	3.51757300	-0.40003300
C	0.00893100	4.17700800	-0.78038500
C	3.12706900	-1.14567300	1.40621400
C	2.81902600	-2.62125000	1.67839000
C	4.63538100	-0.90708800	1.29392000

C	3.13185800	-0.73917600	-1.54736400
C	3.13007600	-2.21749300	-1.94544600
C	2.63070100	0.12891800	-2.70595300
H	3.33732800	-2.93766800	2.59084000
H	2.48385400	1.54633100	1.34034900
H	0.01202000	5.25161100	-0.94045600
H	2.10375500	4.05566000	-0.25773200
H	4.87686200	0.14191400	1.08941200
H	3.16271800	-3.26613200	0.86261900
H	3.25768900	1.78578600	-0.22456400
H	2.74749700	-0.56971200	2.26152200
H	4.16030300	-0.43398800	-1.31482700
H	5.07527400	-1.52061200	0.49921100
H	5.12200100	-1.18656900	2.23517100
H	1.74728800	-2.78989300	1.81843500
H	3.61185600	-2.85030100	-1.19398600
H	1.60194700	-0.13336200	-2.97652400
H	2.10620100	-2.58151900	-2.09503700
H	3.26487000	-0.03647600	-3.58421900
H	3.67361700	-2.34688000	-2.88834600
H	2.66066200	1.19863400	-2.47189200
H	0.03030200	-0.39598200	1.53161000
H	-0.04336200	-2.02915800	0.24305800
P	-2.19462200	-0.42674700	-0.16410600
C	-2.33932400	1.20808200	-1.02250000
C	-1.12815600	2.06391200	-0.75616600
C	-1.15597400	3.44054900	-0.96172600
C	-3.10401600	-1.55836500	-1.32728300
C	-2.82260600	-3.04369200	-1.08094300
C	-4.60887500	-1.28767300	-1.40652700
C	-3.29752200	-0.20998900	1.31717400
C	-3.36295100	-1.47594800	2.17594700
C	-2.86229600	0.98867000	2.16537300
H	-3.29072300	-3.63729800	-1.87460200
H	-2.37300100	0.99781300	-2.09960400
H	-2.08107300	3.91743800	-1.27069400
H	-4.83345900	-0.22854300	-1.57455700
H	-3.23702300	-3.38421200	-0.12629900
H	-3.26083300	1.74428100	-0.77382100
H	-2.65374600	-1.29785200	-2.29465300
H	-4.29780500	0.00200500	0.91814100
H	-5.11766300	-1.60407300	-0.48874600
H	-5.04019000	-1.85822300	-2.23682200
H	-1.74970900	-3.25686500	-1.08253500
H	-3.81429200	-2.31748700	1.64197800
H	-1.87543300	0.81996300	2.60902800
H	-2.36142400	-1.77679400	2.50711600
H	-3.57756900	1.13338500	2.98303100
H	-3.96853600	-1.28528300	3.06937500
H	-2.82380700	1.92024300	1.59007100
H	-0.09361500	-0.89602700	-1.49191700
O	0.65965500	1.50791200	3.26332600
H	0.43661400	2.35641600	2.86256400
H	0.44069100	0.84418400	2.57991700

6-Ir

Ir	-0.00872200	-0.40163700	-0.31298500
P	2.28878800	-0.07779000	-0.21917600
N	-0.02123000	1.67422400	0.34540900
C	2.34144000	1.36934700	0.94075900

C	1.10111400	2.22528300	0.85834300	Fe	0.00200600	-0.39346100	-0.22026800
C	1.10907000	3.53795300	1.32262100	P	-2.24163200	-0.16794400	-0.36361000
C	-0.06203000	4.28381700	1.26978700	N	-0.04214800	1.67221500	0.04517700
C	3.36870600	-1.31503200	0.64512100	C	-2.32102200	1.61940700	-0.81371900
C	3.18559500	-2.74379500	0.12363800	C	-1.17123100	2.37115500	-0.20586400
C	4.84689900	-0.91702800	0.67513900	C	-1.25707300	3.73850800	0.03842700
C	3.20273700	0.52234000	-1.71325100	C	-0.14445300	4.41072700	0.52902700
C	3.30418700	-0.55695400	-2.79451700	C	-3.15922400	-0.94713800	-1.78116000
C	2.56170800	1.79512000	-2.27585300	C	-3.33818600	-2.46367300	-1.64758300
H	3.75280700	-3.43432300	0.75787000	C	-4.50638200	-0.28576400	-2.09052200
H	2.40210500	0.94839200	1.95216400	C	-3.34954000	-0.30800500	1.12377600
H	-0.07950400	5.30603600	1.63713200	C	-3.26066000	-1.69371100	1.77450400
H	2.02530100	3.95760300	1.72608400	C	-3.03584300	0.77966600	2.15894400
H	4.99675400	0.10351200	1.04391000	H	-3.64484700	-2.87595300	-2.61529800
H	3.55640700	-2.85405700	-0.90069900	H	-2.21460600	1.66471100	-1.90561500
H	3.23580400	1.98459700	0.79711200	H	-0.18627100	5.47859000	0.72453900
H	2.98072100	-1.28788000	1.67233600	H	-2.18641000	4.26080100	-0.16624100
H	4.21173300	0.77346800	-1.36083500	H	-4.41654000	0.78786400	-2.28052900
H	5.29671000	-0.99160500	-0.32145400	H	-4.12644400	-2.70429800	-0.92647700
H	5.39425100	-1.59675300	1.33755800	H	-3.27669900	2.08810600	-0.56126600
H	2.13496000	-3.04916500	0.13987500	H	-2.47977700	-0.75935000	-2.62358800
H	3.87921800	-1.42554100	-2.46045000	H	-4.37412500	-0.15347300	0.76033400
H	1.54136500	1.60130500	-2.62499000	H	-5.22042900	-0.43184900	-1.27213400
H	2.30870000	-0.90027900	-3.10034200	H	-4.93632300	-0.74677100	-2.98717300
H	3.15059300	2.14825800	-3.12951000	H	-2.42214200	-2.97504700	-1.33913900
H	3.80498600	-0.14454600	-3.67750600	H	-3.49170200	-2.50513300	1.07993800
H	2.52470700	2.60570900	-1.54025600	H	-1.99910100	0.70249200	2.50472200
H	0.05721200	-2.91805500	1.57144400	H	-2.25888600	-1.87025000	2.17897900
H	0.00373500	-1.92796300	-0.80549800	H	-3.69369000	0.65312000	3.02641600
P	-2.30232200	-0.07620100	-0.39855100	H	-3.97144000	-1.75242400	2.60664900
C	-2.34658800	1.77789000	-0.42633000	H	-3.19695200	1.78913200	1.76741100
C	-1.15739600	2.40255100	0.25949600	H	-0.05431400	-0.17408300	-1.72304400
C	-1.20870800	3.71048000	0.73231200	P	2.23240600	-0.06001400	-0.20352000
C	-3.20566600	-0.51192400	-1.96063600	C	2.29542200	1.52289200	0.74367900
C	-3.00340000	-1.96611300	-2.39720200	C	1.04637200	2.32721200	0.50460300
C	-4.69110200	-0.14215200	-1.93352100	C	1.02549300	3.69720100	0.75364100
C	-3.41390600	-0.50692500	1.02240900	C	3.35819900	-1.13890200	0.81249900
C	-3.50753900	-2.02109800	1.23296300	C	3.22643800	-2.63567500	0.51532200
C	-2.96592100	0.19771000	2.30860700	C	4.82433500	-0.69756800	0.76773500
H	-3.45094600	-2.11031000	-3.38699600	C	3.12651100	0.33136200	-1.78101500
H	-2.30837300	2.06830800	-1.48465300	C	3.17911400	-0.88076000	-2.71581600
H	-2.13649000	4.26970000	0.66237500	C	2.49928700	1.53490700	-2.49303900
H	-4.85809100	0.89322200	-1.61701000	H	3.87313300	-3.19601600	1.20007100
H	-3.48812200	-2.66796000	-1.71050600	H	2.34533600	1.25369700	1.80553900
H	-3.28058200	2.17931400	-0.02065600	H	1.92210800	4.18669200	1.12095600
H	-2.70184100	0.12541100	-2.69999500	H	4.94534200	0.37193000	0.97084200
H	-4.40685500	-0.12505000	0.75208700	H	3.53575800	-2.88015500	-0.50618500
H	-5.25000500	-0.80155000	-1.25980700	H	3.18499500	2.11948000	0.51719900
H	-5.11427800	-0.25865600	-2.93737100	H	2.98339300	-0.97350500	1.83173100
H	-1.94268800	-2.22569400	-2.46042700	H	4.14969100	0.60316000	-1.49199300
H	-3.94485800	-2.53225100	0.37015500	H	5.27246300	-0.91396500	-0.20880100
H	-1.96008900	-0.11913300	2.60244300	H	5.39439900	-1.24949600	1.52333600
H	-2.51934700	-2.45647400	1.42224300	H	2.20268700	-2.99255200	0.65605700
H	-3.65811700	-0.05911700	3.11847400	H	3.72911900	-1.71906700	-2.27796500
H	-4.14047100	-2.23265300	2.10213800	H	1.46200700	1.32788000	-2.77912900
H	-2.96759600	1.28833700	2.20746300	H	2.16917700	-1.22647400	-2.96738500
H	-0.04848000	-0.00445700	-1.83635600	H	3.06644800	1.74924400	-3.40574100
C	0.19094000	-2.11289400	2.32061000	H	3.68179000	-0.60358300	-3.64926600
O	0.16515100	-0.91997500	1.87678500	H	2.51182900	2.43906500	-1.87518900
O	0.34998400	-2.42812800	3.51663600	H	0.30384300	-2.45890500	2.03751000
				C	0.06168800	-2.06537900	-0.67404300
				O	0.11166300	-3.15279900	-1.08655100

6-Fe

C	0.29391900	-1.48604400	2.57032700
O	0.13006600	-0.44991800	1.85483100
O	0.43820400	-1.49131800	3.81038100

6-Co

Co	0.00477200	-0.39359200	0.22511000
P	-2.19374900	-0.20964100	0.23715400
N	-0.00827500	1.58389800	-0.23220900
C	-2.34409600	1.26752700	-0.86922400
C	-1.12532200	2.14646400	-0.73963200
C	-1.14939000	3.48306700	-1.12877700
C	0.00342900	4.24761000	-0.99324300
C	-3.23515600	-1.47412900	-0.63451500
C	-2.98282200	-2.90607900	-0.15177700
C	-4.72975400	-1.14086600	-0.63003800
C	-3.09208900	0.29879000	1.77572900
C	-3.10741000	-0.81728400	2.82422100
C	-2.49606900	1.58294700	2.36250300
H	-3.52693400	-3.60550700	-0.79655700
H	-2.40001200	0.88853300	-1.89687800
H	0.01028100	5.29036600	-1.29832100
H	-2.06306000	3.90839500	-1.53242900
H	-4.92991500	-0.11989900	-0.97289200
H	-3.33584800	-3.05805300	0.87343800
H	-3.25624500	1.84521700	-0.68676400
H	-2.86924600	-1.40592600	-1.66790000
H	-4.12367900	0.51123300	1.46631000
H	-5.15732100	-1.25588700	0.37257900
H	-5.25989300	-1.82943400	-1.29741800
H	-1.92023900	-3.16436000	-0.18688500
H	-3.65357500	-1.70059200	2.48053600
H	-1.45350800	1.43143900	2.66425900
H	-2.08791600	-1.12369800	3.08759000
H	-3.06748100	1.87271800	3.25128000
H	-3.59690700	-0.45680900	3.73591400
H	-2.53125700	2.42068300	1.65803600
H	0.02002800	-2.80217300	-1.62155800
H	0.00606900	-1.81908100	0.61677100
P	2.18147600	-0.17119700	0.46312200
C	2.27624400	1.67129300	0.61679700
C	1.10402400	2.33010000	-0.06364500
C	1.14381400	3.66669000	-0.45010500
C	2.96968600	-0.74854400	2.04302500
C	2.68197700	-2.21747000	2.36903700
C	4.46797600	-0.44496700	2.12900600
C	3.38480100	-0.53047100	-0.90582000
C	3.50756900	-2.03081400	-1.18901700
C	3.02267700	0.23788400	-2.18270300
H	3.07979300	-2.45072400	3.36321700
H	2.21750100	1.90425800	1.68798400
H	2.05619300	4.23868100	-0.31244100
H	4.69506000	0.60102200	1.89544600
H	3.16122100	-2.89490100	1.65452000
H	3.22373000	2.08002500	0.25190500
H	2.44962500	-0.13898100	2.79421300
H	4.35528500	-0.15966100	-0.55083600
H	5.04144200	-1.08155800	1.44566900
H	4.82330300	-0.64665100	3.14567700
H	1.60870200	-2.42801200	2.37224400
H	3.90425400	-2.58202600	-0.33126700
H	2.05440800	-0.08540100	-2.57698200
H	2.53811200	-2.46729700	-1.45574400

H	3.78656200	0.04786000	-2.94520500
H	4.19005200	-2.19025400	-2.03156000
H	2.98168300	1.32040400	-2.01996700
H	0.03057900	-0.11146600	1.66359700
C	-0.08380700	-1.94102700	-2.31059100
O	-0.10773300	-0.78844100	-1.77446100
O	-0.16543900	-2.16337700	-3.53598900

7-Ir

Ir	0.04999400	-0.38409200	-0.34210600
P	2.31944700	0.09046400	-0.27355900
N	-0.03116100	1.29437800	1.02088600
C	2.39517100	1.08848500	1.28456200
C	1.09661000	1.80789100	1.57422200
C	1.07981000	2.91110000	2.40654700
C	-0.16911800	3.49898400	2.70503300
C	3.56041700	-1.25112100	0.06265000
C	3.47585000	-2.42218600	-0.92178100
C	4.99855200	-0.74289700	0.19693200
C	3.05436200	1.22042400	-1.54750500
C	3.12224300	0.56967400	-2.93170400
C	2.29111200	2.54772500	-1.61317300
H	4.10580000	-3.24376000	-0.56217700
H	2.57692500	0.36943400	2.09405100
H	-0.21719600	4.36281100	3.36496300
H	2.00436600	3.29558000	2.82511500
H	5.08166300	0.08996800	0.90348700
H	3.83543000	-2.14231700	-1.91735300
H	3.23467800	1.79161700	1.28886800
H	3.23369700	-1.62348500	1.04374100
H	4.07506400	1.43172600	-1.20293400
H	5.39203800	-0.41187400	-0.77104600
H	5.64253200	-1.55340900	0.55644600
H	2.45237000	-2.79615600	-1.02298500
H	3.77464400	-0.30812300	-2.94569300
H	1.26121900	2.39148300	-1.95357100
H	2.12545600	0.26239800	-3.26989400
H	2.78639700	3.21499300	-2.32742600
H	3.51676600	1.29013800	-3.65720800
H	2.25720400	3.06039700	-0.64589300
H	0.70814500	-3.35623200	0.56986300
H	0.09163900	-1.64854100	-1.35121100
P	-2.27382800	-0.21079100	-0.21341000
C	-2.41470100	1.32624600	0.67153700
C	-1.26794500	1.84801600	1.29092700
C	-1.31919200	2.98108300	2.17184600
C	-3.18317400	0.04396300	-1.82112600
C	-3.21634800	-1.18590900	-2.73261200
C	-4.59175500	0.61577800	-1.63682500
C	-3.26891800	-1.51678200	0.68338100
C	-2.88230200	-2.93685200	0.25063000
C	-3.12915900	-1.37998700	2.20240000
H	-3.55832200	-0.89206900	-3.73185900
H	-2.11670500	2.71570100	-0.83053400
H	-2.28836100	3.42010700	2.39314600
H	-4.58635800	1.53186500	-1.03763900
H	-3.91688600	-1.94043600	-2.35762500
H	-3.38112000	1.71427300	0.98918900
H	-2.56857200	0.80933200	-2.31255400
H	-4.32082500	-1.34409000	0.41744800

H	-5.25950300	-0.10735400	-1.15371400
H	-5.02352500	0.85715600	-2.61548300
H	-2.23020800	-1.65195000	-2.83466100
H	-2.95080900	-3.08778400	-0.82972400
H	-2.08115400	-1.48565500	2.50763300
H	-1.85463100	-3.16408900	0.55397300
H	-3.70658800	-2.16923900	2.69890800
H	-3.54400400	-3.66547900	0.73423100
H	-3.49197900	-0.41289900	2.56198100
H	-0.10317000	0.52320400	-1.61755800
C	0.65149300	-2.85219000	1.55542200
O	0.34154000	-1.61948000	1.54084000
O	0.89006700	-3.52233700	2.58145300
O	-1.94775300	3.40695800	-1.51053300
H	-1.24069100	3.04229500	-2.05602800

7-Fe

P	-2.27111200	0.03464600	0.24891900
N	0.00040300	1.46424000	-0.75041500
C	-2.40791500	1.30024200	-1.08299400
C	-1.11922300	2.07386000	-1.21000800
C	-1.11519500	3.32368600	-1.80330100
C	0.12394900	3.98038800	-1.95809400
C	-3.51363200	-1.23042000	-0.32117300
C	-3.44162600	-2.56461800	0.42757800
C	-4.95302300	-0.70831700	-0.36279100
C	-3.00344600	0.87537700	1.73409000
C	-2.91949800	-0.00297800	2.98613600
C	-2.34244700	2.23465000	1.98938600
H	-4.10271500	-3.28937600	-0.06149900
H	-2.57652000	0.74892600	-2.01684800
H	0.16591600	4.96121800	-2.42769100
H	-2.04368600	3.76846500	-2.14710100
H	-5.03649500	0.24681100	-0.89213800
H	-3.77325300	-2.46642600	1.46644700
H	-3.25960900	1.97502000	-0.94890900
H	-3.19038500	-1.41817000	-1.35471100
H	-4.05966000	1.05322100	1.49457100
H	-5.35459600	-0.57552400	0.64838600
H	-5.59167300	-1.43449100	-0.87852200
H	-2.43087300	-2.98188000	0.43073800
H	-3.47232600	-0.94033400	2.87588600
H	-1.27495500	2.11919500	2.20913500
H	-1.87685100	-0.24669800	3.22264800
H	-2.81645600	2.71023500	2.85559200
H	-3.34195800	0.53452600	3.84279500
H	-2.44446000	2.91577100	1.13815400
H	-0.77110000	-3.02168200	-1.25825700
P	2.20307800	-0.22033000	0.13715400
C	2.37317400	1.46546400	-0.38297900
C	1.22498700	2.08767600	-0.89196400
C	1.27304900	3.37847000	-1.52052800
C	3.12650800	-0.33609800	1.75870600
C	3.29243800	-1.75921400	2.30098400
C	4.48591200	0.36973500	1.72486400
C	3.21716100	-1.31058000	-1.00328300
C	2.78354100	-2.78088100	-0.93133800
C	3.16021500	-0.82154400	-2.45313000
H	3.67925100	-1.71545900	3.32597800
H	2.06379200	2.49196800	1.37465000
H	2.23973600	3.86301500	-1.63052300
H	4.39536000	1.42093400	1.43568800

H	4.01517100	-2.32798100	1.70454400
H	3.33981900	1.91685300	-0.59963600
H	2.47433600	0.21584800	2.44826800
H	4.25871400	-1.23965300	-0.65967700
H	5.17552200	-0.11974300	1.02621700
H	4.94627600	0.33214100	2.71962300
H	2.35081200	-2.31594800	2.32092400
H	2.76157700	-3.17081200	0.08983200
H	2.12771200	-0.81492000	-2.82324300
H	1.78311100	-2.90892200	-1.35748400
H	3.74377300	-1.49295800	-3.09498200
H	3.47479000	-3.40268100	-1.51324300
H	3.56351600	0.18968700	-2.55933800
H	0.09541700	0.31072800	1.52455600
C	-0.64244400	-2.29884400	-2.09028500
O	-0.31066800	-1.11831200	-1.76786600
O	-0.83266400	-2.70681000	-3.25676400
O	1.90029800	3.02998500	2.18362100
H	1.21361500	2.54749500	2.65910500
Fe	-0.06122100	-0.38736000	0.18294200
C	-0.09648600	-1.83652900	1.12147700
O	-0.11661600	-2.76343800	1.83191600

7-Co

Co	-0.05453800	-0.41343300	0.22632600
P	-2.23938000	-0.08538300	0.30160000
N	-0.03701500	1.24042900	-0.93546200
C	-2.42996100	0.92469200	-1.23410300
C	-1.17343300	1.72456300	-1.48900100
C	-1.20275800	2.87103100	-2.26237700
C	0.01636500	3.54652400	-2.48703600
C	-3.40941900	-1.49561700	-0.00255600
C	-3.21811300	-2.67100400	0.96149200
C	-4.87919400	-1.07252300	-0.07419600
C	-2.98772700	0.98064400	1.62245000
C	-2.92479800	0.31658500	3.00074600
C	-2.32439500	2.36175800	1.66145400
H	-3.81193000	-3.52476000	0.61533200
H	-2.56932100	0.21178300	-2.05667500
H	0.03256600	4.44674300	-3.09836200
H	-2.13811500	3.22616400	-2.68314800
H	-5.03805700	-0.23783300	-0.76555300
H	-3.55496400	-2.42439400	1.97374200
H	-3.31159800	1.57390400	-1.21356100
H	-3.10019300	-1.83608800	-1.00041400
H	-4.04008000	1.11730800	1.34118500
H	-5.25366800	-0.77603800	0.91240000
H	-5.48840200	-1.91553700	-0.41961000
H	-2.17110600	-2.98403000	1.01903000
H	-3.49831900	-0.61397400	3.03959800
H	-1.26147400	2.28058500	1.91676900
H	-1.88845400	0.09267000	3.28109300
H	-2.81049300	2.97501400	2.42859500
H	-3.33831600	0.99521800	3.75547200
H	-2.40672700	2.89317400	0.70759500
H	-0.29774200	-3.34982500	-0.51304500
H	-0.05949100	-1.59473900	1.13676100
P	2.15584800	-0.21830600	0.25628300
C	2.31118800	1.39437900	-0.47791200
C	1.16595000	1.89123000	-1.12118000
C	1.17852100	3.07296800	-1.93630000
C	2.96423700	-0.10833300	1.93551800

C	2.61210300	-1.24170000	2.90387900
C	4.47865200	0.10715000	1.86684800
C	3.26837700	-1.34412300	-0.73876600
C	3.25175200	-2.79538700	-0.24864000
C	2.93339600	-1.27867100	-2.23236900
H	3.01774200	-1.01157900	3.89654000
H	1.99037600	2.70402900	1.04901400
H	2.12467600	3.58412200	-2.09425800
H	4.74813400	0.91508100	1.17690300
H	3.03875800	-2.19997700	2.59064400
H	3.27932500	1.81726100	-0.74556500
H	2.51153700	0.80866100	2.33419000
H	4.28310000	-0.94341400	-0.60865300
H	4.99691400	-0.80383600	1.54495300
H	4.86263400	0.37126400	2.85928100
H	1.52963900	-1.36795100	2.99956600
H	3.65711700	-2.89804300	0.76187300
H	1.94059000	-1.69377300	-2.43417900
H	2.23300600	-3.20260600	-0.24902700
H	3.66858100	-1.86205400	-2.79961300
H	3.86070900	-3.42004000	-0.91330500
H	2.95309400	-0.25029700	-2.60707500
H	0.07841700	0.39828900	1.44023500
C	-0.39549400	-2.82975400	-1.48659400
O	-0.31915100	-1.56268800	-1.45907900
O	-0.56740300	-3.51957900	-2.51443000
O	1.84135700	3.38312400	1.74858700
H	1.16622600	3.00119700	2.32170100

8-Ir

Ir	-0.07806700	-0.58471400	0.01966600
P	2.24642000	-0.31921500	-0.10683600
N	-0.04576700	1.52273700	-0.49678300
C	2.33817000	1.45598800	-0.15584300
C	1.17070500	2.17342700	-0.46465100
C	1.17987400	3.58600100	-0.72018700
C	0.01362700	4.24974600	-0.99145600
C	3.22185400	-0.85090300	1.38723700
C	2.95820600	-2.28516200	1.85647800
C	4.72193600	-0.57593900	1.24844900
C	3.17205600	-0.95774900	-1.59047800
C	3.23608300	-2.48604300	-1.65756800
C	2.58195500	-0.38982900	-2.88383800
H	3.44805000	-2.44443400	2.82428400
H	2.14409000	2.08128400	1.79068700
H	0.02945700	5.32158700	-1.17718400
H	2.13085100	4.11053100	-0.68638600
H	4.92405900	0.45256100	0.92891100
H	3.35940600	-3.02768600	1.16000600
H	3.29409000	1.96287700	-0.28251200
H	2.82059700	-0.17980800	2.15826600
H	4.19174800	-0.56304100	-1.48192400
H	5.18480600	-1.25648500	0.52427800
H	5.21871100	-0.73199500	2.21293200
H	1.88860200	-2.47951100	1.98141700
H	3.82493900	-2.91471200	-0.84226100
H	1.58218600	-0.79815700	-3.07059600
H	2.23070600	-2.92388900	-1.62215600
H	3.22145600	-0.66431100	-3.73055600
H	3.70264200	-2.79512800	-2.60022100

H	2.50470900	0.70195900	-2.85384500
H	-0.08638000	-2.18437400	0.19725300
P	-2.37576000	-0.25011200	-0.06835700
C	-2.44207200	1.35747500	-0.97995200
C	-1.18804400	2.18509300	-0.81216300
C	-1.20959000	3.54537300	-1.04732800
C	-3.43203200	-1.35677600	-1.11755300
C	-3.23931700	-2.84661400	-0.81962400
C	-4.91387400	-0.97215000	-1.10683000
C	-3.30118500	0.09956700	1.50013800
C	-3.37201800	-1.12388200	2.41749200
C	-2.70122500	1.29944000	2.24126100
H	-3.79490800	-3.43639100	-1.55729100
H	-2.52942400	1.09695800	-2.04291700
H	-2.14210300	4.04404600	-1.29060600
H	-5.06897600	0.09180700	-1.31617000
H	-3.61816000	-3.11564300	0.17188600
H	-3.33166900	1.94062900	-0.72111300
H	-3.03002200	-1.16833400	-2.12241900
H	-4.31778500	0.36939700	1.18578900
H	-5.37420100	-1.20265700	-0.13927600
H	-5.44617200	-1.54669900	-1.87288200
H	-2.18576900	-3.13581900	-0.87389100
H	-3.91592300	-1.95494400	1.95884400
H	-1.68318800	1.08800800	2.58636700
H	-2.36763400	-1.47535600	2.68253700
H	-3.31266500	1.51961400	3.12322100
H	-3.89055400	-0.85703000	3.34515100
H	-2.67189400	2.20253200	1.62260200
H	-0.16256300	-0.90443300	-1.54758800
O	1.99618900	2.46308300	2.68538400
H	2.72509200	2.13636400	3.22477900
H	0.07967500	0.01991000	1.68437800
H	-0.04438600	-0.82251500	1.75473000

8-Fe

Fe	-0.08815900	-0.42081400	0.10875300
P	2.15021000	-0.30745200	-0.14655200
N	-0.01797100	1.58018700	-0.41849800
C	2.36872100	1.44804200	-0.20515800
C	1.21330900	2.20838200	-0.42929900
C	1.26037500	3.62792600	-0.63903900
C	0.10750300	4.33785900	-0.83899600
C	3.23740100	-0.88455000	1.25975800
C	2.87677000	-2.24907600	1.85435600
C	4.73157100	-0.80044400	0.93268600
C	2.91342900	-1.02899800	-1.68761800
C	2.79923800	-2.55408400	-1.75942800
C	2.32587200	-0.38837400	-2.94713800
H	3.54675900	-2.46582100	2.69484900
H	0.44790400	0.03641600	1.61383900
H	0.14846000	5.41455600	-0.99022800
H	2.23035300	4.11788100	-0.62858700
H	5.00568200	0.16937000	0.50241300
H	2.98320800	-3.06240800	1.12928500
H	3.34110600	1.91008500	-0.36883100
H	3.01999300	-0.13233100	2.02959600
H	3.97582300	-0.75537300	-1.63664000
H	5.03020200	-1.58389700	0.22648500
H	5.31823100	-0.93984600	1.84801300
H	1.85158900	-2.26444500	2.23553800
H	3.32863100	-3.05271400	-0.94219300

H	1.27407500	-0.66793000	-3.07577900
H	1.74924100	-2.87067100	-1.73101400
H	2.87822600	-0.73568200	-3.82809400
H	3.22955400	-2.91427500	-2.70132500
H	2.38674200	0.70440900	-2.91511800
H	-0.36958100	0.06216500	1.67179100
P	-2.29598500	-0.15052700	-0.06892500
C	-2.42093300	1.52059900	-0.83360000
C	-1.13969200	2.29886000	-0.67503600
C	-1.13380300	3.66728300	-0.86828100
C	-3.25127200	-1.19158400	-1.28158700
C	-2.99512900	-2.69697400	-1.17150300
C	-4.75177600	-0.88387500	-1.28362500
C	-3.35256400	-0.00811100	1.45313100
C	-3.43324400	-1.33095500	2.22004400
C	-2.86545900	1.11689400	2.37231500
H	-3.58730500	-3.21711300	-1.93296700
H	-2.59029600	1.36878800	-1.90699200
H	-2.06210500	4.19418300	-1.06447700
H	-4.95748700	0.18989600	-1.35357600
H	-3.28637600	-3.09718000	-0.19463100
H	-3.27916000	2.08574700	-0.45672500
H	-2.83171600	-0.86192700	-2.24180500
H	-4.35459600	0.26023700	1.09539000
H	-5.23738400	-1.26745900	-0.37916000
H	-5.22180200	-1.37241800	-2.14430000
H	-1.94369200	-2.94112800	-1.34328800
H	-3.91885100	-2.11981600	1.63769000
H	-1.90265400	0.87119700	2.83443600
H	-2.43332800	-1.68071000	2.50525300
H	-3.58886800	1.25803300	3.18289900
H	-4.01350700	-1.18986300	3.13892800
H	-2.75883900	2.07380100	1.85017100
H	-0.19333800	-0.80038700	-1.35051600
C	-0.12867100	-2.13312500	0.43394200
O	-0.15149100	-3.28093900	0.59894300
O	2.28764900	2.32720300	2.70504100
H	1.82338700	3.17190500	2.68897000
H	2.30713300	2.02997000	1.76735500

8-Co

Co	-0.07924400	-0.53334800	0.05946900
P	2.12671000	-0.42783100	-0.09923100
N	-0.05971000	1.40961600	-0.46173700
C	2.31304900	1.33778600	-0.13174700
C	1.15269000	2.06873700	-0.43582700
C	1.16144200	3.47931000	-0.69680700
C	-0.00458500	4.13501100	-0.99344400
C	3.09499300	-1.02652300	1.37571500
C	2.73466400	-2.43472000	1.85960400
C	4.60809100	-0.86757000	1.19953000
C	2.98585100	-1.11461300	-1.60121000
C	2.94822100	-2.64345200	-1.67554700
C	2.40747200	-0.50216200	-2.87949800
H	3.25095300	-2.63609500	2.80571100
H	0.13332100	0.04917500	1.62056700
H	0.00872800	5.20546200	-1.18792400
H	2.10998900	4.00792200	-0.65462100
H	4.87929400	0.14063400	0.86644800
H	3.04138400	-3.20728700	1.14753900
H	3.28105900	1.81957900	-0.26328400
H	2.76840100	-0.32348900	2.15357100

H	4.03143200	-0.78870800	-1.51268500
H	5.00124700	-1.58565000	0.47041000
H	5.11488500	-1.05413000	2.15342700
H	1.65894000	-2.53966000	2.03064900
H	3.51387900	-3.11405200	-0.86670000
H	1.37757700	-0.83980300	-3.04387900
H	1.91648300	-3.01432200	-1.63311300
H	3.00681500	-0.81494400	-3.74227600
H	3.38517300	-2.97879100	-2.62348900
H	2.40541200	0.59220000	-2.84341100
H	-0.10467600	-0.71728700	1.69760800
P	-2.26443300	-0.37693100	-0.06679300
C	-2.42883500	-1.21405300	-0.98646400
C	-1.19340800	2.06480800	-0.81165700
C	-1.22104000	3.42227300	-1.06848900
C	-3.21902100	-1.57005500	-1.11779600
C	-2.93335800	-3.04021700	-0.79687200
C	-4.72356000	-1.28727200	-1.14184900
C	-3.24258000	-0.07778700	1.48201600
C	-3.25577500	-1.29823700	2.40602000
C	-2.72740600	1.15915800	2.22690900
H	-3.42742700	-3.67397600	-1.54191200
H	-2.51268400	0.95504900	-2.04991900
H	-2.15200100	3.91013300	-1.33867800
H	-4.94564900	-0.23959300	-1.37238200
H	-3.32025900	-3.32485200	0.18713400
H	-3.33609700	1.76498900	-0.71881000
H	-2.81070000	-1.36743500	-2.11735300
H	-4.26856500	0.12925800	1.15057800
H	-5.18683600	-1.53235200	-0.17922900
H	-5.20075000	-1.90892200	-1.90751600
H	-1.86173500	-3.25856900	-0.81917100
H	-3.74554100	-2.16123800	1.94557300
H	-1.70800300	1.00712900	2.59809700
H	-2.23711700	-1.59152000	2.68740500
H	-3.37075400	1.35222300	3.09249800
H	-3.80101200	-1.05670700	3.32538200
H	-2.73302700	2.05819700	1.60169000
H	-0.16335400	-0.95238100	-1.33512600
O	2.03186500	2.16005200	2.77294900
H	1.57706300	3.00939700	2.73952900
H	2.12479000	1.88318900	1.83243700
H	-0.07358700	-1.98984300	0.30295600

9-Ir

Ir	0.02504700	-0.49372400	0.02323900
P	2.33617600	-0.09587200	0.04103700
N	-0.04963600	1.66782600	-0.13766300
C	2.33949400	1.67357000	0.15804800
C	1.13736400	2.36466700	0.02995100
C	1.06175300	3.80451800	0.06320100
C	-0.13612900	4.44190300	-0.09482000
C	3.25852900	-0.71392800	1.53842300
C	3.03237900	-2.19057800	1.87774200
C	4.75167500	-0.37431800	1.50383400
C	3.37476500	-0.55288000	-1.43486500
C	3.54299500	-2.06375300	-1.61857100
C	2.81607100	0.07956400	-2.71188000
H	3.48639600	-2.41240200	2.85078200
H	0.06568900	-0.16324300	1.77186100
H	-0.18077500	5.52868400	-0.06257500

H	1.98013700	4.36409400	0.21945000
H	4.92907800	0.68207900	1.27352100
H	3.49218100	-2.85750100	1.14190800
H	3.26534600	2.23979100	0.23728500
H	2.79183900	-0.11847200	2.33494600
H	4.35927600	-0.10607500	-1.23847900
H	5.28025900	-0.98007500	0.75856400
H	5.20261800	-0.58504000	2.48041600
H	1.96740800	-2.43464800	1.93708900
H	4.11818100	-2.52226200	-0.80970500
H	1.86040900	-0.37925300	-2.99001400
H	2.56815100	-2.56420000	-1.67254900
H	3.51906000	-0.07796100	-3.53786300
H	4.07446400	-2.26459200	-2.55614100
H	2.65698000	1.15681900	-2.59866200
H	0.01046800	-1.01145000	1.69731200
H	0.10667800	-2.09987300	-0.05445100
P	-2.28499600	-0.27247300	-0.11558400
C	-2.42507700	1.47542800	-0.70140200
C	-1.22188500	2.32000600	-0.34616000
C	-1.31987300	3.69606900	-0.31718700
C	-3.21957900	-1.21233800	-1.41410700
C	-2.93870200	-2.71778800	-1.40193200
C	-4.72358800	-0.92496900	-1.40720000
C	-3.29791500	-0.29878100	1.43732800
C	-3.32924400	-1.68545800	2.08540300
C	-2.81086000	0.75495300	2.43788400
H	-3.42014000	-3.18125100	-2.27039300
H	-2.48201500	1.42167800	-1.79640700
H	-2.27597700	4.18147600	-0.48361400
H	-4.94237000	0.14842100	-1.41001600
H	-3.34066000	-3.20008500	-0.50490000
H	-3.35054300	1.94940300	-0.35918800
H	-2.79113300	-0.80628100	-2.34077200
H	-4.31488300	-0.02655200	1.12645700
H	-5.20672600	-1.37137400	-0.53055900
H	-5.18395600	-1.36409900	-2.29912600
H	-1.86656400	-2.92868000	-1.45258000
H	-3.80306500	-2.43305700	1.44252100
H	-1.80823600	0.51789800	2.80960500
H	-2.31588400	-2.03018500	2.32411800
H	-3.48852500	0.77349200	3.29851800
H	-3.89850800	-1.64055900	3.02059400
H	-2.78831100	1.76283500	2.01003700
H	0.02171300	-0.55567200	-1.57670700

9-Fe

Fe	-0.02602000	-0.33099200	-0.14665000
P	-2.25684900	-0.01301300	-0.03252400
N	0.05534200	1.71943600	0.09826900
C	-2.33459600	1.74953100	-0.09555700
C	-1.12820800	2.43596600	-0.02089400
C	-1.05369300	3.87562400	-0.05953300
C	0.14845900	4.51236100	0.06228100
C	-3.28224800	-0.60056000	-1.48257800
C	-2.97561800	-2.01867400	-1.97343700
C	-4.78658600	-0.39831800	-1.27783200
C	-3.18938500	-0.57115600	1.48251200
C	-3.22777500	-2.09339400	1.64204300
C	-2.63479200	0.08399100	2.74910000
H	-3.58476800	-2.23612500	-2.85892300
H	-0.44723000	-0.03153100	-1.72660100

H	0.19611700	5.59904100	0.02734500
H	-1.97718700	4.43391300	-0.18895400
H	-5.02250800	0.61321700	-0.92861200
H	-3.20525500	-2.77935800	-1.22010600
H	-3.27077500	2.30183200	-0.14040000
H	-2.95487600	0.09302100	-2.26906000
H	-4.21467500	-0.20487600	1.33689600
H	-5.19043700	-1.11315400	-0.55146300
H	-5.31369800	-0.55778900	-2.22560800
H	-1.92484100	-2.12850800	-2.25823500
H	-3.73049100	-2.59051400	0.80730200
H	-1.62637000	-0.28281100	2.97186200
H	-2.21445400	-2.50492800	1.72517500
H	-3.27933700	-0.15946500	3.60183800
H	-3.76891900	-2.35645900	2.55855700
H	-2.58778400	1.17380800	2.65605900
H	0.36952700	-0.09035300	-1.74066100
P	2.18774000	-0.21342500	0.10068100
C	2.43078600	1.53886600	0.61286400
C	1.22466300	2.38194600	0.28193200
C	1.33099100	3.75889200	0.25400800
C	3.00120200	-1.13615700	1.49715000
C	2.62298000	-2.61698600	1.58770800
C	4.52086300	-0.94862100	1.53583300
C	3.30780600	-0.38800000	-1.37181300
C	3.30758500	-1.81453400	-1.92806800
C	2.95096500	0.61741600	-2.47169800
H	3.13192400	-3.06463800	2.44891300
H	2.55188400	1.54007400	1.70344800
H	2.29471200	4.23570800	0.40125600
H	4.81323200	0.10464700	1.46216300
H	2.92478000	-3.17700200	0.69638100
H	3.34609500	1.96816600	0.19350500
H	2.57128500	-0.63787200	2.37645900
H	4.31470800	-0.14557900	-1.00919300
H	5.01004200	-1.49766500	0.72319700
H	4.91184000	-1.33983900	2.48163800
H	1.54740700	-2.75087300	1.72990800
H	3.70042400	-2.54017500	-1.20949600
H	1.99443500	0.37207900	-2.94679400
H	2.29395600	-2.12512500	-2.21018600
H	3.71912000	0.58487300	-3.25215900
H	3.93453400	-1.86076300	-2.82574400
H	2.89428300	1.64702000	-2.10239100
H	-0.01773400	-0.51407200	1.35459900
C	-0.12106900	-2.06843400	-0.24766100
O	-0.19214700	-3.22627200	-0.26842500

9-Co

Co	0.03381900	-0.43522000	0.09747900
P	2.23423100	-0.19231100	0.05995000
N	-0.04931000	1.56229200	-0.10448600
C	2.32781000	1.57118800	0.18895100
C	1.13151400	2.27169700	0.05844000
C	1.05208300	3.71081500	0.07577600
C	-0.14452700	4.34110200	-0.12385000
C	3.15559600	-0.87208100	1.53260400
C	2.83058300	-2.32626300	1.88860100
C	4.66809000	-0.64470300	1.44984700
C	3.21043400	-0.70488000	-1.44027700
C	3.26786600	-2.22236000	-1.63677800
C	2.66718000	-0.02457300	-2.69918200

H	3.31684700	-2.58573300	2.83657000
H	0.14932200	-0.08295200	1.73458500
H	-0.19397300	5.42820100	-0.10986600
H	1.96504600	4.27595700	0.24424800
H	4.91506900	0.39428700	1.20420400
H	3.19377200	-3.02750400	1.13065400
H	3.26671100	2.11584700	0.26409500
H	2.76143600	-0.24109400	2.34075900
H	4.22845000	-0.33005600	-1.26537500
H	5.12713700	-1.29235200	0.69373900
H	5.13308200	-0.88189600	2.41379600
H	1.75407600	-2.48334700	2.00597800
H	3.81743000	-2.72701900	-0.83736900
H	1.67178400	-0.40770600	-2.95230400
H	2.25913900	-2.65151400	-1.68262400
H	3.33280100	-0.22915600	-3.54570400
H	3.77283500	-2.45433000	-2.58188400
H	2.59293300	1.06080600	-2.57639800
H	-0.05981800	-0.85947400	1.68812200
H	0.11807900	-1.91106000	0.11984200
P	-2.15085900	-0.38426300	-0.11237100
C	-2.39220700	1.33919300	-0.72463900
C	-1.21176800	2.20982400	-0.36198500
C	-1.31769600	3.58680200	-0.36868500
C	-2.97473100	-1.41382000	-1.41708900
C	-2.59547900	-2.89672200	-1.36223200
C	-4.49378600	-1.22770500	-1.46602800
C	-3.21491600	-0.45233100	1.40745600
C	-3.18874800	-1.83072200	2.07329500
C	-2.81858200	0.63842800	2.40883800
H	-3.01683900	-3.40942400	-2.23425700
H	-2.44417800	1.27959400	-1.81940100
H	-2.27094300	4.06337300	-0.57329900
H	-4.78208500	-0.17147200	-1.50425900
H	-2.99326100	-3.38620100	-0.46714800
H	-3.33504100	1.77868900	-0.38381000
H	-2.54378600	-0.99891500	-2.33860300
H	-4.23627300	-0.24202200	1.06404800
H	-4.97632800	-1.68324600	-0.59372100
H	-4.89432300	-1.71816600	-2.36020100
H	-1.51064500	-3.03680100	-1.37455000
H	-3.60108100	-2.61098100	1.42670200
H	-1.81736500	0.46115400	2.81557100
H	-2.16598700	-2.11725700	2.34684400
H	-3.52411200	0.63153800	3.24704100
H	-3.78740900	-1.80691500	2.99087100
H	-2.83576300	1.64078800	1.96787000
H	0.04242800	-0.63748000	-1.34736400

10-Ir

Ir	-0.00221900	-0.54702400	-0.02830800
P	-2.29621900	-0.21917700	-0.03173500
N	-0.00145700	1.63425100	0.03949000
C	-2.36308400	1.53565100	-0.62894600
C	-1.12479700	2.31930400	-0.26857500
C	-1.13920100	3.71202500	-0.27664800
C	0.02683200	4.40535600	0.02265200
C	-3.37859400	-1.08847400	-1.26775900
C	-3.17927800	-2.60740500	-1.27843800
C	-4.86046900	-0.71961600	-1.15247000

C	-3.22290500	-0.17066700	1.57332700
C	-3.30246900	-1.55163500	2.23029600
C	-2.61105300	0.85209800	2.53611100
H	-3.75198200	-3.04191100	-2.10556100
H	-2.43018000	1.48508900	-1.72285800
H	0.03944000	5.49157500	0.01042900
H	-2.05716300	4.23632200	-0.52361700
H	-5.01937300	0.36416600	-1.13449300
H	-3.53257900	-3.07125600	-0.35155200
H	-3.25810200	2.06063000	-0.27926400
H	-3.00406700	-0.70156500	-2.22526700
H	-4.23751500	0.16345700	1.32166900
H	-5.30503100	-1.14627500	-0.24604700
H	-5.40600900	-1.12510400	-2.01176200
H	-2.12699700	-2.87588800	-1.41334200
H	-3.85532000	-2.27071800	1.61846000
H	-1.58618600	0.57532500	2.80680900
H	-2.30017400	-1.95626200	2.41490000
H	-3.20732100	0.88400800	3.45480000
H	-3.81615400	-1.46990600	3.19476500
H	-2.59422900	1.86378800	2.11672400
H	-0.00266400	-2.14980900	-0.09811600
P	2.28467500	-0.25294600	0.19488100
C	2.31931700	1.49361700	0.81862400
C	1.12892100	2.30102200	0.36576300
C	1.17457500	3.69198400	0.34831800
C	3.17808300	-1.16016800	1.54771600
C	2.97716100	-2.67766900	1.49736900
C	4.66230000	-0.79949000	1.65364200
C	3.41821500	-0.19893400	-1.27280300
C	3.52043000	-1.56438800	-1.95973900
C	2.96913600	0.88254200	-2.26372100
H	3.41994000	-3.13122200	2.39138500
H	2.27663700	1.42813800	1.91380300
H	2.09906900	4.20089500	0.60271700
H	4.82730400	0.28319200	1.68015200
H	3.46547100	-3.12344400	0.62441000
H	3.25202300	2.00882800	0.56821600
H	2.66546600	-0.79168500	2.44669000
H	4.40734900	0.07755200	-0.88545000
H	5.23024300	-1.21203500	0.81191000
H	5.07783200	-1.22519600	2.57384700
H	1.91621700	-2.94295500	1.46881100
H	3.95958700	-2.32361100	-1.30545300
H	1.95622500	0.67864300	-2.62643900
H	2.53442500	-1.91923000	-2.28160600
H	3.65195900	0.89248200	-3.12129900
H	4.15664700	-1.48253600	-2.84839000
H	2.98570700	1.88355600	-1.81906000
H	0.01607900	-0.67744400	1.56273800
O	-0.06635500	-0.38585400	-2.24086200
H	-0.72024400	-1.02074000	-2.54894800

10-Fe

Fe	-0.03334500	-0.48940400	-0.04385800
P	2.20707900	-0.29127100	0.17236300
N	0.01878700	1.59997400	0.04077100
C	2.26919900	1.38540300	0.94095400
C	1.14511400	2.23943800	0.42628700
C	1.24573000	3.62721000	0.40223900
C	0.14749900	4.37872600	0.00078100
C	3.10134300	-1.32784900	1.43187200

C	3.37153200	-2.75517800	0.94300000
C	4.39549200	-0.69852000	1.95788200
C	3.36615500	-0.19426100	-1.28455400
C	3.14245500	-1.36438100	-2.25195900
C	3.25374800	1.13859400	-2.03501300
H	3.70684800	-3.36928600	1.78619500
H	2.10506300	1.22718000	2.01513100
H	0.20012900	5.46367500	-0.02282100
H	2.17294500	4.10250700	0.70710700
H	4.23066900	0.28196500	2.41402500
H	4.16848200	-2.76766200	0.19097500
H	3.23402900	1.88849800	0.83146900
H	2.37968600	-1.37879800	2.25799600
H	4.38255800	-0.26823200	-0.87525200
H	5.14058900	-0.58601200	1.16190400
H	4.82971100	-1.35195600	2.72337900
H	2.48460600	-3.22945500	0.51201300
H	3.18896200	-2.33865100	-1.75734400
H	2.23686600	1.30524900	-2.40766400
H	2.16531700	-1.27768000	-2.73841200
H	3.92735000	1.12391100	-2.89968100
H	3.91193000	-1.34747400	-3.03251000
H	3.53473000	1.99351200	-1.41248700
H	0.02073800	-0.51633700	1.49051400
P	-2.25748000	-0.14437200	-0.06240900
C	-2.30434600	1.58149900	-0.71709300
C	-1.05607100	2.32776000	-0.32899000
C	-1.02206400	3.72072900	-0.35598600
C	-3.36289900	-1.03044200	-1.27105100
C	-3.15763600	-2.54805600	-1.28887900
C	-4.84447600	-0.67060200	-1.12617800
C	-3.20800800	-0.02822500	1.52863000
C	-3.29232800	-1.38793600	2.22906000
C	-2.60331100	1.02335300	2.46503600
H	-3.81299800	-2.99375600	-2.04617600
H	-2.34158200	1.50337700	-1.80921500
H	-1.90818500	4.27089900	-0.65758300
H	-5.00881200	0.41242900	-1.10300000
H	-3.40193600	-3.00974600	-0.32602300
H	-3.19469500	2.13303700	-0.39758000
H	-3.01179800	-0.64489800	-2.23606900
H	-4.22140900	0.29793600	1.26291600
H	-5.27306800	-1.10079200	-0.21365700
H	-5.40306500	-1.07639900	-1.97719400
H	-2.12669300	-2.81162300	-1.54189000
H	-3.82754400	-2.13122500	1.62972800
H	-1.57710300	0.76000500	2.74453700
H	-2.29111400	-1.77974900	2.44638500
H	-3.20073100	1.07890200	3.38219600
H	-3.82518700	-1.28172700	3.18093000
H	-2.59078000	2.02280000	2.01707400
C	-0.08405300	-2.20879500	0.10693800
O	-0.11954400	-3.35793400	0.30668100
O	-0.19292600	-0.23215000	-2.08363000
H	-0.03171800	-1.07521200	-2.51657700

10-Co

Co	-0.00085600	-0.51782700	-0.10702500
P	-2.19598700	-0.33691700	-0.05769600
N	-0.00837300	1.51935900	0.03020100
C	-2.35481400	1.41141800	-0.64442300
C	-1.12698900	2.20739500	-0.27926000

C	-1.14808700	3.60005400	-0.26648200
C	0.01054200	4.29165600	0.06606200
C	-3.23399500	-1.26612200	-1.28737500
C	-2.95723600	-2.77311000	-1.29857300
C	-4.73297600	-0.97667100	-1.16838800
C	-3.12440600	-0.33587300	1.54851300
C	-3.13779400	-1.72166300	2.20029000
C	-2.55356800	0.70757200	2.51482000
H	-3.50748500	-3.23671000	-2.12536400
H	-2.43912100	1.37430100	-1.73680900
H	0.01986200	5.37808100	0.07353500
H	-2.06471400	4.12489300	-0.51779800
H	-4.94922000	0.09728400	-1.15827300
H	-3.28580600	-3.25495300	-0.37171800
H	-3.25698200	1.90515100	-0.26814300
H	-2.88108400	-0.86065800	-2.24470700
H	-4.15504800	-0.04710100	1.30500400
H	-5.15163600	-1.41862300	-0.25687000
H	-5.25998500	-1.41720700	-2.02220600
H	-1.89283300	-2.98863000	-1.43346300
H	-3.65879500	-2.46339500	1.58754100
H	-1.51405700	0.47706200	2.77399400
H	-2.11708500	-2.08050900	2.37979700
H	-3.14149900	0.70512600	3.43956100
H	-3.65079900	-1.66901300	3.16729200
H	-2.58730600	1.72210300	2.10339100
H	0.00575800	-1.99896400	-0.14848400
P	2.17858800	-0.36956500	0.18118500
C	2.28866700	1.35858200	0.83730900
C	1.10976800	2.18424800	0.38977000
C	1.15384500	3.57578000	0.40229300
C	2.97762600	-1.35208100	1.54176500
C	2.70362800	-2.85658700	1.45381600
C	4.47351600	-1.07156700	1.70763300
C	3.37229500	-0.35365800	-1.24200400
C	3.43458000	-1.71551900	-1.94130000
C	3.02181300	0.75585700	-2.24106000
H	3.09512200	-3.34892100	2.35135700
H	2.25167100	1.28569400	1.93203300
H	2.07214300	4.08130200	0.68484000
H	4.69279400	0.00042000	1.76356600
H	3.19724100	-3.30966500	0.58756700
H	3.23208000	1.85213900	0.58340900
H	2.45408900	-0.97621400	2.43121000
H	4.35848400	-0.13098400	-0.81413800
H	5.05029700	-1.49590900	0.87779500
H	4.83342300	-1.53682600	2.63223800
H	1.63275900	-3.06935700	1.38635800
H	3.81354900	-2.50171100	-1.28125600
H	2.02946600	0.58678300	-2.67094400
H	2.44485200	-2.01949000	-2.30232000
H	3.75990500	0.75880200	-3.05172100
H	4.10521300	-1.65559200	-2.80623200
H	3.03596600	1.74959200	-1.78002300
H	0.03243600	-0.65931000	1.37154200
O	-0.09981200	-0.36020200	-2.11441500
H	-0.52095900	-1.15257900	-2.46073300

11-Ir

Ir	0.03505400	-0.51433500	0.00019300
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P	2.33615900	-0.07138800	-0.02858000
N	-0.07440700	1.63051000	-0.22694300
C	2.29637000	1.69341700	0.17993500
C	1.08224000	2.35888500	0.01135100
C	0.96121500	3.79433200	0.07305300
C	-0.24828900	4.39885800	-0.12741800
C	3.38288800	-0.71704100	1.37481400
C	3.20188800	-2.20804000	1.67723400
C	4.86456600	-0.35365600	1.23357400
C	3.30195800	-0.42261100	-1.58346000
C	3.49576100	-1.91710000	-1.85511200
C	2.64984700	0.25804600	-2.78988900
H	3.75618400	-2.46487200	2.58778200
H	0.58556900	0.75960800	2.43572300
H	-0.32691000	5.48303200	-0.07532900
H	1.85340600	4.37865300	0.28242800
H	5.00872400	0.71203700	1.02365600
H	3.58395200	-2.84139500	0.87030900
H	3.20472200	2.28213900	0.29436800
H	2.98397000	-0.15737000	2.23135200
H	4.28523000	0.04103900	-1.42486500
H	5.34098500	-0.92714200	0.42992400
H	5.39410300	-0.58720900	2.16451600
H	2.14981100	-2.46536100	1.83582500
H	4.12167300	-2.40200300	-1.10078000
H	1.68995500	-0.21171800	-3.03340700
H	2.53107100	-2.43885600	-1.88582200
H	3.30324700	0.16274300	-3.66483100
H	3.98294100	-2.05662400	-2.82742300
H	2.47221800	1.32352400	-2.61054500
H	0.12236100	-2.11425500	0.22924800
P	-2.27149800	-0.34081400	-0.18740100
C	-2.40789500	1.36694700	-0.88793900
C	-1.25673000	2.25265100	-0.46974800
C	-1.39871500	3.62456900	-0.41813700
C	-3.15084000	-1.36141500	-1.46385100
C	-3.09210400	-2.86479900	-1.17818200
C	-4.58912700	-0.91159500	-1.73638100
C	-3.33943300	-0.33544300	1.33334100
C	-3.06605000	-1.56917900	2.20222200
C	-3.15767800	0.94836000	2.15258200
H	-3.44731400	-3.41613900	-2.05588700
H	-2.35032200	1.24066600	-1.97769100
H	-2.36069800	4.08619100	-0.61566700
H	-4.65720600	0.15734800	-1.96315000
H	-3.73891100	-3.13511100	-0.33638900
H	-3.36999900	1.84123000	-0.67344600
H	-2.55039200	-1.16690700	-2.36321900
H	-4.37845000	-0.37277100	0.98181600
H	-5.24164800	-1.12363700	-0.88200400
H	-4.98561600	-1.46179800	-2.59723000
H	-2.07425500	-3.19953200	-0.95330500
H	-3.20884000	-2.50666400	1.65702100
H	-2.11546500	1.07424900	2.46345900
H	-2.03938600	-1.55156200	2.58391200
H	-3.77494900	0.88924900	3.05644600
H	-3.74805300	-1.57308500	3.06021900
H	-3.46441700	1.84168100	1.60013200
H	0.04252200	-0.81741500	-1.53053200
O	0.06755700	-0.04775300	2.30644800
H	0.55229100	-0.73776400	2.77734300

11-Fe

Fe	-0.05027900	-0.42189300	-0.00137300
P	-2.28516600	0.00185800	0.00817500
N	0.09311300	1.62822300	0.19699500
C	-2.24541600	1.74507700	-0.31163700
C	-1.02684500	2.38908300	-0.10488800
C	-0.87259900	3.81916200	-0.19759400
C	0.33602100	4.40383400	0.05844300
C	-3.34956400	-0.70514400	-1.35819800
C	-3.13067600	-2.19432400	-1.64237500
C	-4.83876500	-0.38762000	-1.18706200
C	-3.26026900	-0.26925000	1.57522000
C	-3.39266000	-1.75061200	1.94073100
C	-2.65159100	0.51701600	2.73918700
H	-3.76581400	-2.50371600	-2.48112300
H	0.44278300	5.48468600	-0.01105700
H	-1.74089400	4.41460500	-0.46759200
H	-5.01289700	0.67487200	-0.98320300
H	-3.38768500	-2.82324900	-0.78356100
H	-3.14014500	2.33913900	-0.48825100
H	-2.99534800	-0.14977600	-2.23662800
H	-4.26054200	0.13983300	1.38026900
H	-5.28023100	-0.96823500	-0.36873000
H	-5.37970500	-0.64666300	-2.10468700
H	-2.09218700	-2.40541700	-1.91501600
H	-3.96368800	-2.31581600	1.19809000
H	-1.67046000	0.11385700	3.01486900
H	-2.40582200	-2.21960600	2.04117400
H	-3.30567700	0.44479700	3.61606900
H	-3.90979600	-1.85243500	2.90230200
H	-2.52709400	1.57662000	2.49220000
P	2.19304300	-0.33503600	0.19293300
C	2.37535000	1.33174700	0.95706400
C	1.26777300	2.23997300	0.49047800
C	1.44645400	3.60796300	0.42940400
C	3.06477800	-1.42957300	1.41746600
C	3.20506700	-2.87772700	0.93642600
C	4.42479500	-0.89063600	1.87315500
C	3.28193200	-0.31756500	-1.31741500
C	2.93317800	-1.47683800	-2.26068100
C	3.20797100	1.01687200	-2.06925800
H	3.54138500	-3.50517000	1.76938800
H	2.25265200	1.17647000	2.03735900
H	2.40935900	4.04727800	0.66920700
H	4.35407200	0.10789400	2.31428900
H	3.95664100	-2.95657000	0.14280100
H	3.36041900	1.78165600	0.80347500
H	2.38232500	-1.41903900	2.27792400
H	4.31168200	-0.45289600	-0.96065900
H	5.13902900	-0.84900600	1.04276600
H	4.84356100	-1.56086600	2.63268400
H	2.26380500	-3.29068600	0.56145500
H	2.96052700	-2.45036700	-1.76308500
H	2.18220100	1.23485700	-2.38571000
H	1.93250100	-1.34050500	-2.68341100
H	3.83334400	0.96123200	-2.96791200
H	3.64983500	-1.50395400	-3.08976800
H	3.56823500	1.85555000	-1.46581000
H	-0.03814500	-0.61253500	1.49732500
C	-0.18929700	-2.14582500	-0.02719500
O	-0.28806500	-3.30455100	0.06160000
O	-0.07031900	0.06221900	-2.10941300

H	-0.48314900	-0.61773700	-2.65692300
H	-0.63453100	0.84522000	-2.20552700

11-Co

Co	-0.04152700	-0.48164300	-0.07100500
P	-2.25117700	-0.18497600	-0.01235000
N	0.06539600	1.50846700	0.19277600
C	-2.27341000	1.56627200	-0.30840900
C	-1.07398800	2.24545000	-0.08584300
C	-0.94984600	3.67976600	-0.12927700
C	0.24834700	4.27839300	0.15048100
C	-3.29542400	-0.93667800	-1.36449500
C	-3.04274500	-2.42657300	-1.61665600
C	-4.79088600	-0.64829600	-1.19703800
C	-3.17572000	-0.50608800	1.57420600
C	-3.26085500	-1.99352600	1.92839100
C	-2.55381500	0.28282400	2.72946100
H	-3.61272300	-2.75010700	-2.49580700
H	-0.62827300	0.67181000	-2.30844600
H	0.33164200	5.36310400	0.11878600
H	-1.82832500	4.26893300	-0.37939000
H	-4.98768100	0.41498700	-1.01966700
H	-3.36073600	-3.04625200	-0.77201000
H	-3.19000600	2.13518800	-0.45305400
H	-2.95178000	-0.38983600	-2.25245800
H	-4.19096500	-0.12038400	1.40938100
H	-5.21564700	-1.21771100	-0.36219200
H	-5.32913500	-0.94285600	-2.10547000
H	-1.98406100	-2.63206400	-1.80331200
H	-3.85456000	-2.56216500	1.20694900
H	-1.55582200	-0.10018500	2.97239000
H	-2.26113200	-2.44294400	1.97788200
H	-3.18019300	0.18444400	3.62372400
H	-3.73093900	-2.11502100	2.91152700
H	-2.46141600	1.34779300	2.49193200
H	-0.11707700	-1.95963400	-0.27035500
P	2.14952100	-0.45803500	0.18616000
C	2.34853900	1.21152200	0.95225000
C	1.22894600	2.12439300	0.51157400
C	1.37768000	3.49763500	0.49706600
C	2.92274000	-1.57515000	1.45080900
C	2.76454800	-3.06431800	1.13003100
C	4.38236700	-1.23749100	1.76726700
C	3.27907000	-0.44301100	-1.29070100
C	3.01951000	-1.64923600	-2.20151300
C	3.16010800	0.86284500	-2.08641300
H	3.05553200	-3.65722900	2.00439200
H	2.25500000	1.05942100	2.03596700
H	2.32886700	3.95223500	0.75452700
H	4.52224400	-0.17992700	2.01432300
H	3.41425600	-3.36383000	0.30051100
H	3.33022600	1.66028200	0.77402800
H	2.31661500	-1.35895600	2.34117400
H	4.30189400	-0.51029000	-0.89801600
H	5.03912300	-1.48305700	0.92521800
H	4.71547800	-1.82923200	2.62745400
H	1.73280700	-3.32159600	0.87047600
H	3.12998300	-2.60296300	-1.67763300
H	2.13887100	1.01008400	-2.45202100
H	2.00848200	-1.60721000	-2.62098400
H	3.82780900	0.81726500	-2.95456500
H	3.73200900	-1.64076800	-3.03439500

H	3.44571300	1.73857700	-1.49554900
H	-0.05380900	-0.77837900	1.35334300
O	-0.05051200	-0.08998200	-2.15017500
H	-0.43089100	-0.81383500	-2.66385600

12-Ir

Ir	0.00438900	-0.47740700	-0.07173800
P	2.31371900	-0.11225900	-0.01209700
N	-0.04892000	1.67642200	-0.16069100
C	2.36017700	1.66044700	-0.03462300
C	1.15910100	2.36175700	-0.06309800
C	1.10648200	3.80248100	0.00535500
C	-0.08965800	4.45856500	-0.04206200
C	3.13440300	-0.61118700	1.58958600
C	2.80385200	-2.02937500	2.06611800
C	4.64312200	-0.34849100	1.59961800
C	3.41696300	-0.71574700	-1.38047900
C	3.59636700	-2.23648700	-1.38439000
C	2.89903400	-0.23618700	-2.73912500
H	3.23908000	-2.19196800	3.05950300
H	-0.11612400	5.54482800	0.01785200
H	2.04247200	4.34625800	0.10176400
H	4.88366900	0.67009700	1.27500800
H	3.20962700	-2.79609100	1.39844400
H	3.29417700	2.21542700	0.02788300
H	2.66587600	0.08755500	2.29619100
H	4.39234200	-0.24303000	-1.19952600
H	5.17502800	-1.04899700	0.94526700
H	5.03744300	-0.47944000	2.61407500
H	1.72253500	-2.18359200	2.13854400
H	4.12699200	-2.59767300	-0.49895100
H	1.94958700	-0.72418600	-2.98917200
H	2.62638800	-2.74660100	-1.43346000
H	3.62407100	-0.48936100	-3.52114800
H	4.17821600	-2.53697000	-2.26354300
H	2.74093400	0.84696100	-2.75713900
H	0.05369600	-2.09098100	0.04854900
P	-2.29306700	-0.23853500	-0.09415500
C	-2.47480300	1.54854900	-0.53059500
C	-1.22425200	2.35653400	-0.25657500
C	-1.29849800	3.73190400	-0.18271200
C	-3.38411400	-1.08284700	-1.32933900
C	-3.12687300	-2.58937800	-1.42942100
C	-4.87017800	-0.77180000	-1.12963500
C	-3.07088800	-0.35555900	1.58236600
C	-3.20933100	-1.79990000	2.07074700
C	-2.21913200	0.46442900	2.55944100
H	-3.71397300	-3.00264200	-2.25727000
H	-2.66723600	1.58443500	-1.61071700
H	-2.25771200	4.23377800	-0.25823500
H	-5.06260800	0.30501200	-1.07093200
H	-3.42410900	-3.11581000	-0.51667200
H	-3.34340600	2.00092700	-0.04073400
H	-3.05829100	-0.63030800	-2.27633800
H	-4.06827200	0.09785700	1.51127700
H	-5.25320300	-1.23803200	-0.21464800
H	-5.44591100	-1.17096300	-1.97205000
H	-2.07071100	-2.80442700	-1.61870900
H	-3.91346000	-2.37737400	1.46464900
H	-1.19666000	0.06490700	2.60853900

H	-2.24150800	-2.31574800	2.05719000
H	-2.65219900	0.41364000	3.56453700
H	-3.57784500	-1.80254700	3.10281500
H	-2.15664000	1.52006300	2.27330700
H	0.04177400	-0.70400500	-1.59077200

12-Fe

Fe	-0.00092200	-0.33186000	-0.11320800
P	2.24392100	-0.03707000	-0.03338200
N	-0.06567300	1.69854300	-0.18805900
C	2.33946000	1.72737100	-0.06807900
C	1.13368600	2.40921100	-0.08453900
C	1.07271300	3.85086400	0.00541000
C	-0.12357900	4.50075900	-0.03724700
C	3.05117100	-0.53143800	1.58024000
C	2.66097600	-1.91762100	2.10361600
C	4.57109100	-0.34196000	1.57383800
C	3.34935100	-0.68294600	-1.38329900
C	3.45063000	-2.21075700	-1.40329900
C	2.90192900	-0.16050000	-2.75119000
H	3.14671500	-2.09256000	3.07114400
H	-0.15931200	5.58574600	0.03834200
H	2.00734900	4.39480900	0.11334800
H	4.85928400	0.65024400	1.20874200
H	2.97170600	-2.72112100	1.42768900
H	3.27266700	2.28004000	0.01531700
H	2.62361100	0.20874600	2.27021100
H	4.34312600	-0.26602100	-1.16957200
H	5.06475200	-1.09241900	0.94542300
H	4.96393700	-0.45290400	2.59121700
H	1.57971000	-2.00012700	2.25269500
H	3.89463700	-2.61394600	-0.48847000
H	1.93464500	-0.58918000	-3.03738900
H	2.46352100	-2.66984200	-1.53517000
H	3.63689200	-0.44592100	-3.51278600
H	4.07995700	-2.52704800	-2.24339800
H	2.80665500	0.93004300	-2.75964300
P	-2.22924600	-0.18372800	-0.12335900
C	-2.48362400	1.58279600	-0.56380800
C	-1.23990100	2.39077800	-0.28368400
C	-1.32516000	3.76212200	-0.19509000
C	-3.30940500	-1.07102100	-1.34124900
C	-2.99082600	-2.56282700	-1.47614300
C	-4.80228900	-0.83013100	-1.09710400
C	-2.99193100	-0.32758000	1.56033800
C	-3.04941400	-1.77471600	2.05758400
C	-2.18838100	0.54362100	2.53399400
H	-3.62855700	-2.99890700	-2.25338300
H	-2.67758000	1.61569700	-1.64336700
H	-2.28933200	4.25462100	-0.26945400
H	-5.04005200	0.23575300	-1.01131900
H	-3.17897500	-3.11028400	-0.54668500
H	-3.35752400	2.01748300	-0.06772900
H	-3.03347100	-0.59134000	-2.29043600
H	-4.01339600	0.06896200	1.49088900
H	-5.14113400	-1.33021400	-0.18266600
H	-5.38145400	-1.23807600	-1.93292200
H	-1.94867600	-2.72691500	-1.76500100
H	-3.71221100	-2.39740000	1.44936300
H	-1.14737000	0.19902100	2.59534100
H	-2.05308100	-2.23340300	2.05809500
H	-2.62508200	0.47932500	3.53683700

H	-3.42675500	-1.79286200	3.08634900
H	-2.17880300	1.59858100	2.23909600
H	0.00812600	-0.57754500	-1.58333500
C	0.07199800	-2.05923200	0.00185700
O	0.12600800	-3.22265700	0.01508600

12-Co

Co	0.00538000	-0.40761200	-0.09781400
P	2.21121400	-0.21240700	-0.04732800
N	-0.04777100	1.57995300	-0.15184400
C	2.35479100	1.55190300	-0.07911400
C	1.16331600	2.26671500	-0.07781100
C	1.11925300	3.70771600	-0.00211200
C	-0.07487000	4.36754500	-0.03021400
C	2.97158600	-0.75351500	1.57112300
C	2.52648900	-2.13492800	2.06234500
C	4.49624000	-0.60947700	1.59302600
C	3.28000300	-0.90449000	-1.39902200
C	3.33263100	-2.43498600	-1.39916400
C	2.82342300	-0.38576000	-2.76534100
H	2.95084500	-2.32364900	3.05583700
H	-0.09703000	5.45377800	0.03266800
H	2.05924100	4.24684400	0.08093400
H	4.81808100	0.38218000	1.25545300
H	2.86447900	-2.93878900	1.40034100
H	3.30363300	2.08089000	-0.02101400
H	2.55315800	-0.01051700	2.26373300
H	4.28894300	-0.51489400	-1.20483800
H	4.97745700	-1.35927000	0.95426600
H	4.86977500	-0.75522100	2.61329700
H	1.43642400	-2.19928100	2.13993700
H	3.80892300	-2.83744800	-0.50063500
H	1.83914500	-0.79108800	-3.02758300
H	2.32565900	-2.86358000	-1.47342200
H	3.53523200	-0.70175500	-3.53661300
H	3.91000200	-2.78329400	-2.26347800
H	2.75841100	0.70680300	-2.78657900
H	0.05087400	-1.89520700	0.01181900
P	-2.18534400	-0.32870900	-0.11242800
C	-2.47275000	1.45724800	-0.47124000
C	-1.21945600	2.27006800	-0.22948400
C	-1.28892100	3.64469600	-0.15500000
C	-3.22376800	-1.20019500	-1.37091700
C	-2.86842100	-2.68183000	-1.52719300
C	-4.72535400	-0.99345400	-1.15193100
C	-2.92779600	-0.56505100	1.56860500
C	-2.97158900	-2.03508000	1.99456400
C	-2.11490400	0.26229900	2.57309700
H	-3.43452500	-3.10293900	-2.36562000
H	-2.73041400	1.53364900	-1.53520500
H	-2.24796100	4.14919900	-0.21406600
H	-4.98582100	0.06644300	-1.05772200
H	-3.12202000	-3.25906900	-0.63228500
H	-3.32057100	1.86331500	0.09056400
H	-2.93586200	-0.69251100	-2.30178200
H	-3.95210700	-0.17115900	1.53064000
H	-5.06990600	-1.51168000	-0.24984900
H	-5.28094400	-1.40237300	-2.00311900
H	-1.80221500	-2.81952600	-1.73113500
H	-3.65056600	-2.62718300	1.37407200
H	-1.07673400	-0.09403300	2.61826800
H	-1.97535100	-2.49102400	1.94532800

H	-2.54933100	0.16222600	3.57389400
H	-3.32235400	-2.10361600	3.03056000
H	-2.09773500	1.32784000	2.31934500
H	0.02283700	-0.63799000	-1.51109500

TS_{1,2-Ir}

Ir	-0.03527800	-0.46347500	-0.33218800
P	2.25258600	-0.12082700	-0.26753400
N	-0.06092500	1.67162100	0.12375000
C	2.31101000	1.45133600	0.71420100
C	1.06532200	2.28564500	0.54950900
C	1.07006200	3.64256700	0.86243700
C	-0.10846400	4.37010500	0.75231800
C	3.35460800	-1.24187500	0.72567500
C	3.13873900	-2.72538200	0.41132500
C	4.83812700	-0.86760200	0.66557200
C	3.17855000	0.30650600	-1.81801600
C	3.27307500	-0.88415100	-2.77582000
C	2.56120400	1.51929600	-2.52133000
H	3.72881400	-3.33280400	1.10691600
H	2.37639700	1.14930000	1.76731300
H	-0.12790700	5.42712800	1.00235700
H	1.99034500	4.11091900	1.19730600
H	5.00899100	0.19293600	0.88040600
H	3.46104100	-2.97666600	-0.60479200
H	3.20221700	2.04828700	0.49451100
H	3.00170600	-1.06878800	1.75148100
H	4.18915700	0.58221100	-1.49045400
H	5.26427600	-1.09121600	-0.31899800
H	5.39191100	-1.45404000	1.40711200
H	2.08737600	-3.00905600	0.51644300
H	3.82236100	-1.72466200	-2.34066100
H	1.53990300	1.30426300	-2.85444700
H	2.27473100	-1.23731000	-3.06061300
H	3.16038200	1.76760500	-3.40441800
H	3.79661400	-0.58033700	-3.68927800
H	2.53364700	2.40621900	-1.87912600
H	0.00184800	-0.88840100	1.33974200
H	-0.01549300	-2.02925200	-0.67591100
P	-2.32614700	-0.16828500	-0.36906500
C	-2.40597600	1.67000000	-0.58968000
C	-1.20621200	2.37751100	-0.01256700
C	-1.26080500	3.72988700	0.31152900
C	-3.30366200	-0.77253800	-1.82823800
C	-3.11948100	-2.26763300	-2.10448200
C	-4.78720900	-0.39754700	-1.77901200
C	-3.35632800	-0.47132700	1.14537000
C	-3.32503400	-1.94293800	1.56789100
C	-2.92170300	0.43240000	2.30391300
H	-3.59949400	-2.52144900	-3.05631700
H	-2.40340400	1.84253900	-1.67405700
H	-2.19660100	4.26904800	0.20183300
H	-4.94308400	0.66573500	-1.56637200
H	-3.58389300	-2.88260900	-1.32635100
H	-3.33306100	2.10253300	-0.20091500
H	-2.83315400	-0.22467100	-2.65620800
H	-4.38343400	-0.20039800	0.87023200
H	-5.31792200	-0.98079000	-1.01794800

H	-5.25134900	-0.61780600	-2.74680400
H	-2.06182800	-2.53961500	-2.17141600
H	-3.71983900	-2.60734700	0.79347900
H	-1.87741000	0.25248600	2.58021700
H	-2.30109200	-2.25904400	1.80047000
H	-3.54232500	0.21844100	3.18123100
H	-3.93391100	-2.08003600	2.46861900
H	-3.03535000	1.49578000	2.06948000
H	-0.09263300	-0.17098400	-1.94191100
C	0.49277100	-1.16263000	2.90884000
O	0.66334500	-0.06921100	3.34366600
O	0.46618200	-2.34891800	2.97789000

TS_{1,2-Fe}

Fe	-0.04174600	-0.41372300	-0.26481600
P	-2.25280300	-0.16859600	-0.37546200
N	-0.04976700	1.67867100	-0.13398200
C	-2.37951000	1.60922300	-0.85422400
C	-1.18342600	2.37797600	-0.36814000
C	-1.24007100	3.76053600	-0.21735000
C	-0.09472600	4.45119400	0.15812000
C	-3.22526500	-0.96742000	-1.75103000
C	-3.02419700	-2.48031700	-1.87367200
C	-4.71650200	-0.61785800	-1.73301900
C	-3.31834600	-0.27944600	1.14535400
C	-3.26089200	-1.68056100	1.76185200
C	-2.92988300	0.78356000	2.17833100
H	-3.60109700	-2.85122100	-2.72874700
H	-2.37873200	1.63964300	-1.95147400
H	-0.11356100	5.53088000	0.27728300
H	-2.17490200	4.27948000	-0.40570400
H	-4.89508100	0.45737000	-1.62399300
H	-3.37303700	-3.01461700	-0.98352700
H	-3.30982300	2.07942400	-0.52123600
H	-2.77519500	-0.50730300	-2.64102600
H	-4.34665100	-0.07471100	0.82308600
H	-5.23476200	-1.13522300	-0.91758400
H	-5.17705300	-0.94059300	-2.67350100
H	-1.97611500	-2.74006300	-2.04045800
H	-3.62361600	-2.45111800	1.07424200
H	-1.88528200	0.67779300	2.48905900
H	-2.23496200	-1.93742300	2.05225800
H	-3.55791900	0.67111000	3.06947500
H	-3.88500500	-1.71602100	2.66215400
H	-3.07089900	1.80182800	1.80121200
H	-0.13490100	-0.30560800	-1.80925900
P	2.17530100	-0.12851400	-0.28147000
C	2.31195600	1.54810400	0.47922900
C	1.06713300	2.35120400	0.22181500
C	1.07636300	3.73623400	0.36979600
C	3.31803900	-1.10623100	0.82235200
C	3.12118800	-2.62290800	0.74333100
C	4.79499700	-0.73463000	0.65780000
C	3.07335900	0.06849300	-1.89795500
C	3.09264000	-1.23757500	-2.69716200
C	2.47646600	1.20432100	-2.73521700
H	3.81183200	-3.11241800	1.43970700
H	2.40828300	1.39911800	1.56184100
H	1.99760300	4.23512200	0.65457500
H	4.96080400	0.34750000	0.69768600
H	3.32871800	-3.01412300	-0.25846000
H	3.20002700	2.09593100	0.14722600

H	3.00279200	-0.79093600	1.82624000
H	4.10402900	0.34415200	-1.64255900
H	5.19431700	-1.10786700	-0.29217600
H	5.37752800	-1.19342700	1.46453900
H	2.10521700	-2.91441700	1.02063800
H	3.62707700	-2.03616700	-2.17334500
H	1.43528200	0.99273400	-3.00231900
H	2.07326200	-1.58560400	-2.90410100
H	3.05011300	1.30997000	-3.66303100
H	3.59383800	-1.07567200	-3.65831500
H	2.50818300	2.16764300	-2.21484300
H	0.03263600	-0.44924900	1.34022700
C	-0.03957600	-2.13689700	-0.35235300
O	-0.04156500	-3.30226600	-0.40337500
C	0.47430200	-0.59423600	3.02563600
O	0.65487500	0.54053000	3.31640800
O	0.40781800	-1.76448400	3.19700500

TS_{1,2-co}

Co	-0.03372300	-0.44809500	-0.30039200
P	2.14529600	-0.25624200	-0.29409900
N	-0.04429400	1.55986000	-0.01704200
C	2.30317000	1.34747800	0.61678600
C	1.07120700	2.19046500	0.40819700
C	1.07943100	3.56034200	0.65841800
C	-0.08819100	4.29029000	0.47216600
C	3.21134300	-1.39578800	0.71751700
C	2.92963500	-2.87908400	0.45842800
C	4.70859400	-1.08899300	0.62133500
C	3.06350000	0.06549800	-1.87638100
C	3.07363400	-1.16142700	-2.79224900
C	2.49186700	1.28186200	-2.61198800
H	3.50506500	-3.48652600	1.16631900
H	2.37859200	1.10127800	1.68327800
H	-0.10695100	5.35851400	0.66947200
H	1.99360400	4.03727400	0.99824600
H	4.92756800	-0.02949600	0.79391300
H	3.22641700	-3.17855000	-0.55238800
H	3.20513200	1.90714500	0.34773000
H	2.88588700	-1.17463400	1.74284300
H	4.09500500	0.29969700	-1.58353600
H	5.10804400	-1.36579300	-0.36097800
H	5.24995200	-1.67169800	1.37502800
H	1.86967500	-3.11693800	0.58650100
H	3.59191000	-2.01273300	-2.34055600
H	1.44935900	1.11140400	-2.90357700
H	2.05205800	-1.47391500	-3.04010200
H	3.07386500	1.46022800	-3.52314700
H	3.58729500	-0.91735600	-3.72905000
H	2.53439600	2.19418300	-2.00731300
H	0.02180800	-0.73075600	1.25117200
H	-0.02394900	-1.91384100	-0.50642800
P	-2.20445200	-0.28660900	-0.44409500
C	-2.35186100	1.52329300	-0.79999000
C	-1.17423200	2.26938300	-0.22913000
C	-1.22951500	3.63746000	0.02010700
C	-3.08663100	-1.04736000	-1.89277400
C	-2.80734800	-2.54361800	-2.06282500
C	-4.59066600	-0.76168400	-1.92148900
C	-3.30716800	-0.51967900	1.03367200
C	-3.25395700	-1.95806600	1.55682900
C	-2.96307800	0.47485300	2.14731700

H	-3.25123300	-2.89033000	-3.00305200
H	-2.32356500	1.63164100	-1.89210000
H	-2.15605000	4.17661700	-0.15148200
H	-4.81670900	0.30160000	-1.78493000
H	-3.24907600	-3.13288200	-1.25221100
H	-3.29690100	1.95703500	-0.45868100
H	-2.61836900	-0.52799100	-2.73979100
H	-4.32716800	-0.30335500	0.69183100
H	-5.11566400	-1.32585200	-1.14217800
H	-5.00331600	-1.07123800	-2.88823500
H	-1.73434900	-2.75385000	-2.09326400
H	-3.59426900	-2.68355200	0.81172800
H	-1.92781600	0.35738300	2.48356200
H	-2.23412500	-2.22767000	1.85602500
H	-3.61747000	0.29658900	3.00806500
H	-3.90041600	-2.05496200	2.43655100
H	-3.10299300	1.51487700	1.83518200
H	-0.09780200	-0.31427600	-1.79846900
C	0.38990300	-0.96366400	2.92668500
O	0.56258000	0.14834800	3.30082100
O	0.31650300	-2.14264000	3.02580800

TS_{4,5-Ir}

Ir	-0.02747900	-0.56592100	0.03091300
P	2.28089300	-0.28208400	-0.02206600
N	0.00357800	1.60717000	-0.20369800
C	2.38112700	1.51554400	0.40816500
C	1.15732300	2.28721100	-0.01647800
C	1.20582400	3.67057400	-0.16439100
C	0.04449400	4.36084600	-0.48878000
C	3.34074400	-1.07409200	1.27849900
C	3.08405800	-2.57678800	1.42967000
C	4.83327800	-0.77327500	1.11751100
C	3.17900600	-0.40834900	-1.63764400
C	3.21016500	-1.84349000	-2.17002000
C	2.58715500	0.54494900	-2.68074900
H	3.65254000	-2.95490600	2.28673000
H	2.41819900	1.55062600	1.50472300
H	0.05910000	5.44182800	-0.59543800
H	2.14590800	4.19172700	-0.01311300
H	5.03134800	0.29762800	0.99897100
H	3.40551600	-3.13684400	0.54527100
H	3.28862900	1.98954600	0.02111900
H	2.98345800	-0.58718300	2.19593900
H	4.20578100	-0.08429000	-1.42410900
H	5.25140600	-1.29812100	0.25094900
H	5.37242000	-1.11850300	2.00652600
H	2.02457800	-2.78847900	1.60213600
H	3.74290700	-2.52343700	-1.49838300
H	1.55016400	0.28000300	-2.91469500
H	2.19428600	-2.22962800	-2.31565100
H	3.17149200	0.47391700	-3.60475300
H	3.72087200	-1.86322100	-3.13919700
H	2.61008200	1.58983700	-2.35357400
H	-0.13780900	-0.83356900	1.76174300
H	-0.03704800	-2.16446300	0.07853300
P	-2.31542900	-0.26120000	-0.18246000
C	-2.35659600	1.45726300	-0.87490500
C	-1.12352200	2.26530200	-0.55427600
C	-1.13399500	3.65102700	-0.68476000

C	-3.23243900	-1.22799400	-1.47454400
C	-3.01159200	-2.74043600	-1.37674500
C	-4.72308900	-0.88513000	-1.54552500
C	-3.40038400	-0.15894800	1.31668500
C	-3.51802600	-1.50769400	2.03166900
C	-2.90700100	0.92351300	2.28164100
H	-3.48380700	-3.22899300	-2.23638200
H	-2.40294900	1.34695300	-1.96612500
H	-2.05629600	4.15613100	-0.95390800
H	-4.90012400	0.19411100	-1.60884200
H	-3.46015600	-3.16011400	-0.47032500
H	-3.25930700	2.00012900	-0.57698600
H	-2.75082400	-0.88568500	-2.40074000
H	-4.38990500	0.13696100	0.94511400
H	-5.25894400	-1.26995500	-0.67040600
H	-5.16238400	-1.35046700	-2.43473900
H	-1.94759300	-2.99378100	-1.38121800
H	-3.99618200	-2.26834700	1.40744300
H	-1.91754900	0.67781200	2.68140100
H	-2.53115700	-1.87967200	2.33257700
H	-3.60345300	0.99922300	3.12405900
H	-4.12370700	-1.39028700	2.93712200
H	-2.84763100	1.91063600	1.81042000
H	-0.04589900	-0.71883700	-1.56721600
O	0.75379800	1.02933200	3.09853400
H	0.15860300	0.90038000	3.84682700
H	0.20477600	-0.04849700	1.94325700

TS_{4,5-Fe}

P	2.22101900	-0.19352800	-0.00345600
N	-0.03279000	1.56825600	-0.21419900
C	2.31728700	1.58783600	0.45765200
C	1.07307400	2.30924400	0.02170100
C	1.06608800	3.69610600	-0.10442900
C	-0.10775600	4.34053800	-0.47049300
C	3.27447000	-0.98915400	1.30677200
C	3.01673800	-2.48963400	1.47587900
C	4.76906100	-0.69491600	1.15065600
C	3.16052200	-0.29517000	-1.59932200
C	3.19422900	-1.72377000	-2.14979300
C	2.59377500	0.67342800	-2.64251600
H	3.63808600	-2.87230800	2.29354400
H	2.35166600	1.62229100	1.55338300
H	-0.13916700	5.42257300	-0.56234900
H	1.97687300	4.25287100	0.09281200
H	4.97078800	0.37376800	1.01847900
H	3.27008400	-3.05598000	0.57326400
H	3.21288900	2.08359300	0.06999400
H	2.91866000	-0.49450400	2.22066000
H	4.18486600	0.02027600	-1.36360700
H	5.19114300	-1.23203500	0.29347100
H	5.30270000	-1.02956200	2.04715000
H	1.97164800	-2.69351900	1.72667300
H	3.69010500	-2.42031200	-1.46660000
H	1.55933000	0.41757600	-2.89701800
H	2.18000600	-2.09409100	-2.34150300
H	3.19390100	0.61033500	-3.55715900
H	3.74237800	-1.73923000	-3.09853600
H	2.61653900	1.71422700	-2.30228800
H	-0.13141000	-0.67452600	1.63158500
P	-2.22407700	-0.31631500	-0.17343500
C	-2.33022400	1.32536100	-0.99964600

C	-1.16470200	2.19166700	-0.61369800
C	-1.23805200	3.57604500	-0.73186000
C	-3.18014400	-1.40467100	-1.33604300
C	-3.39628200	-2.82124500	-0.79203800
C	-4.51662400	-0.80541500	-1.78683700
C	-3.26395500	-0.16699600	1.36168200
C	-2.98958100	-1.31468100	2.34180100
C	-3.05137000	1.17938900	2.06343400
H	-3.77420700	-3.46226000	-1.59602900
H	-2.25200000	1.12321500	-2.07625500
H	-2.17088200	4.03668200	-1.04159600
H	-4.39998000	0.16740700	-2.27316500
H	-4.14433800	-2.82313900	0.00848700
H	-3.28121100	1.84017600	-0.83615400
H	-2.51473700	-1.46771200	-2.20763900
H	-4.30966000	-0.22608500	1.03236200
H	-5.20788300	-0.68812800	-0.94449800
H	-4.98932500	-1.48239300	-2.50746800
H	-2.47761700	-3.27208700	-0.40516900
H	-3.08750500	-2.30167700	1.88136900
H	-2.00103700	1.31552100	2.34886900
H	-1.97897700	-1.23414200	2.75716100
H	-3.65253300	1.20793400	2.97942800
H	-3.69957100	-1.25961900	3.17475200
H	-3.35332100	2.02842900	1.44254000
H	-0.02163200	-0.57652900	-1.51907400
O	0.60805800	1.11257300	3.03505300
H	-0.02678500	0.90191300	3.73062100
Fe	0.00245300	-0.50067400	-0.00225600
C	0.07108700	-2.22916300	-0.14603700
O	0.12697000	-3.37383400	-0.33618700
H	0.18768100	0.06972100	1.89878700

TS_{4,5-Co}

Co	-0.03555900	-0.50854300	0.10877900
P	2.15457300	-0.40421100	0.00196800
N	0.01123100	1.49391500	-0.19339400
C	2.38451000	1.38981400	0.38072400
C	1.16759900	2.17482100	-0.03372100
C	1.22813000	3.55289300	-0.21961500
C	0.07203800	4.24181900	-0.56595500
C	3.19352000	-1.23666000	1.29538800
C	2.83941900	-2.71332100	1.49847200
C	4.69824900	-1.04519000	1.08655500
C	3.00331900	-0.63275300	-1.62973700
C	2.92339800	-2.08068100	-2.12168700
C	2.44817500	0.32894300	-2.68534600
H	3.41021900	-3.10838900	2.34645100
H	2.46766400	1.46165700	1.47225400
H	0.09390400	5.31911500	-0.70477100
H	2.17343300	4.06959500	-0.08585600
H	4.96541900	0.00602700	0.93218500
H	3.08971100	-3.31746300	0.61999400
H	3.29230200	1.81194400	-0.06222400
H	2.89880000	-0.70058900	2.20737200
H	4.05543000	-0.37410800	-1.45356400
H	5.05481000	-1.61997800	0.22412900
H	5.23819500	-1.40334500	1.97010700
H	1.77459900	-2.84623400	1.71168500
H	3.42518200	-2.77765300	-1.44359500
H	1.39003700	0.12678800	-2.88575800
H	1.88033100	-2.40021200	-2.23334200

H	3.00152200	0.19484100	-3.62142700
H	3.40716800	-2.16179100	-3.10153100
H	2.54740100	1.37847300	-2.38864900
H	-0.17829200	-0.70668700	1.71074700
H	-0.05632800	-1.97716600	0.19840100
P	-2.19748800	-0.37245700	-0.16216400
C	-2.33658400	1.33193500	-0.86651000
C	-1.10619200	2.15188900	-0.57088500
C	-1.10935100	3.53274900	-0.74697600
C	-3.00981700	-1.41756200	-1.46333900
C	-2.69745400	-2.91174100	-1.33745200
C	-4.51584400	-1.17112500	-1.58722800
C	-3.33647200	-0.32975400	1.30190900
C	-3.40639700	-1.68448400	2.01246000
C	-2.93237700	0.77409500	2.28459300
H	-3.10722000	-3.43925800	-2.20615400
H	-2.41602400	1.22762900	-1.95612400
H	-2.02759200	4.03317300	-1.03826700
H	-4.75718500	-0.10604300	-1.67500200
H	-3.14987600	-3.34929800	-0.44148900
H	-3.24116400	1.85139200	-0.53440400
H	-2.52203100	-1.05799800	-2.37953600
H	-4.32877600	-0.08488900	0.90120100
H	-5.05571100	-1.57463800	-0.72302800
H	-4.89654400	-1.67685200	-2.48149600
H	-1.62004000	-3.09682300	-1.30138400
H	-3.83498000	-2.46475500	1.37665000
H	-1.95662900	0.56562300	2.73551600
H	-2.41030000	-2.01157300	2.33466300
H	-3.67266800	0.82792600	3.09059500
H	-4.03650000	-1.59849200	2.90485200
H	-2.88387700	1.76128600	1.81219400
H	-0.05687300	-0.75171200	-1.33755800
O	0.76491100	1.05496700	3.04561600
H	0.19542600	0.90275300	3.80952600
H	0.20576100	0.01715700	1.96146400

TS_{4,8-Ir}

Ir	-0.09484100	-0.59541500	0.02121600
P	2.22950900	-0.34173800	-0.07827600
N	-0.01933900	1.55449600	-0.32813100
C	2.34371700	1.43779800	0.24595600
C	1.17416100	2.19539400	-0.20377000
C	1.23778900	3.58504800	-0.42728700
C	0.09171400	4.28385500	-0.75207200
C	3.24464100	-1.12380800	1.26316800
C	2.99228200	-2.62211400	1.45532500
C	4.73986300	-0.81891900	1.13649100
C	3.10601700	-0.64888900	-1.68575800
C	3.10016900	-2.12290200	-2.09918500
C	2.52450500	0.22654100	-2.79989400
H	3.51299900	-2.96331600	2.35746500
H	2.31871300	1.61098900	1.59151500
H	0.13356900	5.35781100	-0.91482300
H	2.19399400	4.08990500	-0.32790200
H	4.93229300	0.25136700	1.00199500
H	3.36928800	-3.21328400	0.61479200
H	3.28174300	1.89815800	-0.08139400
H	2.86232200	-0.60885100	2.15422000
H	4.14295100	-0.33130000	-1.51147600

H	5.18363300	-1.35647300	0.29037300
H	5.26075600	-1.14318900	2.04454000
H	1.92661500	-2.84028100	1.57474600
H	3.65686700	-2.75302300	-1.39996100
H	1.48850800	-0.05460100	-3.02099000
H	2.07518900	-2.50740300	-2.16738700
H	3.11289100	0.09058100	-3.71428200
H	3.56558200	-2.23058600	-3.08569800
H	2.54348400	1.29045800	-2.54174000
H	-0.13002100	-2.19694000	0.07081400
P	-2.38598300	-0.21881400	-0.08331900
C	-2.40147400	1.43470900	-0.91521300
C	-1.14040300	2.23105800	-0.67816200
C	-1.12232000	3.60199300	-0.88004100
C	-3.44046800	-1.25039500	-1.20711700
C	-3.27226200	-2.75644500	-0.98521100
C	-4.91671700	-0.84505000	-1.19556100
C	-3.33190500	0.07060200	1.48380900
C	-3.44791400	-1.19899900	2.33141500
C	-2.71511400	1.21281200	2.29851000
H	-3.82345800	-3.29798400	-1.76203500
H	-2.47021700	1.23230000	-1.99200700
H	-2.03638800	4.12087400	-1.15026600
H	-5.05450200	0.22987500	-1.35537000
H	-3.67116400	-3.07199100	-0.01559800
H	-3.28514300	2.02210700	-0.64580800
H	-3.02102000	-1.01503700	-2.19474800
H	-4.33580000	0.38219900	1.16738200
H	-5.39251900	-1.11536500	-0.24601600
H	-5.44662000	-1.37413600	-1.99520800
H	-2.22194900	-3.05717900	-1.03824600
H	-4.00738400	-1.98829900	1.82072500
H	-1.70668000	0.95921200	2.64337400
H	-2.45716200	-1.59155400	2.58993400
H	-3.33341300	1.39695000	3.18385300
H	-3.97249600	-0.96882800	3.26534800
H	-2.65826500	2.14868900	1.73286500
H	-0.16714800	-0.78735700	-1.56584500
O	2.23220200	1.88084200	2.83125700
H	2.99721800	1.48296300	3.26326300
H	0.05467800	-0.14480300	1.74479300
H	-0.09197700	-0.97934400	1.73955300

TS_{4,8-Fe}

Fe	-0.11641200	-0.42700100	0.15397500
P	2.11778300	-0.35291700	-0.10559100
N	0.02336400	1.60791900	-0.24064200
C	2.40995700	1.40642200	0.15855400
C	1.24507700	2.20986600	-0.20153400
C	1.36241300	3.59493700	-0.43032700
C	0.23505200	4.35083500	-0.68052700
C	3.23184100	-1.16530500	1.14684100
C	2.88447100	-2.61629300	1.49088700
C	4.71723100	-1.02028800	0.80151400
C	2.81540100	-0.77531000	-1.77675800
C	2.62580000	-2.24923100	-2.14515400
C	2.23499200	0.13297000	-2.86419300
H	3.58426000	-2.98273500	2.25106100
H	0.40963100	-0.12525000	1.70049500
H	0.31575700	5.42184100	-0.84833400
H	2.34831500	4.04889000	-0.39500300
H	4.98386200	0.01084500	0.54395500

H	2.96106000	-3.28080500	0.62396500
H	3.33632000	1.79572000	-0.27656600
H	3.03144700	-0.56229700	2.04193900
H	3.89028600	-0.56421200	-1.70229600
H	4.99504300	-1.66630900	-0.03950500
H	5.32511100	-1.31964500	1.66290600
H	1.87487200	-2.70462100	1.90130900
H	3.14648200	-2.92034100	-1.45546300
H	1.16035000	-0.04057000	-2.99000700
H	1.56256300	-2.51905800	-2.14979500
H	2.72635000	-0.08282100	-3.81986600
H	3.02189800	-2.43315600	-3.15059500
H	2.38683600	1.19377700	-2.63888900
H	-0.40713600	-0.05401000	1.74250700
P	-2.31314100	-0.09341000	-0.03877000
C	-2.38809300	1.63185500	-0.68386400
C	-1.07502200	2.35101400	-0.52109200
C	-1.01048000	3.72101500	-0.72649300
C	-3.26537200	-1.01723400	-1.34596300
C	-3.04578100	-2.53226700	-1.35059100
C	-4.75864400	-0.67519400	-1.35176400
C	-3.39333600	-0.03994100	1.47140400
C	-3.52606500	-1.41831600	2.12515500
C	-2.88902100	0.98950800	2.48809300
H	-3.63723200	-2.97543600	-2.15975800
H	-2.60926100	1.57225200	-1.75650200
H	-1.91859100	4.27567700	-0.94089800
H	-4.94063600	0.40513300	-1.34495300
H	-3.36241200	-3.00158000	-0.41328000
H	-3.20367300	2.20370300	-0.22994400
H	-2.81890000	-0.62424600	-2.26932600
H	-4.38029600	0.28700700	1.12070300
H	-5.27077000	-1.11438500	-0.48820600
H	-5.22106100	-1.08695900	-2.25549600
H	-1.99787600	-2.78767300	-1.52661900
H	-4.01968500	-2.14295200	1.47064500
H	-1.94744600	0.67090400	2.94919000
H	-2.54232200	-1.81808300	2.40074300
H	-3.62662600	1.09199700	3.29155100
H	-4.12237800	-1.33532700	3.04073000
H	-2.73533400	1.98080700	2.04846200
H	-0.22421400	-0.68695500	-1.32916500
C	-0.21231100	-2.15980300	0.33682200
O	-0.27423000	-3.31465800	0.40515700
O	2.59810600	1.93231300	2.72198600
H	3.40183000	1.53318900	3.07527000
H	2.53743500	1.62253600	1.49839900

TS_{4,8-Co}

Co	-0.10051200	-0.54983200	0.08213000
P	2.10321100	-0.45177400	-0.06069500
N	-0.03179800	1.43263300	-0.28647500
C	2.30852500	1.30736500	0.31134300
C	1.15600600	2.08138200	-0.15033400
C	1.22548900	3.46779500	-0.38740600
C	0.08731100	4.15942700	-0.75507900
C	3.10638400	-1.32956000	1.23111100
C	2.75416900	-2.80938300	1.41068700
C	4.61462400	-1.13137300	1.05289500
C	2.92254300	-0.76376400	-1.69716500
C	2.83769400	-2.22754800	-2.13796400
C	2.34847100	0.15904200	-2.77649900

H	3.29459700	-3.20757000	2.27733500
H	0.07074300	-0.12145700	1.70146600
H	0.13150500	5.23105000	-0.93263200
H	2.17890000	3.97459500	-0.27161600
H	4.87935500	-0.07522300	0.92980500
H	3.04106600	-3.40840500	0.54049700
H	3.26191300	1.74666300	-0.00094900
H	2.80068900	-0.80459300	2.14539600
H	3.97792400	-0.49722400	-1.54946400
H	4.98686800	-1.68203600	0.18111500
H	5.14357200	-1.51038600	1.93477000
H	1.68297100	-2.95164000	1.58251900
H	3.38101600	-2.89651100	-1.46452400
H	1.29123800	-0.06332200	-2.96259500
H	1.79470100	-2.56347600	-2.18819900
H	2.89495100	0.00801600	-3.71432300
H	3.27384100	-2.33732100	-3.13758500
H	2.43320000	1.21598400	-2.50348500
H	-0.13434300	-0.90090800	1.69228400
P	-2.27836200	-0.34821200	-0.08628500
C	-2.38010100	1.28654200	-0.93863100
C	-1.13837100	2.10405600	-0.68435200
C	-1.11968100	3.47133200	-0.91175200
C	-3.22957400	-1.47050400	-1.21412200
C	-2.97276600	-2.95866600	-0.95913800
C	-4.72857300	-1.16107600	-1.24991900
C	-3.28605900	-0.09558200	1.45057700
C	-3.35146600	-1.35906700	2.31275900
C	-2.75448000	1.08923100	2.26526700
H	-3.46566500	-3.54762000	-1.74072600
H	-2.43530300	1.07981500	-2.01525700
H	-2.02648500	3.98095500	-1.22153800
H	-4.92974200	-0.09985200	-1.43251000
H	-3.37913400	-3.28269700	0.00454200
H	-3.28342200	1.84549400	-0.67422200
H	-2.79953500	-1.22671700	-2.19508300
H	-4.29803400	0.15469600	1.10651300
H	-5.21268600	-1.44523100	-0.30860000
H	-5.20142300	-1.73648600	-2.05343800
H	-1.90455700	-3.19316300	-0.97674400
H	-3.85649500	-2.18369200	1.80129500
H	-1.74296200	0.89656200	2.63947500
H	-2.34738700	-1.69533100	2.59815200
H	-3.40468600	1.25084200	3.13207100
H	-3.90775500	-1.14661000	3.23256700
H	-2.73391700	2.01973600	1.68833200
H	-0.17136000	-0.84995900	-1.34220100
O	2.24356000	1.69239100	2.90846000
H	1.79011000	0.95330000	3.33115800
H	2.26997600	1.44692900	1.66903400
H	-0.12993200	-2.01738600	0.18852200

TS_{6,7-Ir}

Ir	0.06144400	-0.38828800	-0.35065000
P	2.33528900	0.06622000	-0.25868200
N	-0.03169500	1.38383900	0.89885400
C	2.37938300	1.11579300	1.26958600
C	1.08655700	1.86375400	1.49599000
C	1.04955200	2.98193900	2.31491300
C	-0.18033800	3.60910200	2.53852200
C	3.54470400	-1.27950700	0.15952500
C	3.44109500	-2.49634100	-0.76548500

C	4.99068400	-0.79056100	0.27906500
C	3.11355600	1.14261600	-1.55082700
C	3.21590400	0.43385300	-2.90402100
C	2.35631800	2.46768500	-1.68999600
H	4.07096500	-3.30294900	-0.37342300
H	2.52883300	0.42434700	2.10856900
H	-0.23893700	4.47915900	3.18781700
H	1.96227400	3.34586700	2.77619200
H	5.08338700	0.07525700	0.94364100
H	3.78836500	-2.26876300	-1.77866900
H	3.22664000	1.80957000	1.27326200
H	3.20212100	-1.59510400	1.15456500
H	4.12513800	1.36339300	-1.18607700
H	5.39685200	-0.51522300	-0.70106600
H	5.61695900	-1.59332100	0.68408600
H	2.41378500	-2.86758200	-0.83323400
H	3.86348800	-0.44678800	-2.86230600
H	1.33167100	2.30079900	-2.04153900
H	2.22705800	0.11683500	-3.25630400
H	2.86762500	3.10089900	-2.42357800
H	3.63445100	1.12116300	-3.64782700
H	2.30797900	3.02338400	-0.74735800
H	0.41315800	-3.34680600	0.68726300
H	0.11688100	-1.70696800	-1.27276800
P	-2.25732700	-0.18695300	-0.24218700
C	-2.37784600	1.54354300	0.28946400
C	-1.23336800	1.99969000	1.07551000
C	-1.31797500	3.12093600	1.92604100
C	-3.20190500	-0.23501100	-1.84288400
C	-2.96648200	-1.49183300	-2.68572100
C	-4.69749800	0.04493500	-1.67183400
C	-3.25635100	-1.16660800	0.98657100
C	-3.23258700	-2.67245000	0.70683300
C	-2.79755800	-0.87614200	2.42008200
H	-3.42126200	-1.35619900	-3.67404500
H	-2.28159300	2.32099700	-0.83153300
H	-2.28273400	3.59742300	2.07339800
H	-4.88257800	0.94251300	-1.07119500
H	-3.42224100	-2.37958900	-2.23521200
H	-3.33355300	1.81706200	0.74884500
H	-2.75849600	0.61163200	-2.38243600
H	-4.28860000	-0.80576200	0.88330900
H	-5.20836100	-0.79893500	-1.19342900
H	-5.16012000	0.19691300	-2.65394500
H	-1.89970100	-1.69062200	-2.82652300
H	-3.69507900	-2.92411600	-0.25173900
H	-1.76705200	-1.21121000	2.57888700
H	-2.20541700	-3.05688900	0.69971600
H	-3.44409100	-1.41144800	3.12541500
H	-3.78426900	-3.20439500	1.49092000
H	-2.85128400	0.19115300	2.65866800
H	-0.09206300	0.44006600	-1.68151600
C	0.53665800	-2.78894800	1.63669200
O	0.39901100	-1.52619500	1.57080500
O	0.79458100	-3.42858500	2.67683600
O	-2.19234300	3.12287100	-1.80260700
H	-1.56397100	2.72309300	-2.41617000

TS_{6,7-Fe}

P	-2.28186000	0.03322200	0.23075700
N	0.03216400	1.50237800	-0.58966200
C	-2.35278800	1.32520100	-1.08419700

C	-1.05863200	2.09542800	-1.13026200
C	-1.00517000	3.35191600	-1.71553200
C	0.22169800	4.02011100	-1.75725900
C	-3.53899100	-1.19416800	-0.38723800
C	-3.44211900	-2.57154600	0.27613800
C	-4.97742200	-0.66885100	-0.35096100
C	-3.03012900	0.87273000	1.70785700
C	-3.06161300	-0.04877200	2.93083800
C	-2.30048500	2.17984600	2.03778800
H	-4.16264300	-3.25017600	-0.19470500
H	-2.48294600	0.79539500	-2.03565900
H	0.29627900	5.00120600	-2.22001500
H	-1.90530900	3.79215300	-2.13305900
H	-5.07312500	0.31909100	-0.81422000
H	-3.67689800	-2.53012500	1.34489900
H	-3.20341700	2.00536100	-0.97082100
H	-3.24866400	-1.31813800	-1.43970500
H	-4.06053900	1.12346600	1.42548700
H	-5.34733800	-0.60143100	0.67869700
H	-5.63289500	-1.35929400	-0.89360400
H	-2.44704400	-3.01030200	0.16366500
H	-3.68738100	-0.93157300	2.76919000
H	-1.25416900	1.99323200	2.30546800
H	-2.05197900	-0.38694900	3.19362100
H	-2.78895300	2.65867100	2.89402400
H	-3.46858400	0.49467300	3.79114500
H	-2.31921000	2.89039700	1.20474300
H	-0.70132900	-2.94299800	-1.44445800
P	2.18676100	-0.24964100	0.19516100
C	2.33968400	1.54854600	0.12325500
C	1.22636300	2.15550400	-0.59501800
C	1.33558500	3.42513300	-1.19899100
C	3.13243900	-0.71178400	1.73239100
C	3.29922700	-2.22018500	1.94537300
C	4.49502900	-0.01872100	1.83777600
C	3.20399900	-0.94807000	-1.20865500
C	2.90722000	-2.42998600	-1.47308800
C	3.00315700	-0.14224900	-2.49705800
H	3.66085700	-2.40474900	2.96358900
H	2.15937700	2.03033200	1.39863000
H	2.30098800	3.92289100	-1.20435600
H	4.41024200	1.07004700	1.78017600
H	4.04312200	-2.63495400	1.25600100
H	3.31252900	1.92911100	-0.20334000
H	2.48922600	-0.32322800	2.53306900
H	4.25533100	-0.85105400	-0.90411900
H	5.17724700	-0.35420800	1.04753600
H	4.95958500	-0.26945300	2.79901500
H	2.36451800	-2.77337800	1.81498100
H	2.97961300	-3.04899800	-0.57533900
H	1.95224000	-0.16297000	-2.80919000
H	1.90064800	-2.55340600	-1.88504900
H	3.60241000	-0.58131900	-3.30375800
H	3.61723600	-2.82363800	-2.21028700
H	3.30539500	0.90301300	-2.38186500
H	0.07270000	0.15184900	1.59914400
C	-0.63810500	-2.14448700	-2.21200600
O	-0.33249800	-0.98488200	-1.79822900
O	-0.86698300	-2.45246000	-3.40130800
O	1.98918600	2.56520200	2.52271400
H	1.28385900	2.05353100	2.93759800
Fe	-0.07425100	-0.41868700	0.19891200

C	-0.14461900	-1.92781400	1.03896800
O	-0.18784100	-2.88951900	1.69798800

TS_{6,7-Co}

Co	-0.07963100	-0.42246700	0.25130000
P	-2.25759600	-0.05633600	0.31514900
N	-0.01295000	1.28758600	-0.83110500
C	-2.40428900	0.98784600	-1.20489400
C	-1.12926300	1.76458400	-1.42826100
C	-1.10839400	2.90491400	-2.21751000
C	0.10948400	3.56801400	-2.39939700
C	-3.45560100	-1.43230800	-0.02921000
C	-3.28465300	-2.63768100	0.90101800
C	-4.91584300	-0.97481200	-0.08282000
C	-2.99158400	1.00537700	1.64639300
C	-2.97918300	0.30545000	3.00828600
C	-2.27605000	2.35834200	1.73088300
H	-3.90837900	-3.46402300	0.54138600
H	-2.55190900	0.29817600	-2.04511100
H	0.15847400	4.45880300	-3.02103600
H	-2.02303200	3.26181500	-2.68070800
H	-5.05823400	-0.11745800	-0.74966900
H	-3.59868900	-2.40861900	1.92461600
H	-3.26845900	1.65999800	-1.18011200
H	-3.15696400	-1.75059600	-1.03749400
H	-4.03253700	1.18814200	1.34936800
H	-5.27982100	-0.69810700	0.91336900
H	-5.54440100	-1.79413800	-0.44957400
H	-2.24648700	-2.98216900	0.93301500
H	-3.59070300	-0.60146900	3.01395500
H	-1.22036000	2.23081000	1.99744200
H	-1.95782500	0.03299700	3.30016200
H	-2.74984600	2.96925800	2.50745000
H	-3.37825500	0.98177900	3.77265800
H	-2.32653600	2.91804600	0.79098200
H	-0.38880700	-3.30623100	-0.68981100
H	-0.11843900	-1.64743600	1.08983700
P	2.12685000	-0.26842000	0.30079600
C	2.31067800	1.46641100	-0.18313300
C	1.17339400	1.93856800	-0.96772800
C	1.24742800	3.09059000	-1.77779800
C	2.96684400	-0.37143600	1.95772800
C	2.63813100	-1.62911100	2.76778900
C	4.47941100	-0.14453600	1.88185800
C	3.20314500	-1.22678100	-0.88112000
C	3.18886800	-2.73506700	-0.61466800
C	2.82287100	-0.92956800	-2.33605600
H	3.05559400	-1.53073500	3.77693900
H	2.24017000	2.22038600	0.96530500
H	2.20271800	3.59530600	-1.89042500
H	4.73266900	0.75073300	1.30276600
H	3.07113400	-2.53018900	2.32101600
H	3.27374200	1.72663800	-0.63476000
H	2.52142400	0.48462000	2.48061900
H	4.22332300	-0.85293600	-0.71894900
H	4.98871900	-1.00206600	1.42637200
H	4.88635800	-0.01735100	2.89183400
H	1.55843000	-1.78091300	2.85929100
H	3.61053900	-2.98679600	0.36268100
H	1.81347100	-1.28898900	-2.56105900
H	2.16943800	-3.13705000	-0.65784900
H	3.52537700	-1.43612400	-3.00844200

H	3.78468800	-3.25283800	-1.37582500
H	2.86001100	0.14238100	-2.55707000
H	0.05884800	0.30868100	1.51278700
C	-0.47446700	-2.71247700	-1.62148700
O	-0.35675800	-1.45365700	-1.50186700
O	-0.67494000	-3.31683300	-2.69641200
O	2.17887800	2.92412100	2.00041800
H	1.96340000	3.81553400	1.70114500

TS_{9,1-Ir}

Ir	-0.01297500	-0.58365700	-0.03441300
P	-2.32257400	-0.20034500	-0.12847100
N	0.03518300	1.55098500	0.14020900
C	-2.05711300	1.37631600	-0.97911400
C	-1.03046600	2.20499400	-0.40740600
C	-1.00562500	3.62113500	-0.47324100
C	0.09908500	4.30408600	-0.01523400
C	-3.34569900	-1.16450700	-1.34025000
C	-3.27272200	-2.68356100	-1.15659700
C	-4.79767800	-0.68156000	-1.41434800
C	-3.34592300	0.05063700	1.39851700
C	-3.63228500	-1.26582500	2.12806400
C	-2.67725100	1.05293800	-2.34433400
H	-3.78311000	-3.17332900	-1.99384900
H	-0.95250200	0.42558300	-1.69551900
H	0.12395100	5.39023800	-0.05981000
H	-1.86090200	4.14572700	-0.88884700
H	-4.86822200	0.40329500	-1.54833400
H	-3.76569000	-3.00952200	-0.23516100
H	-2.91593500	1.90824600	-1.39384700
H	-2.85382900	-0.92276400	-2.29205700
H	-4.29499500	0.48267600	1.05406300
H	-5.35233200	-0.95119600	-0.50821300
H	-5.29972500	-1.15829500	-2.26377200
H	-2.23775900	-3.03729200	-1.13372200
H	-4.24926300	-1.94613700	1.53423900
H	-1.71501700	0.67155500	2.70532700
H	-2.69968700	-1.78315500	2.38485000
H	-3.32250900	1.21647000	3.21480400
H	-4.16976100	-1.05886700	3.06055000
H	-2.50566400	2.02233700	1.86609500
H	-0.24622900	-0.23330300	-1.82779200
H	-0.03851400	-2.17578200	-0.28507200
P	2.27589800	-0.28386100	0.16560500
C	2.28835400	1.36558700	1.02355400
C	1.14088900	2.22098800	0.54943700
C	1.20457900	3.60018700	0.49674300
C	3.24396500	-1.35002800	1.33728200
C	3.03600800	-2.85023000	1.10765000
C	4.73278400	-0.99798400	1.39896800
C	3.33012400	-0.01424900	-1.33721400
C	3.46051900	-1.29069500	-2.17327300
C	2.79103300	1.13570100	-2.19427900
H	3.52457400	-3.40956200	1.91347200
H	2.15811600	1.14772900	2.09157000
H	2.09849000	4.11783600	0.82967300
H	4.90127300	0.07164800	1.56395900
H	3.47605500	-3.18199000	0.16150500
H	3.24063200	1.89272500	0.90685600
H	2.78744300	-1.10034400	2.30478800
H	4.32100400	0.27283000	-0.96286300
H	5.24650500	-1.28801500	0.47529200

H	5.20291700	-1.54331500	2.22491400
H	1.97465300	-3.11485700	1.10267100
H	3.96939300	-2.09315400	-1.63115200
H	1.78041400	0.91725800	-2.55843000
H	2.47445600	-1.65744100	-2.48357000
H	3.44078600	1.27129300	-3.06601600
H	4.04130900	-1.07925500	-3.07810300
H	2.76257200	2.08506000	-1.64981400
H	0.08459500	-0.98070700	1.51106300

TS_{9,1-Fe}

Fe	0.02038200	-0.50015000	-0.05582100
P	-2.23630300	-0.26107600	-0.09732300
N	-0.00057700	1.52434000	0.08096400
C	-2.06471700	1.26221900	-1.04633600
C	-1.07828300	2.14237400	-0.48159100
C	-1.11607100	3.55530600	-0.56364600
C	-0.05753900	4.29152900	-0.07945900
C	-3.21584200	-1.37815200	-1.20779900
C	-3.53212500	-2.72651900	-0.55119200
C	-4.49683700	-0.73630500	-1.74958300
C	-3.28640300	-0.01971400	1.42278300
C	-2.98471600	-1.08205000	2.48734700
C	-3.10979000	1.38237400	2.01313900
H	-3.94759300	-3.40905300	-1.30095900
H	-0.94387200	0.38074500	-1.69437000
H	-0.07853900	5.37751500	-0.12980900
H	-1.98496100	4.03533100	-1.00432300
H	-4.29375800	0.17359400	-2.32146400
H	-4.28183600	-2.61193600	0.24020900
H	-2.93665600	1.74666900	-1.48769200
H	-2.53338100	-1.55576000	-2.05010300
H	-4.33028700	-0.13037200	1.09977700
H	-5.19361600	-0.48625300	-0.94079800
H	-5.00588500	-1.44331500	-2.41502300
H	-2.64561300	-3.20002500	-0.11729600
H	-3.05891900	-2.10273200	2.10064400
H	-2.06495600	1.56270000	2.29543400
H	-1.97309700	-0.94667800	2.88627000
H	-3.72121600	1.47919600	2.91782400
H	-3.69317600	-0.98363000	3.31809800
H	-3.41258500	2.16496400	1.31096400
H	-0.15271800	-0.17792200	-1.73710800
P	2.21814000	-0.19612100	0.18714300
C	2.22208700	1.45391100	1.02714200
C	1.05302300	2.25442300	0.52244900
C	1.05757300	3.63571100	0.46996100
C	3.18911100	-1.23184700	1.39072300
C	2.98866100	-2.74032200	1.21793800
C	4.67761000	-0.87502900	1.44160000
C	3.31354200	0.06055300	-1.29317400
C	3.45561500	-1.22766000	-2.10992900
C	2.79165800	1.19899200	-2.17641100
H	3.56465200	-3.27064200	1.98498800
H	2.09556500	1.25777500	2.09935100
H	1.91812400	4.18994800	0.83118800
H	4.84430800	0.20112300	1.55988300
H	3.33511200	-3.09339100	0.24090000
H	3.16115000	2.00115800	0.89696000
H	2.73685000	-0.95289800	2.35193600
H	4.29925800	0.35127500	-0.90870500
H	5.19655600	-1.20421100	0.53406900

H	5.14526100	-1.38274100	2.29269100
H	1.93936600	-3.02446800	1.33239200
H	3.94989400	-2.02519800	-1.54670900
H	1.78860400	0.97564800	-2.55812900
H	2.47444100	-1.59562500	-2.43512100
H	3.45865900	1.32584700	-3.03668200
H	4.05469900	-1.03295000	-3.00680400
H	2.75081100	2.15483000	-1.64387100
H	0.12584700	-0.71709400	1.45472600
C	0.02843200	-2.21309700	-0.33286400
O	0.01876500	-3.36001900	-0.53532700

TS_{9,1-Co}

Co	-0.00576700	-0.55770000	-0.08923300
P	-2.21688200	-0.33588600	-0.14598300
N	0.04054800	1.41708100	0.09384800
C	-2.02359000	1.22692300	-1.03686800
C	-1.01840100	2.07608600	-0.45461200
C	-1.00566600	3.49129900	-0.50075100
C	0.08008300	4.17425500	0.00421800
C	-3.18468200	-1.38297900	-1.33372900
C	-3.05837900	-2.89121600	-1.09616100
C	-4.65289900	-0.95994300	-1.44322000
C	-3.26382400	-0.08927700	1.36662800
C	-3.48756400	-1.39693500	2.13330400
C	-2.64858200	0.97072100	2.28608800
H	-3.53207800	-3.42875900	-1.92570400
H	-0.91829800	0.33116300	-1.71360500
H	0.09740500	5.26128700	-0.01952200
H	-1.85411100	4.01632800	-0.92966900
H	-4.76244900	0.11516900	-1.62188600
H	-3.55869200	-3.20420500	-0.17416700
H	-2.89454000	1.72865000	-1.46333700
H	-2.68934200	-1.15704500	-2.28770700
H	-4.23222600	0.28520100	1.00900400
H	-5.20718500	-1.21331900	-0.53209400
H	-5.12727200	-1.48964200	-2.27719800
H	-2.01165400	-3.20411900	-1.04002100
H	-4.07106800	-2.12191100	1.55896900
H	-1.66421300	0.65343300	2.65010000
H	-2.53195200	-1.86267000	2.40435200
H	-3.29772000	1.11795400	3.15671000
H	-4.03494100	-1.19040500	3.06017100
H	-2.53373700	1.93678600	1.78480200
H	-0.16782000	-0.28118100	-1.76042600
H	-0.01193300	-2.02367200	-0.33165300
P	2.16325900	-0.41428100	0.16955400
C	2.25085700	1.21925800	1.04443100
C	1.11970300	2.08863600	0.55822900
C	1.17280900	3.47000700	0.54084100
C	3.03919900	-1.55561800	1.34284200
C	2.75097500	-3.03785900	1.08576800
C	4.54439600	-1.29248800	1.44171600
C	3.27164900	-0.18519800	-1.30326000
C	3.34068000	-1.45270500	-2.16037400
C	2.82409700	1.01053300	-2.15080400
H	3.20319100	-3.63725300	1.88408500
H	2.11610400	1.00849500	2.11306600
H	2.04944600	3.98767400	0.91719200
H	4.77113900	-0.23623700	1.62319400
H	3.17747000	-3.37679900	0.13595000
H	3.21631600	1.72087800	0.92377400

H	2.57781100	-1.29436800	2.30484600
H	4.27071600	0.03267200	-0.90444200
H	5.06117200	-1.60145000	0.52590300
H	4.96344500	-1.87381700	2.27061400
H	1.67687700	-3.24390000	1.07034900
H	3.78452800	-2.29548600	-1.62212000
H	1.81129200	0.86048600	-2.54248100
H	2.34130400	-1.75075700	-2.50039200
H	3.50199900	1.12267500	-3.00440300
H	3.95511300	-1.26355600	-3.04787100
H	2.83928700	1.95004100	-1.58889300
H	0.05765800	-0.88850900	1.34758700

TS_{10,11-Ir}

Ir	-0.00389700	-0.59535200	-0.02503200
P	-2.31103000	-0.18478100	-0.05233000
N	0.03965700	1.55624300	0.16133700
C	-2.10442900	1.40675800	-0.89525600
C	-1.04067300	2.22608800	-0.32692600
C	-1.01853700	3.63467500	-0.35458500
C	0.10344900	4.30782700	0.09388200
C	-3.43700900	-1.12684000	-1.19422900
C	-3.31306800	-2.64897600	-1.07345600
C	-4.89937900	-0.67762500	-1.10753400
C	-3.23128000	0.03004300	1.54727500
C	-3.42311600	-1.29834300	2.28619000
C	-2.53455700	1.05084400	2.45205400
H	-3.91814500	-3.12595500	-1.85319700
H	-1.25127300	0.75080000	-1.88065800
H	0.12835900	5.39464200	0.07451000
H	-1.88142800	4.17190700	-0.73674300
H	-5.00399700	0.40983200	-1.18830200
H	-3.67395300	-3.01421900	-0.10634900
H	-3.00155800	1.95915500	-1.18277400
H	-3.05671400	-0.84396800	-2.18455200
H	-4.21585100	0.43225200	1.27511800
H	-5.35869000	-0.99650500	-0.16489500
H	-5.47171600	-1.13208000	-1.92416300
H	-2.27714100	-2.97896100	-1.19624700
H	-4.04760300	-2.00058400	1.72632600
H	-1.53155500	0.70967000	2.73431300
H	-2.45769400	-1.78044000	2.48334400
H	-3.11792000	1.17950700	3.37089600
H	-3.91088100	-1.11652100	3.25080900
H	-2.44095800	2.03097700	1.97371300
H	-0.03036200	-2.18980800	-0.26631600
P	2.28423500	-0.30848600	0.20822900
C	2.28900700	1.34699800	1.05684200
C	1.14614200	2.20800300	0.57961500
C	1.21220500	3.59341100	0.56324800
C	3.20669800	-1.36788000	1.42218700
C	3.08733900	-2.86737800	1.13428100
C	4.66926100	-0.95853400	1.61613000
C	3.37744700	-0.06667700	-1.27144600
C	3.35800300	-1.29979400	-2.18059400
C	2.97071500	1.18571800	-2.05764100
H	3.50746600	-3.43186300	1.97430000
H	2.14742200	1.13457600	2.12464600
H	2.10963100	4.10039800	0.90305800
H	4.78131600	0.11235800	1.81655900

H	3.64539300	-3.14985700	0.23528700
H	3.24247600	1.87424600	0.95345400
H	2.66308500	-1.16684300	2.35565100
H	4.39542600	0.08088500	-0.88899500
H	5.27009100	-1.20731100	0.73409500
H	5.09104200	-1.50469600	2.46732700
H	2.04520100	-3.17399000	1.00313000
H	3.71146300	-2.20070700	-1.67058300
H	1.92943300	1.11903300	-2.39196500
H	2.34388800	-1.49322600	-2.55035100
H	3.60904400	1.27780600	-2.94390000
H	4.00702700	-1.12897700	-3.04692900
H	3.08777000	2.10159400	-1.46923700
H	0.04228000	-0.93893700	1.50813800
O	-0.31753900	0.08146300	-2.22810000
H	-0.65499400	-0.63833200	-2.77427300

TS_{10,11-Fe}

P	-2.26677300	-0.14907500	-0.05242900
N	0.04404700	1.52492600	0.08180000
C	-2.06247600	1.37059300	-1.01089400
C	-1.00593900	2.20168800	-0.45746800
C	-0.97087400	3.60848700	-0.52732300
C	0.13059600	4.28661300	-0.03847600
C	-3.41337800	-1.14129300	-1.13611600
C	-3.34696900	-2.65681800	-0.92429900
C	-4.86239800	-0.64475200	-1.09030000
C	-3.20378600	0.19116800	1.51863200
C	-3.39255800	-1.08050500	2.35240800
C	-2.52122800	1.28048700	2.35198300
H	-4.00795100	-3.15266200	-1.64491500
H	-1.18281000	0.63869100	-1.89281500
H	0.16632500	5.37248700	-0.08321000
H	-1.81255900	4.13910600	-0.96256800
H	-4.93527100	0.43894400	-1.23246500
H	-3.67605800	-2.94838800	0.07851100
H	-2.95097400	1.90823100	-1.34800900
H	-3.01929900	-0.93391500	-2.13981600
H	-4.18942300	0.56608200	1.21413900
H	-5.33792000	-0.89683100	-0.13535000
H	-5.44161900	-1.12811700	-1.88536900
H	-2.33669200	-3.04522800	-1.07632700
H	-4.00949800	-1.82533800	1.84112800
H	-1.51674200	0.97094600	2.66402200
H	-2.42568200	-1.54145700	2.59018700
H	-3.11137000	1.46955900	3.25618700
H	-3.88735400	-0.83340100	3.29893800
H	-2.43371100	2.22431100	1.80456000
P	2.20706300	-0.30124000	0.21017800
C	2.23031300	1.32756800	1.08800600
C	1.12299600	2.18861700	0.54607100
C	1.20232800	3.57330800	0.50997400
C	3.13517400	-1.39801700	1.38927500
C	3.42911000	-2.78646900	0.81041900
C	4.42251600	-0.77205100	1.93601900
C	3.32700200	-0.08922900	-1.26159300
C	3.09050100	-1.20682100	-2.28599400
C	3.14940600	1.28030700	-1.92800000
H	3.79221500	-3.44193200	1.60978300
H	2.02468600	1.10218700	2.14263500
H	2.08491500	4.07793500	0.89006900
H	4.24102500	0.17204500	2.45778600

H	4.21342400	-2.73493300	0.04681800
H	3.19504100	1.84109300	1.04155200
H	2.42622900	-1.51495500	2.21986100
H	4.35774100	-0.16049700	-0.88952200
H	5.15038100	-0.58851800	1.13722700
H	4.88549300	-1.46303800	2.64984500
H	2.54594100	-3.25459800	0.36544200
H	3.20092800	-2.20602100	-1.85531500
H	2.11205300	1.43519400	-2.24649900
H	2.08249100	-1.12906300	-2.70797900
H	3.78545600	1.33489400	-2.81900500
H	3.81195500	-1.11301500	-3.10596000
H	3.43194200	2.10538600	-1.26704300
H	0.03008800	-0.66353600	1.48579500
O	-0.23291200	-0.06970100	-2.11148400
H	-0.54227200	-0.82587700	-2.62312100
Fe	-0.01855200	-0.53583200	-0.02910000
C	-0.04004600	-2.26716700	-0.00654300
O	-0.03873600	-3.42757600	0.10197000

TS_{10,11-Co}

Co	-0.00003000	-0.57655000	-0.10135800
P	-2.21636600	-0.31709100	-0.08320500
N	0.03047400	1.42281300	0.11994400
C	-2.07287700	1.25276500	-0.97450400
C	-1.03677300	2.09367700	-0.38998800
C	-1.02614100	3.50215100	-0.40252500
C	0.06901600	4.17636700	0.10854300
C	-3.29142500	-1.34911400	-1.19538200
C	-3.11117000	-2.86008500	-1.01608700
C	-4.77139300	-0.95651800	-1.13945600
C	-3.15347100	-0.09058200	1.50542700
C	-3.27909900	-1.40206800	2.28787700
C	-2.51177200	0.99272400	2.37802500
H	-3.68150800	-3.38860300	-1.78881800
H	-1.17066900	0.57701800	-1.89621600
H	0.08572200	5.26363400	0.10771500
H	-1.87727300	4.03834200	-0.81177400
H	-4.91904300	0.12137000	-1.26780100
H	-3.47831300	-3.20366400	-0.04346800
H	-2.98011500	1.77410300	-1.28618100
H	-2.91264800	-1.08967100	-2.19267300
H	-4.15718800	0.25163700	1.22125300
H	-5.22547000	-1.25267000	-0.18682300
H	-5.31805100	-1.46864800	-1.93950200
H	-2.06110300	-3.15394000	-1.10599400
H	-3.86750200	-2.15242400	1.75201600
H	-1.48995500	0.71703600	2.66478700
H	-2.29110200	-1.82900400	2.50014700
H	-3.09791800	1.11402500	3.29619500
H	-3.77586900	-1.21362300	3.24664900
H	-2.47515000	1.96265900	1.87219800
H	-0.01006800	-2.05179100	-0.29971000
P	2.17388400	-0.42748600	0.21595200
C	2.22663800	1.20197200	1.10357400
C	1.10504300	2.07685000	0.60335600
C	1.15936900	3.46331300	0.62141400
C	2.99533600	-1.56994900	1.42829300
C	2.76724500	-3.05401500	1.12586000
C	4.48221000	-1.27374500	1.64204800
C	3.34607900	-0.19416800	-1.20566700
C	3.35565000	-1.41928500	-2.12594200

C	3.00608200	1.07308000	-2.00006100
H	3.15989600	-3.65579700	1.95338300
H	2.06232400	0.98302100	2.16647700
H	2.03410600	3.97087900	1.01549700
H	4.67102600	-0.21543300	1.85244300
H	3.28878400	-3.36683900	0.21515200
H	3.19309500	1.70861600	1.01881500
H	2.45865300	-1.33865600	2.35846900
H	4.34553900	-0.06796300	-0.77020000
H	5.07242500	-1.55873700	0.76365600
H	4.85257200	-1.85695500	2.49258000
H	1.70456000	-3.28555900	1.00887700
H	3.69508700	-2.32334500	-1.61181100
H	1.98795100	1.02402700	-2.40054300
H	2.35528700	-1.61204900	-2.53173500
H	3.70187800	1.16824900	-2.84169300
H	4.03299900	-1.24137000	-2.96897600
H	3.09597900	1.98013500	-1.39331000
H	0.02539100	-0.86523400	1.33664200
O	-0.20784700	-0.10126400	-2.13390700
H	-0.49814000	-0.85706100	-2.65743300

H₂

H	0.00000000	0.00000000	0.37262100
H	0.00000000	0.00000000	-0.37262100

OH⁻

O	0.00000000	0.00000000	0.10703600
H	0.00000000	0.00000000	-0.85628700

H₂O

O	0.00000000	0.00000000	0.11742500
H	0.00000000	0.76423300	-0.46969800
H	0.00000000	-0.76423300	-0.46969800

CO₂

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16537400
O	0.00000000	0.00000000	-1.16537400

HCOO⁻

H	0.00000500	1.45505500	0.00003500
C	-0.00013800	0.34168900	-0.00001700
O	1.12709100	-0.21904900	0.00000400
O	-1.12698800	-0.21910000	0.00000400