

Supplementary material for the publication:

"The prediction of 57-Fe Mössbauer parameters by the density functional theory: a benchmark study"

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Contents:

- The atomic coordinates of the 31 complexes used in the non-optimized data set (in Å)
- The isomer shifts and quadrupole splittings predicted by 8 functionals and 2 basis sets for X-ray-based geometries
- The isomer shift calibrations for 8 functionals and 2 basis sets obtained for X-ray-based geometries

The Cartesian coordinates (in Angstrom)

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1. SISKOU			
Fe1	-1.5230000000	-3.5910000000	0.6630000000
Fe2	-0.3600000000	-6.2020000000	2.8070000000
O3	-0.0400000000	-5.1390000000	1.0100000000
O4	-3.0150000000	-2.1680000000	0.6210000000
O5	0.0670000000	-4.4490000000	3.8690000000
O6	-0.9940000000	-2.8980000000	2.6410000000
O7	-2.3500000000	-6.1530000000	3.2450000000
O8	-2.9530000000	-4.9980000000	1.4330000000
O9	2.0100000000	-5.8520000000	1.3840000000
O10	-4.6760000000	-0.9920000000	1.5020000000
O11	0.3060000000	-2.9560000000	-3.7870000000
O12	-0.1240000000	-10.9080000000	3.8710000000
N13	-0.0610000000	-2.3460000000	-0.2840000000
N14	1.1090000000	-1.1310000000	-1.7010000000
N15	-1.9160000000	-4.2600000000	-1.3370000000
N16	-2.1420000000	-4.4420000000	-3.5200000000
N17	0.4810000000	-7.4220000000	4.3080000000
N18	1.3470000000	-9.0550000000	5.4910000000
N19	-0.5440000000	-8.0240000000	1.7130000000
N20	-1.0120000000	-10.1300000000	1.2410000000
C21	-0.6310000000	-2.5760000000	-2.7840000000
C22	0.4460000000	-9.7740000000	3.2560000000
C23	1.2010000000	-5.2020000000	0.7520000000
C24	-3.1820000000	-5.6500000000	2.4490000000
C25	-0.3770000000	-3.2980000000	3.6320000000
C26	-3.8650000000	-1.9090000000	1.5100000000
C27	0.1200000000	-2.0510000000	-1.5580000000
C28	1.5610000000	-0.8210000000	-0.4440000000
C29	0.8530000000	-1.5770000000	0.4100000000
C30	1.6190000000	-0.4660000000	-2.9070000000
C31	-1.5390000000	-3.7620000000	-2.4970000000
C32	-2.9230000000	-5.4120000000	-2.9590000000
C33	-2.7810000000	-5.2940000000	-1.6260000000
C34	-2.0170000000	-4.2710000000	-4.9650000000
C35	0.7430000000	-8.7200000000	4.3250000000
C36	1.4610000000	-7.9160000000	6.2450000000
C37	0.9390000000	-6.9200000000	5.5070000000
C38	1.8480000000	-10.3560000000	5.9550000000
C39	-0.4350000000	-9.2790000000	2.1250000000
C40	-1.5150000000	-9.3660000000	0.2210000000
C41	-1.2220000000	-8.0740000000	0.5120000000
C42	-1.1560000000	-11.5880000000	1.2880000000
C43	1.1450000000	-4.0520000000	-3.4320000000
C44	-1.3900000000	-10.6540000000	4.5020000000
C45	-1.4910000000	-1.4400000000	-3.3490000000
C46	-2.5010000000	-0.9300000000	-2.5490000000
C47	-3.3040000000	0.0940000000	-3.0130000000
C48	-3.1130000000	0.6090000000	-4.2750000000

C49	-2.1140000000	0.0870000000	-5.0870000000
C50	-1.3060000000	-0.9290000000	-4.6190000000
C51	1.7660000000	-10.2290000000	2.5920000000
C52	2.1810000000	-11.5500000000	2.5870000000
C53	3.3090000000	-11.9260000000	1.8880000000
C54	4.0370000000	-10.9930000000	1.1850000000
C55	3.6500000000	-9.6570000000	1.1960000000
C56	2.5130000000	-9.2810000000	1.8930000000
H57	1.5250000000	-4.7030000000	0.0100000000
H58	-4.0970000000	-5.7920000000	2.6570000000
H59	-0.2130000000	-2.6480000000	4.3040000000
H60	-3.8780000000	-2.4830000000	2.2660000000
H61	2.2400000000	-0.1960000000	-0.2210000000
H62	0.9640000000	-1.5820000000	1.3540000000
H63	-3.4610000000	-6.0470000000	-3.4180000000
H64	-3.2120000000	-5.8400000000	-0.9800000000
H65	1.8380000000	-7.8440000000	7.1150000000
H66	0.8920000000	-6.0090000000	5.7730000000
H67	-1.9800000000	-9.6800000000	-0.5440000000
H68	-1.4470000000	-7.3230000000	-0.0250000000
H69	-2.6420000000	-1.2880000000	-1.6810000000
H70	-3.9870000000	0.4480000000	-2.4570000000
H71	-3.6590000000	1.3190000000	-4.5900000000
H72	-1.9830000000	0.4330000000	-5.9630000000
H73	-0.6180000000	-1.2780000000	-5.1720000000
H74	1.6860000000	-12.2010000000	3.0690000000
H75	3.5880000000	-12.8340000000	1.8920000000
H76	4.8060000000	-11.2570000000	0.6920000000
H77	4.1620000000	-9.0060000000	0.7290000000
H78	2.2420000000	-8.3690000000	1.8940000000
H79	2.1810000000	-10.2690000000	6.8410000000
H80	1.7120000000	-3.7970000000	-2.7110000000
H81	-1.6550000000	-11.4190000000	4.9950000000
H82	-2.6430000000	-4.8310000000	-5.4050000000
H83	-1.5660000000	-11.8910000000	0.4870000000
H84	0.8970000000	-0.2840000000	-3.4970000000
H85	2.0400000000	0.3510000000	-2.6640000000
H86	2.2490000000	-1.0300000000	-3.3380000000
H87	-2.1850000000	-3.3640000000	-5.1920000000
H88	-1.1370000000	-4.5060000000	-5.2360000000
H89	1.1430000000	-10.9890000000	5.9420000000
H90	2.5490000000	-10.6470000000	5.3820000000
H91	-1.6980000000	-11.8280000000	2.0320000000
H92	-0.3000000000	-11.9880000000	1.3790000000
H93	0.6100000000	-4.7900000000	-3.1660000000
H94	1.6790000000	-4.2990000000	-4.1790000000
H95	-1.3060000000	-9.9110000000	5.0890000000
H96	-2.0400000000	-10.4610000000	3.8380000000

2. JOHCEP

Fe1	6.6382000000	4.8662000000	6.9818000000
B2	8.6672000000	7.2069000000	6.6453000000
H3	9.3137000000	7.9631000000	6.5406000000
C4	9.1633000000	7.2828000000	9.2481000000
C5	7.4761000000	5.6088000000	9.7243000000
H6	6.8890000000	4.9655000000	10.1027000000
C7	6.8908000000	8.7388000000	5.5156000000
C8	5.1516000000	7.0415000000	5.6497000000
H9	4.3673000000	6.5071000000	5.6008000000
C10	10.2783000000	5.8288000000	5.1679000000
C11	8.8404000000	3.8657000000	5.2294000000
H12	8.4192000000	3.0190000000	5.1428000000
N13	7.5688000000	5.7918000000	8.4550000000
N14	8.4912000000	6.8079000000	8.1589000000
N15	6.2653000000	6.6191000000	6.1887000000
N16	7.2705000000	7.5806000000	6.1105000000

N17	8.3353000000	4.8195000000	5.9513000000
N18	9.1469000000	5.9505000000	5.9038000000
S19	8.4731000000	6.5933000000	10.6693000000
S20	10.4377000000	8.3306000000	9.2790000000
S21	5.2272000000	8.6219000000	5.0444000000
S22	7.7928000000	10.0958000000	5.1933000000
S23	10.3031000000	4.2344000000	4.4512000000
S24	11.4961000000	6.9440000000	4.9660000000
B25	4.6092000000	2.5256000000	7.3183000000
H26	3.9627000000	1.7694000000	7.4231000000
C27	4.1131000000	2.4497000000	4.7155000000
C28	5.8003000000	4.1237000000	4.2394000000
H29	6.3874000000	4.7670000000	3.8609000000
C30	6.3857000000	0.9937000000	8.4480000000
C31	8.1248000000	2.6910000000	8.3139000000
H32	8.9091000000	3.2254000000	8.3628000000
C33	2.9981000000	3.9037000000	8.7957000000
C34	4.4360000000	5.8668000000	8.7342000000
H35	4.8572000000	6.7135000000	8.8208000000
N36	5.7076000000	3.9407000000	5.5086000000
N37	4.7852000000	2.9246000000	5.8047000000
N38	7.0111000000	3.1134000000	7.7749000000
N39	6.0059000000	2.1519000000	7.8531000000
N40	4.9411000000	4.9130000000	8.0123000000
N41	4.1295000000	3.7820000000	8.0598000000
S42	4.8033000000	3.1392000000	3.2943000000
S43	2.8387000000	1.4019000000	4.6847000000
S44	8.0492000000	1.1106000000	8.9193000000
S45	5.4836000000	-0.3633000000	8.7703000000
S46	2.9733000000	5.4981000000	9.5124000000
S47	1.7803000000	2.7885000000	8.9976000000

3. VUNMIA

Fe1	0.5340000000	1.7770000000	1.0750000000
O2	-1.3630000000	1.1510000000	1.1280000000
O3	1.5000000000	1.0300000000	-0.6890000000
C4	-1.9710000000	0.0400000000	1.1100000000
C5	-3.3700000000	0.0380000000	1.6800000000
N6	2.3870000000	3.0310000000	1.4420000000
N7	0.2420000000	3.4960000000	-0.1610000000
N8	0.1720000000	2.6880000000	3.1050000000
N9	1.7810000000	0.4250000000	2.1820000000
C10	1.3170000000	4.2550000000	-0.4070000000
C11	1.2420000000	5.3720000000	-1.2110000000
C12	0.0510000000	5.6740000000	-1.8420000000
C13	-1.0510000000	4.8790000000	-1.6170000000
C14	-0.9220000000	3.8110000000	-0.7560000000
C15	1.1790000000	3.4480000000	3.5800000000
C16	1.3000000000	3.7770000000	4.9110000000
C17	0.3340000000	3.3400000000	5.8030000000
C18	-0.7220000000	2.5970000000	5.3220000000
C19	-0.7540000000	2.2760000000	3.9840000000
C20	2.9790000000	0.9170000000	2.5740000000
C21	3.7130000000	0.3120000000	3.5830000000
C22	3.2220000000	-0.8340000000	4.1780000000
C23	2.0260000000	-1.3700000000	3.7450000000
C24	1.3330000000	-0.7050000000	2.7560000000
C25	2.6300000000	3.7690000000	0.1860000000
C26	2.1210000000	3.9930000000	2.5360000000
C27	3.4790000000	2.1110000000	1.7970000000
H28	2.0030000000	5.9300000000	-1.3300000000
H29	-0.0080000000	6.4230000000	-2.4250000000
H30	-1.8790000000	5.0610000000	-2.0470000000
H31	-1.6870000000	3.2770000000	-0.5770000000
H32	2.0350000000	4.2980000000	5.2150000000
H33	0.3980000000	3.5470000000	6.7290000000

H34	-1.4170000000	2.3100000000	5.9040000000
H35	-1.4670000000	1.7340000000	3.6670000000
H36	4.5430000000	0.6820000000	3.8610000000
H37	3.7060000000	-1.2520000000	4.8820000000
H38	1.6900000000	-2.1760000000	4.1190000000
H39	0.5030000000	-1.0620000000	2.4660000000
H40	2.9440000000	4.2120000000	2.9550000000
H41	1.7370000000	4.7780000000	2.1630000000
H42	3.1880000000	4.5180000000	0.3650000000
H43	3.0600000000	3.1950000000	-0.4360000000
H44	3.8960000000	1.8070000000	0.9990000000
H45	4.1150000000	2.5780000000	2.3260000000
H46	-3.6830000000	0.9640000000	1.8190000000
H47	-3.3510000000	-0.4210000000	2.4350000000
H48	-3.9070000000	-0.3380000000	1.0030000000
C49	1.9710000000	-0.0400000000	-1.1100000000
O50	-1.5000000000	-1.0300000000	0.6890000000
O51	1.3630000000	-1.1510000000	-1.1280000000
C52	3.3700000000	-0.0380000000	-1.6800000000
Fe53	-0.5340000000	-1.7770000000	-1.0750000000
H54	3.6830000000	-0.9640000000	-1.8190000000
H55	3.3510000000	0.4210000000	-2.4350000000
H56	3.9070000000	0.3380000000	-1.0030000000
N57	-2.3870000000	-3.0310000000	-1.4420000000
N58	-0.2420000000	-3.4960000000	0.1610000000
N59	-0.1720000000	-2.6880000000	-3.1050000000
N60	-1.7810000000	-0.4250000000	-2.1820000000
C61	-2.6300000000	-3.7690000000	-0.1860000000
C62	-2.1210000000	-3.9930000000	-2.5360000000
C63	-3.4790000000	-2.1110000000	-1.7970000000
C64	-1.3170000000	-4.2550000000	0.4070000000
C65	0.9220000000	-3.8110000000	0.7560000000
C66	-1.1790000000	-3.4480000000	-3.5800000000
C67	0.7540000000	-2.2760000000	-3.9840000000
C68	-2.9790000000	-0.9170000000	-2.5740000000
C69	-1.3330000000	0.7050000000	-2.7560000000
H70	-3.1880000000	-4.5180000000	-0.3650000000
H71	-3.0600000000	-3.1950000000	0.4360000000
H72	-2.9440000000	-4.2120000000	-2.9550000000
H73	-1.7370000000	-4.7780000000	-2.1630000000
H74	-3.8960000000	-1.8070000000	-0.9990000000
H75	-4.1150000000	-2.5780000000	-2.3260000000
C76	-1.2420000000	-5.3720000000	1.2110000000
C77	1.0510000000	-4.8790000000	1.6170000000
H78	1.6870000000	-3.2770000000	0.5770000000
C79	-1.3000000000	-3.7770000000	-4.9110000000
C80	0.7220000000	-2.5970000000	-5.3220000000
H81	1.4670000000	-1.7340000000	-3.6670000000
C82	-3.7130000000	-0.3120000000	-3.5830000000
C83	-2.0260000000	1.3700000000	-3.7450000000
H84	-0.5030000000	1.0620000000	-2.4660000000
C85	-0.0510000000	-5.6740000000	1.8420000000
H86	-2.0030000000	-5.9300000000	1.3300000000
H87	1.8790000000	-5.0610000000	2.0470000000
C88	-0.3340000000	-3.3400000000	-5.8030000000
H89	-2.0350000000	-4.2980000000	-5.2150000000
H90	1.4170000000	-2.3100000000	-5.9040000000
C91	-3.2220000000	0.8340000000	-4.1780000000
H92	-4.5430000000	-0.6820000000	-3.8610000000
H93	-1.6900000000	2.1760000000	-4.1190000000
H94	0.0080000000	-6.4230000000	2.4250000000
H95	-0.3980000000	-3.5470000000	-6.7290000000
H96	-3.7060000000	1.2520000000	-4.8820000000

4. YUZKAF10

Fe1	5.7006000000	17.0942000000	6.4105000000
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Fe2	4.0966000000	18.3062000000	3.4155000000
O3	7.7986000000	16.9022000000	6.6265000000
O4	5.8026000000	18.3402000000	8.1035000000
O5	7.9976000000	18.4682000000	8.5715000000
O6	5.9096000000	18.8412000000	5.0885000000
O7	5.2366000000	19.9962000000	3.3635000000
O8	3.6666000000	17.3552000000	6.2645000000
O9	2.6496000000	18.5942000000	4.7155000000
O10	1.9096000000	14.6652000000	7.1115000000
O11	-0.2024000000	17.0532000000	3.8905000000
O12	5.8746000000	15.8012000000	4.7075000000
O13	5.2636000000	16.8282000000	2.8105000000
O14	4.7576000000	12.5382000000	4.4235000000
O15	3.6066000000	14.8822000000	0.7465000000
N16	5.2516000000	15.4322000000	7.6755000000
N17	4.7126000000	13.4132000000	8.3415000000
N18	2.9056000000	18.3182000000	1.7445000000
N19	1.1636000000	18.6912000000	0.4045000000
N20	0.8346000000	15.8472000000	5.5025000000
N21	4.2346000000	13.7782000000	2.6345000000
C22	8.4716000000	15.4452000000	6.9495000000
C23	5.0946000000	14.1852000000	7.3345000000
C24	4.5786000000	14.2502000000	9.4225000000
C25	4.8946000000	15.4692000000	8.9935000000
C26	1.6156000000	18.6122000000	1.6635000000
C27	2.2306000000	18.4532000000	-0.3805000000
C28	3.3046000000	18.2262000000	0.4485000000
C29	6.7916000000	18.6712000000	8.8305000000
C30	6.4946000000	19.3142000000	10.2075000000
C31	5.1266000000	19.4112000000	10.6365000000
C32	4.8706000000	19.9812000000	11.8805000000
C33	5.8746000000	20.3802000000	12.6805000000
C34	7.1526000000	20.3422000000	12.2365000000
C35	7.4886000000	19.7792000000	11.0075000000
C36	5.9896000000	19.8482000000	4.3585000000
C37	6.9896000000	20.8952000000	4.6395000000
C38	7.9416000000	20.7552000000	5.6615000000
C39	8.9166000000	21.7282000000	5.8395000000
C40	8.9416000000	22.8882000000	5.1135000000
C41	7.9726000000	23.0432000000	4.1505000000
C42	7.0136000000	22.0212000000	3.9145000000
C43	2.7736000000	18.1332000000	5.8985000000
C44	1.2126000000	15.6162000000	6.8605000000
C45	0.0046000000	16.9582000000	5.0985000000
C46	2.4816000000	19.9592000000	7.4675000000
C47	0.5676000000	15.7332000000	9.2005000000
C48	-1.8534000000	18.3762000000	5.6615000000
C49	1.7976000000	18.7012000000	6.9495000000
C50	1.6406000000	17.7042000000	8.1345000000
C51	0.6716000000	16.5392000000	7.8825000000
C52	-0.6824000000	17.0842000000	7.4235000000
C53	-0.5214000000	17.8722000000	6.1645000000
C54	0.4256000000	19.0382000000	6.3865000000
C55	5.9686000000	16.0022000000	3.4845000000
C56	4.4766000000	14.3102000000	1.3525000000
C57	5.1286000000	13.0432000000	3.4105000000
C58	8.3036000000	16.2542000000	2.9515000000
C59	5.7796000000	14.1032000000	-0.7805000000
C60	7.0456000000	11.4592000000	3.3515000000
C61	7.1176000000	15.3422000000	2.6995000000
C62	6.8306000000	15.2262000000	1.2045000000
C63	5.9356000000	14.1242000000	0.7895000000
C64	6.4376000000	12.7942000000	1.2635000000
C65	6.5286000000	12.8252000000	2.7885000000
C66	7.4346000000	13.9602000000	3.2325000000
C67	2.5096000000	14.8132000000	4.0325000000

C68	1.2226000000	14.8752000000	4.5215000000
C69	0.2646000000	13.9502000000	4.1215000000
C70	0.6696000000	12.9912000000	3.1885000000
C71	1.9256000000	12.9482000000	2.6405000000
C72	2.8346000000	13.8802000000	3.0845000000
C73	-1.1224000000	13.9422000000	4.6985000000
C74	2.2786000000	11.8982000000	1.6035000000
H75	4.5526000000	12.4942000000	8.3265000000
H76	0.2826000000	18.8762000000	0.1235000000
H77	8.1556000000	15.1512000000	7.7495000000
H78	8.2556000000	14.8842000000	6.2245000000
H79	9.3956000000	15.0982000000	6.9645000000
H80	5.2446000000	13.8652000000	6.4615000000
H81	4.3026000000	14.0132000000	10.2965000000
H82	4.8976000000	16.2542000000	9.5415000000
H83	1.0636000000	18.7332000000	2.4185000000
H84	2.2436000000	18.4472000000	-1.3285000000
H85	4.1826000000	18.0322000000	0.1525000000
H86	4.4126000000	19.1152000000	10.0895000000
H87	3.9706000000	20.0832000000	12.1625000000
H88	5.6786000000	20.6912000000	13.5685000000
H89	7.8386000000	20.7142000000	12.7695000000
H90	8.3906000000	19.7122000000	10.7255000000
H91	7.9176000000	19.9962000000	6.2245000000
H92	9.5866000000	21.5992000000	6.5055000000
H93	9.5956000000	23.5672000000	5.2765000000
H94	7.9446000000	23.8352000000	3.6175000000
H95	6.3766000000	22.1592000000	3.2325000000
H96	3.3176000000	19.7122000000	7.8525000000
H97	2.6266000000	20.5712000000	6.7575000000
H98	1.9376000000	20.3702000000	8.1345000000
H99	0.2166000000	16.2772000000	9.8965000000
H100	-0.0154000000	14.9862000000	9.0675000000
H101	1.4326000000	15.4132000000	9.4525000000
H102	-1.7244000000	18.8472000000	4.8465000000
H103	-2.4414000000	17.6382000000	5.5135000000
H104	-2.2294000000	18.9642000000	6.3125000000
H105	2.5106000000	17.3532000000	8.3265000000
H106	1.3386000000	18.2052000000	8.9045000000
H107	-1.2744000000	16.3552000000	7.2605000000
H108	-1.0544000000	17.6472000000	8.0895000000
H109	-0.0014000000	19.6532000000	6.9945000000
H110	0.5436000000	19.4762000000	5.5425000000
H111	8.4896000000	16.3022000000	3.8845000000
H112	9.0696000000	15.9052000000	2.4925000000
H113	7.4896000000	17.1242000000	2.6255000000
H114	6.6396000000	13.9882000000	-1.1795000000
H115	5.2086000000	13.3762000000	-1.0315000000
H116	5.4026000000	14.9212000000	-1.0765000000
H117	7.0846000000	11.4992000000	4.2995000000
H118	6.4466000000	10.7752000000	3.0845000000
H119	7.9106000000	11.2922000000	3.0105000000
H120	6.4196000000	16.0352000000	0.9225000000
H121	7.6456000000	15.1132000000	0.7455000000
H122	5.8376000000	12.1102000000	0.9965000000
H123	7.2926000000	12.6282000000	0.8935000000
H124	8.3266000000	13.7392000000	2.9815000000
H125	7.3856000000	13.9992000000	4.1805000000
H126	3.1636000000	15.4282000000	4.3585000000
H127	0.0286000000	12.3332000000	2.9075000000
H128	-1.2124000000	14.6492000000	5.3205000000
H129	-1.7594000000	14.0302000000	3.9885000000
H130	-1.2834000000	13.0942000000	5.1285000000
H131	2.1736000000	11.0362000000	1.9745000000
H132	1.7036000000	11.9972000000	0.8485000000
H133	3.1756000000	12.0162000000	1.3225000000

H134 8.3809000000 17.3384000000 7.3125000000

5. XIGDIA

Fe1	0.5270000000	0.8030000000	9.1180000000
O2	0.8430000000	1.7010000000	10.9310000000
O3	-0.0140000000	-0.5600000000	7.6230000000
O4	1.8760000000	-0.6380000000	9.7000000000
O5	-1.1830000000	2.0020000000	8.8810000000
N6	1.6000000000	2.0140000000	7.7660000000
C7	2.9160000000	2.0700000000	7.7980000000
H8	3.3510000000	1.5850000000	8.4890000000
C9	3.7130000000	2.7590000000	6.9270000000
H10	4.6580000000	2.7750000000	7.0240000000
C11	3.0920000000	3.4200000000	5.9210000000
H12	3.6000000000	3.9070000000	5.2810000000
C13	1.7640000000	3.3840000000	5.8320000000
H14	1.3150000000	3.8700000000	5.1500000000
C15	1.0550000000	2.6410000000	6.7300000000
H16	0.1160000000	2.5680000000	6.6060000000
C17	-0.0370000000	1.4380000000	11.7920000000
C18	-0.0580000000	2.2610000000	13.0570000000
C19	0.2460000000	3.6270000000	13.0350000000
C20	0.1600000000	4.3660000000	14.2130000000
H21	0.3100000000	5.3030000000	14.1780000000
C22	-0.1370000000	3.7840000000	15.4350000000
C23	-0.3970000000	2.4240000000	15.4450000000
H24	-0.5890000000	2.0030000000	16.2750000000
C25	-0.3860000000	1.6490000000	14.2920000000
C26	-0.1800000000	4.5800000000	16.7540000000
C27	0.7040000000	4.3500000000	11.7570000000
H28	1.6320000000	4.0720000000	11.5560000000
H29	0.1340000000	4.0490000000	11.0050000000
C30	-0.6420000000	0.1470000000	14.4110000000
H31	-1.2210000000	-0.1330000000	13.6590000000
H32	0.2210000000	-0.3280000000	14.3170000000
C33	1.4380000000	-1.7580000000	10.0820000000
C34	2.4190000000	-2.8910000000	10.2050000000
C35	2.5650000000	-3.5520000000	11.4290000000
C36	3.4400000000	-4.6220000000	11.5100000000
H37	3.5440000000	-5.0610000000	12.3450000000
C38	4.1710000000	-5.0770000000	10.4280000000
C39	4.0070000000	-4.3960000000	9.2310000000
H40	4.4970000000	-4.6900000000	8.4720000000
C41	3.1670000000	-3.3080000000	9.0890000000
C42	5.1000000000	-6.2890000000	10.5220000000
C43	3.0120000000	-2.6270000000	7.7280000000
H44	2.2120000000	-3.0040000000	7.2820000000
H45	2.8400000000	-1.6650000000	7.8810000000
O46	-0.9340000000	0.5600000000	11.6300000000
Fe47	-1.4750000000	-0.8030000000	10.1360000000
O48	-1.7910000000	-1.7010000000	8.3220000000
C49	-0.9110000000	-1.4380000000	7.4610000000
O50	0.2350000000	-2.0020000000	10.3720000000
O51	-2.8240000000	0.6380000000	9.5540000000
C52	-2.3860000000	1.7580000000	9.1720000000
C53	-3.3670000000	2.8910000000	9.0480000000
C54	-3.5130000000	3.5520000000	7.8240000000
C55	-4.3880000000	4.6220000000	7.7430000000
H56	-4.4920000000	5.0610000000	6.9080000000
C57	-5.1190000000	5.0770000000	8.8260000000
C58	-4.9550000000	4.3960000000	10.0230000000
H59	-5.4450000000	4.6900000000	10.7820000000
C60	-4.1150000000	3.3080000000	10.1650000000
C61	-3.9600000000	2.6270000000	11.5250000000
H62	-3.1600000000	3.0040000000	11.9720000000
H63	-3.7880000000	1.6650000000	11.3730000000

C64	-6.0480000000	6.2890000000	8.7320000000
C65	-2.7360000000	3.1120000000	6.5870000000
H66	-2.5400000000	2.1440000000	6.6600000000
H67	-1.8700000000	3.5930000000	6.5670000000
N68	-2.5480000000	-2.0140000000	11.4880000000
C69	-3.8640000000	-2.0700000000	11.4560000000
H70	-4.2990000000	-1.5850000000	10.7650000000
C71	-4.6610000000	-2.7590000000	12.3260000000
H72	-5.6060000000	-2.7750000000	12.2300000000
C73	-4.0400000000	-3.4200000000	13.3330000000
H74	-4.5480000000	-3.9070000000	13.9720000000
C75	-2.7120000000	-3.3840000000	13.4220000000
H76	-2.2630000000	-3.8700000000	14.1030000000
C77	-2.0030000000	-2.6410000000	12.5240000000
H78	-1.0640000000	-2.5680000000	12.6480000000
C79	-0.8900000000	-2.2610000000	6.1960000000
C80	-1.1950000000	-3.6270000000	6.2190000000
C81	-1.1080000000	-4.3660000000	5.0400000000
H82	-1.2580000000	-5.3030000000	5.0750000000
C83	-0.8110000000	-3.7840000000	3.8190000000
C84	-0.5510000000	-2.4240000000	3.8090000000
H85	-0.3590000000	-2.0030000000	2.9790000000
C86	-0.5620000000	-1.6490000000	4.9620000000
C87	-0.3060000000	-0.1470000000	4.8430000000
H88	0.2730000000	0.1330000000	5.5950000000
H89	-1.1690000000	0.3280000000	4.9370000000
C90	-0.7680000000	-4.5800000000	2.5000000000
C91	-1.6520000000	-4.3500000000	7.4970000000
H92	-2.5800000000	-4.0720000000	7.6980000000
H93	-1.0820000000	-4.0490000000	8.2480000000
H94	5.5696000000	-6.4635000000	9.5539000000
H95	5.8700000000	-6.1001000000	11.2700000000
H96	4.5232000000	-7.1682000000	10.8092000000
H97	3.8685000000	-2.8709000000	7.0995000000
H98	-4.8170000000	2.8698000000	12.1533000000
H99	-3.3544000000	3.2514000000	5.7003000000
H100	0.2411000000	0.0571000000	3.9226000000
H101	0.7250000000	5.4252000000	11.9349000000
H102	-1.1891000000	-0.0571000000	15.3314000000
H103	-0.4340000000	3.9099000000	17.5753000000
H104	0.7958000000	5.0286000000	16.9403000000
H105	-0.9323000000	5.3654000000	16.6807000000
H106	-6.5174000000	6.4636000000	9.7001000000
H107	-5.4712000000	7.1681000000	8.4446000000
H108	-6.8182000000	6.1000000000	7.9842000000
C109	1.6808000000	-3.1611000000	12.6149000000
H110	1.9345000000	-3.7783000000	13.4768000000
H111	1.8436000000	-2.1115000000	12.8597000000
H112	0.6337000000	-3.3148000000	12.3542000000
H113	-0.5139000000	-3.9099000000	1.6787000000
H114	-0.0158000000	-5.3654000000	2.5734000000
H115	-1.7438000000	-5.0285000000	2.3137000000
H116	-1.6726000000	-5.4252000000	7.3192000000

6. YEQPOA

Fe1	3.4825000000	0.9215000000	3.5624000000
N2	1.8929000000	0.1560000000	4.4701000000
N3	3.8361000000	-0.8432000000	2.7198000000
N4	5.2829000000	1.5321000000	2.9798000000
N5	3.3205000000	2.5467000000	4.6998000000
C6	1.8375000000	-2.0530000000	3.4201000000
H7	1.3512000000	-2.8662000000	3.3450000000
C8	5.9485000000	-0.3667000000	1.5845000000
H9	6.6047000000	-0.7023000000	0.9849000000
C10	5.3117000000	3.7630000000	3.9791000000
H11	5.7837000000	4.5860000000	4.0312000000

C12	1.2139000000	2.0665000000	5.8397000000
H13	0.5486000000	2.4084000000	6.4252000000
C14	1.0251000000	0.7953000000	5.3332000000
C15	1.3311000000	-1.0864000000	4.2675000000
C16	2.9903000000	-1.9328000000	2.6749000000
C17	4.8592000000	-1.1689000000	1.8526000000
C18	6.1557000000	0.8862000000	2.1223000000
C19	5.8494000000	2.7746000000	3.1793000000
C20	4.1451000000	3.6531000000	4.7087000000
C21	2.2928000000	2.8779000000	5.5613000000
C22	-0.0828000000	-0.0606000000	5.6854000000
C23	0.1171000000	-1.2400000000	5.0325000000
C24	3.4827000000	-2.9428000000	1.7658000000
C25	4.6534000000	-2.4677000000	1.2563000000
C26	7.2957000000	1.7178000000	1.8074000000
C27	7.0956000000	2.9005000000	2.4552000000
C28	3.6412000000	4.6761000000	5.6013000000
C29	2.4934000000	4.1868000000	6.1422000000
C30	-1.2288000000	0.3179000000	6.5707000000
H31	-0.9061000000	0.9338000000	7.2748000000
H32	-1.5796000000	-0.4944000000	7.0156000000
C33	-2.3604000000	0.9926000000	5.7924000000
H34	-3.0907000000	1.2176000000	6.4069000000
H35	-2.6911000000	0.3809000000	5.1021000000
H36	-2.0245000000	1.8103000000	5.3712000000
C37	-0.7155000000	-2.4829000000	5.0869000000
H38	-1.2931000000	-2.4449000000	5.8897000000
H39	-0.1161000000	-3.2646000000	5.1852000000
C40	-1.5983000000	-2.6913000000	3.8552000000
H41	-2.1002000000	-3.5277000000	3.9509000000
H42	-1.0354000000	-2.7369000000	3.0534000000
H43	-2.2248000000	-1.9418000000	3.7720000000
C44	2.8164000000	-4.2514000000	1.4784000000
H45	3.0085000000	-4.5099000000	0.5425000000
H46	1.8365000000	-4.1388000000	1.5654000000
C47	3.2698000000	-5.3798000000	2.4080000000
H48	2.7827000000	-6.2009000000	2.1868000000
H49	3.0861000000	-5.1307000000	3.3380000000
H50	4.2314000000	-5.5307000000	2.2939000000
C51	5.5865000000	-3.1247000000	0.2876000000
H52	5.8781000000	-2.4568000000	-0.3818000000
H53	5.0997000000	-3.8404000000	-0.1930000000
C54	6.8237000000	-3.7281000000	0.9579000000
H55	7.4079000000	-4.1195000000	0.2748000000
H56	6.5461000000	-4.4252000000	1.5880000000
H57	7.3095000000	-3.0270000000	1.4400000000
C58	8.4672000000	1.2911000000	0.9735000000
H59	8.9510000000	2.0948000000	0.6566000000
H60	8.1388000000	0.8019000000	0.1775000000
C61	9.4343000000	0.3973000000	1.7471000000
H62	10.1936000000	0.1638000000	1.1737000000
H63	8.9717000000	-0.4205000000	2.0248000000
H64	9.7577000000	0.8747000000	2.5391000000
C65	7.9614000000	4.1220000000	2.4434000000
H66	7.3855000000	4.9206000000	2.3376000000
H67	8.5633000000	4.0792000000	1.6584000000
C68	8.8075000000	4.2869000000	3.7050000000
H69	9.3392000000	5.1073000000	3.6367000000
H70	9.4060000000	3.5162000000	3.8001000000
H71	8.2198000000	4.3428000000	4.4878000000
C72	4.2689000000	6.0180000000	5.8317000000
H73	5.2538000000	5.9274000000	5.7855000000
H74	4.0359000000	6.3322000000	6.7408000000
C75	3.8142000000	7.0618000000	4.8087000000
H76	4.2892000000	7.9045000000	4.9682000000
H77	2.8494000000	7.2090000000	4.8978000000

H78	4.0137000000	6.7415000000	3.9044000000
C79	1.5835000000	4.8507000000	7.1342000000
H80	2.1095000000	5.4900000000	7.6778000000
H81	1.2140000000	4.1641000000	7.7454000000
C82	0.4277000000	5.5972000000	6.4645000000
H83	-0.1503000000	5.9896000000	7.1522000000
H84	-0.0926000000	4.9715000000	5.9193000000
H85	0.7858000000	6.3094000000	5.8940000000
C86	2.6139000000	1.4818000000	2.1951000000
O87	2.0354000000	1.8047000000	1.2597000000

7. DEDWUE

Fe1	0.0000000000	0.0000000000	0.0000000000
N2	1.3816000000	1.1624000000	-0.8256000000
N3	0.2163000000	0.9707000000	1.7424000000
C4	1.8505000000	1.1498000000	-2.1255000000
C5	2.8330000000	2.1582000000	-2.3433000000
C6	3.0105000000	2.7927000000	-1.1582000000
C7	2.1257000000	2.1748000000	-0.2414000000
C8	1.9399000000	2.5487000000	1.1053000000
C9	1.0411000000	2.0177000000	1.9925000000
C10	0.8480000000	2.4757000000	3.3722000000
C11	-0.0550000000	1.6927000000	3.9170000000
C12	-0.4787000000	0.7452000000	2.9213000000
C13	1.4101000000	0.2192000000	-3.0863000000
C14	3.4878000000	2.4893000000	-3.6450000000
C15	2.7112000000	3.4823000000	-4.4506000000
C16	3.9164000000	3.9490000000	-0.8510000000
C17	3.1877000000	5.2693000000	-0.9546000000
C18	1.5602000000	3.6786000000	3.9278000000
C19	0.9438000000	4.9999000000	3.4649000000
C20	-0.5882000000	1.7078000000	5.3274000000
C21	0.1097000000	0.7318000000	6.2319000000
H22	1.8134000000	0.2818000000	-3.9502000000
H23	2.5108000000	3.2316000000	1.4353000000
H24	3.5761000000	1.6764000000	-4.1342000000
H25	4.3520000000	2.8409000000	-3.4595000000
H26	4.6451000000	3.9610000000	-1.4844000000
H27	4.2726000000	3.8530000000	0.0245000000
H28	2.4666000000	3.6557000000	3.6435000000
H29	1.5287000000	3.6508000000	4.8826000000
H30	-1.5157000000	1.4810000000	5.3120000000
H31	-0.4807000000	2.5741000000	5.6923000000
H32	3.2902000000	4.2007000000	-4.7108000000
H33	2.3835000000	3.0521000000	-5.2383000000
H34	1.9909000000	3.8199000000	-3.9502000000
H35	3.7883000000	5.9564000000	-1.2022000000
H36	2.4894000000	5.1941000000	-1.5825000000
H37	2.8127000000	5.4936000000	-0.0981000000
H38	1.6314000000	5.5741000000	3.1528000000
H39	0.3214000000	4.8383000000	2.7725000000
H40	0.5033000000	5.4156000000	4.1956000000
H41	0.1043000000	-0.1304000000	5.8272000000
H42	1.0165000000	1.0050000000	6.3547000000
H43	-0.3310000000	0.6851000000	7.0662000000
N44	-1.3816000000	-1.1624000000	0.8256000000
N45	-0.2163000000	-0.9707000000	-1.7424000000
C46	-1.4101000000	-0.2192000000	3.0863000000
C47	0.4787000000	-0.7452000000	-2.9213000000
C48	-1.8505000000	-1.1498000000	2.1255000000
C49	-2.1257000000	-2.1748000000	0.2414000000
C50	-1.0411000000	-2.0177000000	-1.9925000000
H51	-1.8134000000	-0.2818000000	3.9502000000
C52	0.0550000000	-1.6927000000	-3.9170000000
C53	-2.8330000000	-2.1582000000	2.3433000000
C54	-3.0105000000	-2.7927000000	1.1582000000

C55	-1.9399000000	-2.5487000000	-1.1053000000
C56	-0.8480000000	-2.4757000000	-3.3722000000
C57	0.5882000000	-1.7078000000	-5.3274000000
C58	-3.4878000000	-2.4893000000	3.6450000000
C59	-3.9164000000	-3.9490000000	0.8510000000
H60	-2.5108000000	-3.2316000000	-1.4353000000
C61	-1.5602000000	-3.6786000000	-3.9278000000
C62	-0.1097000000	-0.7318000000	-6.2319000000
H63	1.5157000000	-1.4810000000	-5.3120000000
H64	0.4807000000	-2.5741000000	-5.6923000000
C65	-2.7112000000	-3.4823000000	4.4506000000
H66	-3.5761000000	-1.6764000000	4.1342000000
H67	-4.3520000000	-2.8409000000	3.4595000000
C68	-3.1877000000	-5.2693000000	0.9546000000
H69	-4.6451000000	-3.9610000000	1.4844000000
H70	-4.2726000000	-3.8530000000	-0.0245000000
C71	-0.9438000000	-4.9999000000	-3.4649000000
H72	-2.4666000000	-3.6557000000	-3.6435000000
H73	-1.5287000000	-3.6508000000	-4.8826000000
H74	-0.1043000000	0.1304000000	-5.8272000000
H75	-1.0165000000	-1.0050000000	-6.3547000000
H76	0.3310000000	-0.6851000000	-7.0662000000
H77	-3.2902000000	-4.2007000000	4.7108000000
H78	-2.3835000000	-3.0521000000	5.2383000000
H79	-1.9909000000	-3.8199000000	3.9502000000
H80	-3.7883000000	-5.9564000000	1.2022000000
H81	-2.4894000000	-5.1941000000	1.5825000000
H82	-2.8127000000	-5.4936000000	0.0981000000
H83	-1.6314000000	-5.5741000000	-3.1528000000
H84	-0.3214000000	-4.8383000000	-2.7725000000
H85	-0.5033000000	-5.4156000000	-4.1956000000

8. BUYKUB10

Fe1	0.0000000000	1.1814000000	2.1385000000
N2	1.6277000000	1.1962000000	1.0308000000
N3	0.0000000000	3.1680000000	2.1385000000
N4	0.0000000000	-0.8207000000	2.1385000000
C5	2.1987000000	0.1245000000	0.3960000000
C6	3.3999000000	0.5146000000	-0.2842000000
C7	3.5713000000	1.8431000000	-0.0614000000
C8	2.4567000000	2.2759000000	0.7527000000
C9	2.1922000000	3.5698000000	1.1092000000
C10	1.0102000000	4.0111000000	1.7226000000
C11	0.6404000000	5.3836000000	1.8996000000
C12	0.4409000000	-3.0938000000	1.5267000000
C13	0.7474000000	-1.6228000000	1.3212000000
C14	1.7106000000	-1.1789000000	0.4648000000
C15	4.3104000000	-0.4132000000	-1.0420000000
C16	5.3188000000	-1.1352000000	-0.1436000000
C17	4.7022000000	2.7306000000	-0.4935000000
C18	5.7398000000	2.9440000000	0.6123000000
C19	1.5163000000	6.5644000000	1.5756000000
C20	2.5748000000	6.8211000000	2.6416000000
C21	1.7462000000	-3.8892000000	1.6049000000
C22	1.6517000000	-5.3446000000	1.9620000000
H23	2.8663000000	4.2173000000	0.9238000000
H24	2.0786000000	-1.8164000000	-0.1369000000
H25	-0.0656000000	-3.4117000000	0.7870000000
H26	4.7917000000	0.0948000000	-1.6851000000
H27	3.7852000000	-1.0583000000	-1.4884000000
H28	4.3322000000	3.5697000000	-0.7442000000
H29	5.1199000000	2.3377000000	-1.2489000000
H30	0.9627000000	7.3447000000	1.5055000000
H31	1.9473000000	6.4128000000	0.7442000000
H32	2.2974000000	-3.4749000000	2.2583000000
H33	2.1661000000	-3.8224000000	0.7528000000

H34	5.2950000000	-2.0691000000	-0.3165000000
H35	6.1920000000	-0.8213000000	-0.3165000000
H36	5.0980000000	-0.9793000000	0.7699000000
H37	6.4327000000	2.2903000000	0.5303000000
H38	6.1264000000	3.8066000000	0.5303000000
H39	5.3168000000	2.8589000000	1.4627000000
H40	2.9100000000	7.7080000000	2.5405000000
H41	2.1880000000	6.7287000000	3.4986000000
H42	3.2820000000	6.1916000000	2.5405000000
H43	0.8533000000	-5.7020000000	1.5996000000
H44	2.3849000000	-5.8126000000	1.5996000000
H45	1.6410000000	-5.4493000000	2.8998000000
N46	-1.6277000000	1.1962000000	3.2462000000
C47	-1.0102000000	4.0111000000	2.5544000000
C48	-0.7474000000	-1.6228000000	2.9558000000
C49	-0.6404000000	5.3836000000	2.3774000000
C50	-0.4409000000	-3.0938000000	2.7503000000
C51	-2.1987000000	0.1245000000	3.8810000000
C52	-2.4567000000	2.2759000000	3.5243000000
C53	-2.1922000000	3.5698000000	3.1678000000
C54	-1.7106000000	-1.1789000000	3.8122000000
C55	-1.5163000000	6.5644000000	2.7014000000
C56	-1.7462000000	-3.8892000000	2.6721000000
H57	0.0656000000	-3.4117000000	3.4900000000
C58	-3.3999000000	0.5146000000	4.5612000000
C59	-3.5713000000	1.8431000000	4.3384000000
H60	-2.8663000000	4.2173000000	3.3532000000
H61	-2.0786000000	-1.8164000000	4.4139000000
C62	-2.5748000000	6.8211000000	1.6354000000
H63	-0.9627000000	7.3447000000	2.7715000000
H64	-1.9473000000	6.4128000000	3.5328000000
C65	-1.6517000000	-5.3446000000	2.3150000000
H66	-2.2974000000	-3.4749000000	2.0187000000
H67	-2.1661000000	-3.8224000000	3.5242000000
C68	-4.3104000000	-0.4132000000	5.3190000000
C69	-4.7022000000	2.7306000000	4.7705000000
H70	-2.9100000000	7.7080000000	1.7365000000
H71	-2.1880000000	6.7287000000	0.7784000000
H72	-3.2820000000	6.1916000000	1.7365000000
H73	-0.8533000000	-5.7020000000	2.6774000000
H74	-2.3849000000	-5.8126000000	2.6774000000
H75	-1.6410000000	-5.4493000000	1.3772000000
C76	-5.3188000000	-1.1352000000	4.4206000000
H77	-4.7917000000	0.0948000000	5.9621000000
H78	-3.7852000000	-1.0583000000	5.7654000000
C79	-5.7398000000	2.9440000000	3.6647000000
H80	-4.3322000000	3.5697000000	5.0212000000
H81	-5.1199000000	2.3377000000	5.5259000000
H82	-5.2950000000	-2.0691000000	4.5935000000
H83	-6.1920000000	-0.8213000000	4.5935000000
H84	-5.0980000000	-0.9793000000	3.5071000000
H85	-6.4327000000	2.2903000000	3.7467000000
H86	-6.1264000000	3.8066000000	3.7467000000
H87	-5.3168000000	2.8589000000	2.8143000000

9. FATBOR

Fe1	0.0000000000	0.0000000000	0.0000000000
Fe2	2.8180000000	-1.3702000000	0.5859000000
S3	0.7449000000	-2.3706000000	0.0810000000
S4	1.5587000000	0.0172000000	1.9817000000
S5	2.2415000000	0.1366000000	-1.1045000000
O6	4.2270000000	-2.8422000000	-1.5329000000
O7	3.1191000000	-3.5030000000	2.5755000000
O8	5.1007000000	0.2056000000	1.5464000000
C9	3.6955000000	-2.2864000000	-0.7037000000
C10	3.0002000000	-2.6723000000	1.8189000000

C11	4.2357000000	-0.4174000000	1.1475000000
C12	0.8511000000	-3.2586000000	-1.4662000000
C13	0.7487000000	-2.6440000000	-2.7009000000
C14	0.8031000000	-3.3950000000	-3.8484000000
C15	0.9741000000	-4.7563000000	-3.7820000000
C16	1.0732000000	-5.3688000000	-2.5719000000
C17	1.0139000000	-4.6252000000	-1.4187000000
C18	1.1269000000	-0.8495000000	3.4816000000
C19	-0.0735000000	-1.4914000000	3.6417000000
C20	-0.3713000000	-2.1154000000	4.8328000000
C21	0.5292000000	-2.1427000000	5.8514000000
C22	1.7312000000	-1.5008000000	5.6977000000
C23	2.0279000000	-0.8422000000	4.5180000000
C24	3.0796000000	1.7200000000	-1.0546000000
C25	3.0372000000	2.5685000000	0.0247000000
C26	3.6899000000	3.7883000000	-0.0247000000
C27	4.3539000000	4.1637000000	-1.1532000000
C28	4.3725000000	3.3488000000	-2.2381000000
C29	3.7449000000	2.1070000000	-2.2078000000
H30	0.6410000000	-1.7012000000	-2.7445000000
H31	0.7281000000	-2.9692000000	-4.6944000000
H32	1.0229000000	-5.2713000000	-4.5787000000
H33	1.1764000000	-6.3117000000	-2.5264000000
H34	1.0933000000	-5.0542000000	-0.5728000000
H35	-0.6920000000	-1.5071000000	2.9209000000
H36	-1.2193000000	-2.5297000000	4.9447000000
H37	0.3365000000	-2.6052000000	6.6575000000
H38	2.3630000000	-1.5124000000	6.4071000000
H39	2.8507000000	-0.3776000000	4.4269000000
H40	2.5568000000	2.3126000000	0.8042000000
H41	3.6719000000	4.3693000000	0.7264000000
H42	4.8108000000	4.9954000000	-1.1817000000
H43	4.8196000000	3.6278000000	-3.0291000000
H44	3.7663000000	1.5271000000	-2.9608000000
S45	-0.7449000000	2.3706000000	-0.0810000000
S46	-1.5587000000	-0.0172000000	-1.9817000000
S47	-2.2415000000	-0.1366000000	1.1045000000
Fe48	-2.8180000000	1.3702000000	-0.5859000000
C49	-0.8511000000	3.2586000000	1.4662000000
C50	-1.1269000000	0.8495000000	-3.4816000000
C51	-3.0796000000	-1.7200000000	1.0546000000
C52	-3.6955000000	2.2864000000	0.7037000000
C53	-3.0002000000	2.6723000000	-1.8189000000
C54	-4.2357000000	0.4174000000	-1.1475000000
C55	-0.7487000000	2.6440000000	2.7009000000
C56	-1.0139000000	4.6252000000	1.4187000000
C57	0.0735000000	1.4914000000	-3.6417000000
C58	-2.0279000000	0.8422000000	-4.5180000000
C59	-3.0372000000	-2.5685000000	-0.0247000000
C60	-3.7449000000	-2.1070000000	2.2078000000
O61	-4.2270000000	2.8422000000	1.5329000000
O62	-3.1191000000	3.5030000000	-2.5755000000
O63	-5.1007000000	-0.2056000000	-1.5464000000
C64	-0.8031000000	3.3950000000	3.8484000000
H65	-0.6410000000	1.7012000000	2.7445000000
C66	-1.0732000000	5.3688000000	2.5719000000
H67	-1.0933000000	5.0542000000	0.5728000000
C68	0.3713000000	2.1154000000	-4.8328000000
H69	0.6920000000	1.5071000000	-2.9209000000
C70	-1.7312000000	1.5008000000	-5.6977000000
H71	-2.8507000000	0.3776000000	-4.4269000000
C72	-3.6899000000	-3.7883000000	0.0247000000
H73	-2.5568000000	-2.3126000000	-0.8042000000
C74	-4.3725000000	-3.3488000000	2.2381000000
H75	-3.7663000000	-1.5271000000	2.9608000000
C76	-0.9741000000	4.7563000000	3.7820000000

H77	-0.7281000000	2.9692000000	4.6944000000
H78	-1.1764000000	6.3117000000	2.5264000000
C79	-0.5292000000	2.1427000000	-5.8514000000
H80	1.2193000000	2.5297000000	-4.9447000000
H81	-2.3630000000	1.5124000000	-6.4071000000
C82	-4.3539000000	-4.1637000000	1.1532000000
H83	-3.6719000000	-4.3693000000	-0.7264000000
H84	-4.8196000000	-3.6278000000	3.0291000000
H85	-1.0229000000	5.2713000000	4.5787000000
H86	-0.3365000000	2.6052000000	-6.6575000000
H87	-4.8108000000	-4.9954000000	1.1817000000

10. VUPJUL

Fe1	4.1920000000	3.8750000000	3.9570000000
Fe2	2.3710000000	0.7980000000	4.4730000000
O3	2.3510000000	2.9660000000	4.6440000000
H4	2.1300000000	3.0300000000	5.4660000000
H5	1.6840000000	3.4080000000	4.0780000000
O6	5.3520000000	2.5540000000	5.0730000000
O7	4.3070000000	0.5930000000	5.2010000000
O8	4.2180000000	2.7350000000	2.2190000000
O9	3.0460000000	0.8690000000	2.5090000000
O10	2.9600000000	5.2810000000	2.8910000000
O11	0.9270000000	4.4050000000	3.1050000000
O12	1.6490000000	0.7630000000	6.4510000000
O13	1.5980000000	2.8900000000	7.1020000000
N14	6.0250000000	4.9730000000	3.2210000000
N15	4.4000000000	5.4270000000	5.6300000000
N16	2.2410000000	-1.4570000000	4.3800000000
N17	0.2240000000	0.5990000000	3.6870000000
C18	6.2850000000	5.9960000000	4.2440000000
C19	5.4350000000	6.2870000000	5.1610000000
C20	7.1970000000	4.0660000000	3.1630000000
C21	5.8230000000	5.5550000000	1.9070000000
C22	4.7480000000	4.8470000000	6.9290000000
C23	3.1780000000	6.2150000000	5.8210000000
C24	1.0240000000	-1.7370000000	3.5840000000
C25	-0.0940000000	-0.8220000000	3.9310000000
C26	3.4110000000	-2.0280000000	3.6900000000
C27	2.1730000000	-2.0700000000	5.7130000000
C28	0.1000000000	0.9470000000	2.2620000000
C29	-0.7560000000	1.4280000000	4.4050000000
C30	6.3910000000	0.7800000000	6.2540000000
C31	6.4290000000	-0.5630000000	6.5210000000
C32	7.4650000000	-1.1130000000	7.2710000000
C33	8.4380000000	-0.3160000000	7.7750000000
C34	8.4060000000	1.0260000000	7.5380000000
C35	7.3850000000	1.5870000000	6.7600000000
C36	5.2620000000	1.3560000000	5.4450000000
C37	3.7840000000	1.3890000000	0.3450000000
C38	3.6240000000	0.1230000000	-0.1360000000
C39	3.7860000000	-0.1670000000	-1.4740000000
C40	4.0690000000	0.8330000000	-2.3530000000
C41	4.2130000000	2.0990000000	-1.8990000000
C42	4.0850000000	2.3990000000	-0.5470000000
C43	3.6780000000	1.6940000000	1.8060000000
C44	1.1210000000	6.3740000000	1.8340000000
C45	1.9280000000	7.2600000000	1.1580000000
C46	1.3280000000	8.2910000000	0.4050000000
C47	-0.0360000000	8.4110000000	0.3680000000
C48	-0.8240000000	7.5420000000	1.0270000000
C49	-0.2660000000	6.5140000000	1.7700000000
C50	1.7090000000	5.2650000000	2.6630000000
C51	1.0280000000	1.2320000000	8.6650000000
C52	0.4350000000	2.1340000000	9.5340000000
C53	-0.0330000000	1.7070000000	10.7580000000

C54	0.1150000000	0.4040000000	11.1350000000
C55	0.7150000000	-0.5160000000	10.3040000000
C56	1.1670000000	-0.0830000000	9.0630000000
C57	1.4670000000	1.6710000000	7.3070000000
H58	6.4690000000	6.9160000000	3.7080000000
H59	7.1880000000	5.6840000000	4.7560000000
H60	6.0280000000	6.5190000000	6.0330000000
H61	4.9300000000	7.1800000000	4.8130000000
H62	7.3650000000	3.6210000000	4.1350000000
H63	8.0710000000	4.6250000000	2.8720000000
H64	7.0130000000	3.2880000000	2.4400000000
H65	4.9710000000	6.2200000000	1.9270000000
H66	5.6470000000	4.7690000000	1.1910000000
H67	6.7030000000	6.1080000000	1.6240000000
H68	5.6470000000	4.2520000000	6.8380000000
H69	3.9400000000	4.2200000000	7.2670000000
H70	4.9120000000	5.6370000000	7.6420000000
H71	2.8820000000	6.6660000000	4.8830000000
H72	3.3610000000	6.9900000000	6.5480000000
H73	2.3880000000	5.5720000000	6.1740000000
H74	1.2530000000	-1.6160000000	2.5370000000
H75	0.7180000000	-2.7530000000	3.7730000000
H76	-0.3260000000	-0.9530000000	4.9770000000
H77	-0.9550000000	-1.0840000000	3.3340000000
H78	3.4850000000	-1.5930000000	2.7030000000
H79	3.2960000000	-3.0970000000	3.6050000000
H80	4.3070000000	-1.8100000000	4.2520000000
H81	1.3240000000	-1.6700000000	6.2440000000
H82	3.0790000000	-1.8530000000	6.2620000000
H83	2.0680000000	-3.1390000000	5.6160000000
H84	0.8050000000	0.3600000000	1.6930000000
H85	0.3100000000	1.9970000000	2.1240000000
H86	-0.9030000000	0.7380000000	1.9220000000
H87	-0.7010000000	1.2060000000	5.4610000000
H88	-1.7500000000	1.2140000000	4.0400000000
H89	-0.5370000000	2.4730000000	4.2420000000
H90	5.6460000000	-1.2010000000	6.1450000000
H91	7.4980000000	-2.1780000000	7.4550000000
H92	9.2400000000	-0.7460000000	8.3650000000
H93	9.1740000000	1.6590000000	7.9540000000
H94	7.3730000000	2.6470000000	6.5560000000
H95	3.3650000000	-0.6700000000	0.5490000000
H96	3.6890000000	-1.1830000000	-1.8210000000
H97	4.1740000000	0.6200000000	-3.4050000000
H98	4.4340000000	2.8910000000	-2.5990000000
H99	4.2180000000	3.4100000000	-0.1990000000
H100	3.0040000000	7.1640000000	1.2070000000
H101	1.9410000000	8.9860000000	-0.1440000000
H102	-0.4920000000	9.2160000000	-0.1960000000
H103	-1.8980000000	7.6500000000	0.9740000000
H104	-0.9000000000	5.8220000000	2.2970000000
H105	0.3420000000	3.1730000000	9.2530000000
H106	-0.5200000000	2.4070000000	11.4180000000
H107	-0.2420000000	0.0860000000	12.1020000000
H108	0.8310000000	-1.5470000000	10.6090000000
H109	1.6370000000	-0.7910000000	8.4000000000

11. VUPJOF

Fe1	1.7330000000	3.0670000000	4.8340000000
Fe2	-0.8120000000	4.8910000000	2.9520000000
N3	3.7770000000	2.0990000000	4.9620000000
N4	2.4700000000	4.0330000000	6.7500000000
N5	-1.4870000000	5.8050000000	1.0020000000
N6	-3.0390000000	4.1400000000	2.9020000000
O7	-0.2750000000	3.9360000000	4.8280000000
H8	-0.4790000000	4.5970000000	5.3210000000

H9	-0.9310000000	2.8010000000	5.2340000000
O10	2.5760000000	4.5650000000	3.7040000000
O11	1.0700000000	5.8090000000	2.6340000000
O12	1.2120000000	1.9410000000	3.0990000000
O13	-0.2800000000	3.1740000000	1.9660000000
O14	0.9270000000	1.5300000000	6.0010000000
O15	-1.2350000000	1.6310000000	5.4490000000
O16	-0.8790000000	6.0720000000	6.1510000000
O17	-1.4620000000	6.5180000000	4.0570000000
C18	0.3410000000	2.1090000000	2.2310000000
C19	-0.0310000000	0.9220000000	1.4230000000
C20	2.2360000000	5.4520000000	2.9050000000
C21	3.3750000000	6.1970000000	2.2060000000
C22	-0.2220000000	1.0390000000	5.8950000000
C23	-0.3850000000	-0.4030000000	6.3320000000
C24	-1.3170000000	6.8430000000	5.2740000000
C25	-1.7200000000	8.2190000000	5.6830000000
C26	3.6530000000	3.2330000000	7.1470000000
C27	4.5060000000	2.8910000000	5.9580000000
C28	3.6980000000	0.6860000000	5.4080000000
C29	4.4520000000	2.1200000000	3.6640000000
C30	1.4700000000	3.9760000000	7.8300000000
C31	2.8340000000	5.4460000000	6.5790000000
C32	-3.6570000000	5.0430000000	1.9070000000
C33	-2.8060000000	5.2150000000	0.6900000000
C34	-3.7050000000	4.3000000000	4.2070000000
C35	-0.5060000000	5.4700000000	-0.0750000000
C36	-1.5630000000	7.2590000000	1.1360000000
C37	-3.1980000000	2.7470000000	2.4970000000
H38	3.0100000000	6.8620000000	1.6200000000
H39	3.9000000000	5.5740000000	1.6980000000
H40	3.9310000000	6.6220000000	2.8620000000
H41	-0.7030000000	1.1670000000	0.7830000000
H42	-0.3770000000	0.2370000000	2.0040000000
H43	0.7430000000	0.5900000000	0.9640000000
H44	-1.2960000000	-0.6750000000	6.2070000000
H45	-0.1530000000	-0.4820000000	7.2620000000
H46	0.1920000000	-0.9640000000	5.8080000000
H47	-2.0250000000	8.7050000000	4.9150000000
H48	-0.9660000000	8.6720000000	6.0670000000
H49	-2.4260000000	8.1660000000	6.3290000000
H50	4.1770000000	3.7370000000	7.7710000000
H51	3.3550000000	2.4190000000	7.5620000000
H52	5.2670000000	2.3870000000	6.2570000000
H53	4.8040000000	3.7050000000	5.5460000000
H54	3.2620000000	0.6450000000	6.2630000000
H55	4.5850000000	0.3260000000	5.4860000000
H56	3.1990000000	0.1750000000	4.7690000000
H57	4.5230000000	3.0240000000	3.3520000000
H58	3.9440000000	1.6050000000	3.0300000000
H59	5.3300000000	1.7420000000	3.7510000000
H60	1.2110000000	3.0650000000	7.9800000000
H61	0.6990000000	4.4910000000	7.5800000000
H62	1.8490000000	4.3360000000	8.6350000000
H63	3.4930000000	5.5250000000	5.8860000000
H64	3.1930000000	5.7860000000	7.3990000000
H65	2.0540000000	5.9500000000	6.3350000000
H66	-4.5040000000	4.6760000000	1.6420000000
H67	-3.7930000000	5.9030000000	2.3130000000
H68	-3.2630000000	5.7900000000	0.0750000000
H69	-2.6710000000	4.3550000000	0.2840000000
H70	-3.6190000000	5.2090000000	4.5000000000
H71	-3.2950000000	3.7150000000	4.8500000000
H72	-4.6340000000	4.0770000000	4.1230000000
H73	-0.4490000000	4.5160000000	-0.1690000000
H74	0.3560000000	5.8220000000	0.1560000000

H75	-0.8000000000	5.8570000000	-0.9050000000
H76	-2.1860000000	7.4850000000	1.8320000000
H77	-1.8570000000	7.6430000000	0.3060000000
H78	-0.6960000000	7.6070000000	1.3610000000
H79	-2.7870000000	2.6150000000	1.6380000000
H80	-4.1330000000	2.5360000000	2.4370000000
H81	-2.7800000000	2.1750000000	3.1430000000

12. PTSQFE10

Fe1	4.2790000000	1.6230000000	0.9160000000
S2	5.1260000000	0.2170000000	-0.8060000000
S3	3.9930000000	-0.1270000000	2.5250000000
S4	5.4270000000	3.5210000000	1.8230000000
S5	2.2710000000	2.7920000000	0.3720000000
O6	1.0340000000	5.8730000000	1.7610000000
O7	3.9540000000	6.5300000000	3.2050000000
O8	5.2370000000	-3.4260000000	-0.9770000000
O9	4.2860000000	-3.6930000000	2.1560000000
C10	4.0070000000	4.4170000000	1.8550000000
C11	2.7590000000	4.1370000000	1.2760000000
C12	2.1290000000	5.3630000000	1.8060000000
C13	3.4980000000	5.6900000000	2.4770000000
C14	4.9190000000	-1.1840000000	0.1370000000
C15	4.4790000000	-1.3210000000	1.4470000000
C16	4.5460000000	-2.8020000000	1.3920000000
C17	4.9880000000	-2.6590000000	-0.0770000000

13. PTHPFE10

Fe1	2.9670000000	7.2270000000	0.0000000000
S2	3.8920000000	5.6960000000	-1.5390000000
S3	3.2740000000	5.9430000000	1.9560000000
S4	3.9290000000	9.3460000000	0.2070000000
S5	0.7340000000	7.7800000000	-0.5010000000
C6	4.5160000000	6.4380000000	-3.0000000000
C7	4.5830000000	5.6990000000	-4.1830000000
C8	5.1970000000	6.2430000000	-5.3160000000
C9	5.6820000000	7.5100000000	-5.3190000000
C10	5.5800000000	8.2690000000	-4.1700000000
C11	4.9860000000	7.7290000000	-3.0440000000
C12	2.4560000000	6.7100000000	3.3060000000
C13	1.7650000000	7.8900000000	3.1810000000
C14	1.1080000000	8.4870000000	4.2530000000
C15	1.1520000000	7.8970000000	5.4810000000
C16	1.8380000000	6.7120000000	5.6550000000
C17	2.4710000000	6.1260000000	4.5910000000
C18	5.7240000000	9.2150000000	0.2640000000
C19	6.3760000000	8.0080000000	0.1690000000
C20	7.7680000000	7.9570000000	0.1540000000
C21	8.4850000000	9.2270000000	0.2620000000
C22	7.7820000000	10.3320000000	0.3860000000
C23	6.4850000000	10.3040000000	0.3790000000
C24	-0.2370000000	6.3100000000	-0.5160000000
C25	-1.6560000000	6.3980000000	-0.4160000000
C26	-2.4270000000	5.2490000000	-0.4960000000
C27	-1.8430000000	4.0190000000	-0.6830000000
C28	-0.4980000000	3.9240000000	-0.7600000000
C29	0.2900000000	5.0350000000	-0.6850000000
H30	4.2470000000	4.8050000000	-4.2150000000
H31	5.2590000000	5.7820000000	-6.1290000000
H32	6.0780000000	7.8680000000	-6.1160000000
H33	5.9240000000	9.1600000000	-4.2000000000
H34	4.9120000000	8.2460000000	-2.2720000000
H35	1.7470000000	8.2900000000	2.3020000000
H36	0.6320000000	9.3080000000	4.1110000000
H37	0.7000000000	8.3150000000	6.1810000000
H38	1.8520000000	6.3120000000	6.5020000000

H39	2.9300000000	5.3120000000	4.7010000000
H40	5.8650000000	7.2030000000	0.0570000000
H41	8.2190000000	7.1200000000	0.0320000000
H42	9.4100000000	9.1940000000	0.1990000000
H43	8.3150000000	11.1710000000	0.4610000000
H44	6.0680000000	11.1320000000	0.4460000000
H45	-2.0470000000	7.2640000000	-0.3290000000
H46	-3.3780000000	5.3640000000	-0.4460000000
H47	-2.4090000000	3.2590000000	-0.7720000000
H48	-0.1320000000	3.0590000000	-0.9090000000
H49	1.2360000000	4.9420000000	-0.7600000000

14. CACZIP10

Fe1	-2.5940000000	0.6370000000	5.1640000000
Fe2	-0.1270000000	2.5890000000	5.1740000000
O3	-0.8410000000	0.9500000000	5.1640000000
O4	-3.0620000000	1.9360000000	6.6660000000
O5	-3.0910000000	2.0070000000	3.7360000000
O6	-1.3340000000	3.3550000000	6.6440000000
O7	-1.3420000000	3.3980000000	3.7490000000
N8	-2.5420000000	-0.9980000000	6.5640000000
N9	-4.7420000000	0.1640000000	5.1380000000
N10	-2.5190000000	-0.9430000000	3.6950000000
N11	-3.2670000000	-2.1450000000	6.3440000000
N12	-5.1750000000	-1.1320000000	5.1000000000
N13	-3.2370000000	-2.0950000000	3.8590000000
N14	1.4070000000	2.1550000000	6.6150000000
N15	0.8350000000	4.5410000000	5.1740000000
N16	1.3960000000	2.1830000000	3.7150000000
N17	2.6960000000	2.5440000000	6.4080000000
N18	2.1900000000	4.6550000000	5.1920000000
N19	2.6870000000	2.5720000000	3.9190000000
C20	-1.8730000000	-1.1900000000	7.6950000000
C21	-2.1540000000	-2.4290000000	8.2310000000
C22	-3.0340000000	-2.9980000000	7.3540000000
C23	-5.8380000000	0.9170000000	5.1140000000
C24	-6.9670000000	0.1290000000	5.0560000000
C25	-6.4980000000	-1.1530000000	5.0490000000
C26	-1.8310000000	-1.0770000000	2.5760000000
C27	-2.0830000000	-2.3040000000	1.9930000000
C28	-2.9780000000	-2.9160000000	2.8280000000
C29	1.3870000000	1.4940000000	7.7660000000
C30	2.6530000000	1.4470000000	8.3070000000
C31	3.4410000000	2.1190000000	7.4340000000
C32	0.3610000000	5.7800000000	5.1780000000
C33	1.3790000000	6.6930000000	5.1940000000
C34	2.5190000000	5.9640000000	5.2000000000
C35	1.3680000000	1.5550000000	2.5350000000
C36	2.6430000000	1.5290000000	1.9700000000
C37	3.4300000000	2.1780000000	2.8660000000
C38	-2.4140000000	2.9190000000	7.1100000000
C39	-3.0010000000	3.6560000000	8.2800000000
C40	-2.4610000000	3.0150000000	3.3210000000
C41	-3.1010000000	3.8400000000	2.2450000000
B42	-4.1380000000	-2.2700000000	5.0870000000
B43	3.0560000000	3.3800000000	5.1740000000
H44	-4.6680000000	-3.2350000000	5.0990000000
H45	3.9890000000	3.5980000000	5.2230000000
H46	-1.2830000000	-0.5580000000	8.0830000000
H47	-1.8110000000	-2.8040000000	9.0320000000
H48	-3.4220000000	-3.8600000000	7.4430000000
H49	-5.8390000000	1.8670000000	5.1340000000
H50	-7.8710000000	0.4160000000	5.0250000000
H51	-7.0340000000	-1.9360000000	5.0120000000
H52	-1.2460000000	-0.4210000000	2.2210000000
H53	-1.7160000000	-2.6480000000	1.1870000000

H54	-3.3520000000	-3.7800000000	2.7040000000
H55	0.6100000000	1.1100000000	8.1550000000
H56	2.9130000000	1.0310000000	9.1210000000
H57	4.3730000000	2.2670000000	7.5360000000
H58	-0.5630000000	6.0020000000	5.1680000000
H59	1.3010000000	7.6390000000	5.2030000000
H60	3.4030000000	6.3120000000	5.2070000000
H61	0.5900000000	1.1790000000	2.1400000000
H62	2.9030000000	1.1450000000	1.1420000000
H63	4.3620000000	2.3310000000	2.7680000000
H64	-3.8640000000	3.3480000000	8.5260000000
H65	-3.0390000000	4.5860000000	8.0890000000
H66	-2.3940000000	3.5050000000	8.9950000000
H67	-3.7550000000	3.3200000000	1.7900000000
H68	-2.4750000000	4.1790000000	1.6140000000
H69	-3.5230000000	4.5610000000	2.6920000000

15. COCJIN10

Fe1	1.2623000000	2.3808000000	13.0232000000
Fe2	3.8887000000	0.2507000000	12.4037000000
O3	2.3455000000	1.2891000000	11.8085000000
O4	1.2314000000	0.9193000000	14.3822000000
O5	2.8740000000	3.1958000000	13.8824000000
O6	2.8674000000	-0.5422000000	13.9338000000
O7	4.5402000000	1.7315000000	13.5772000000
N8	-0.5344000000	1.6657000000	12.1915000000
N9	0.0034000000	3.5985000000	14.2016000000
N10	-1.5137000000	2.5524000000	11.8256000000
N11	1.1647000000	3.9272000000	11.6216000000
N12	-1.0628000000	4.2201000000	13.5990000000
N13	-0.0246000000	4.5190000000	11.3413000000
N14	3.3883000000	-1.3469000000	11.1467000000
N15	5.5970000000	-0.8767000000	12.8828000000
N16	5.0939000000	0.9564000000	10.8244000000
N17	4.3626000000	-1.9507000000	10.3947000000
N18	6.2999000000	-1.5004000000	11.8941000000
N19	5.7857000000	0.0737000000	10.0475000000
B20	-1.3094000000	4.0767000000	12.0965000000
B21	5.7966000000	-1.4266000000	10.4383000000
C22	-0.9960000000	0.4443000000	11.8801000000
C23	-2.2604000000	0.5519000000	11.3320000000
C24	-2.5603000000	1.8909000000	11.3009000000
C25	-0.0813000000	3.8874000000	15.4955000000
C26	-1.1802000000	4.6644000000	15.7493000000
C27	-1.7769000000	4.8478000000	14.5395000000
C28	2.0706000000	4.5389000000	10.8742000000
C29	1.4862000000	5.5332000000	10.1144000000
C30	0.1682000000	5.4814000000	10.4476000000
C31	2.2604000000	-2.0264000000	10.9256000000
C32	2.4939000000	-3.0665000000	10.0428000000
C33	3.8170000000	-2.9907000000	9.7314000000
C34	6.3070000000	-1.0799000000	14.0163000000
C35	7.4305000000	-1.8211000000	13.7625000000
C36	7.3925000000	-2.0722000000	12.4141000000
C37	5.3838000000	2.1698000000	10.3744000000
C38	6.2580000000	2.0822000000	9.2939000000
C39	6.4857000000	0.7472000000	9.1397000000
C40	1.8474000000	-0.1574000000	14.5831000000
C41	1.3500000000	-1.0640000000	15.6808000000
C42	4.0722000000	2.8174000000	14.0101000000
C43	5.0196000000	3.7260000000	14.7450000000
H44	2.0256000000	1.3688000000	11.1156000000
H45	-2.1317000000	4.6644000000	11.6808000000
H46	6.4508000000	-2.0064000000	9.7937000000
H47	0.6243000000	-0.6755000000	16.1541000000
H48	2.0622000000	-1.2433000000	16.2849000000

H49	1.0655000000	-1.8789000000	15.2822000000
H50	4.4775000000	4.1843000000	15.3787000000
H51	5.3858000000	4.3516000000	14.1315000000
H52	5.7219000000	3.2757000000	15.1997000000
H53	-0.5257000000	-0.3666000000	12.0109000000
H54	-2.8156000000	-0.1554000000	11.0408000000
H55	-3.3600000000	2.2794000000	10.9739000000
H56	0.5408000000	3.6004000000	16.1541000000
H57	-1.4725000000	4.9872000000	16.5994000000
H58	-2.5685000000	5.3558000000	14.3838000000
H59	2.9964000000	4.3197000000	10.8602000000
H60	1.9069000000	6.1170000000	9.4901000000
H61	-0.5098000000	6.0532000000	10.1035000000
H62	1.4222000000	-1.8291000000	11.3211000000
H63	1.8624000000	-3.7001000000	9.7174000000
H64	4.2788000000	-3.5726000000	9.1428000000
H65	6.0580000000	-0.7432000000	14.8711000000
H66	8.0867000000	-2.1021000000	14.3884000000
H67	8.0387000000	-2.5683000000	11.9283000000
H68	5.0501000000	2.9828000000	10.7326000000
H69	6.6160000000	2.7975000000	8.7816000000
H70	7.0487000000	0.3606000000	8.4811000000

16. PIMTAG

Fe1	5.9819000000	3.3633000000	10.2127000000
Fe2	8.9063000000	5.2382000000	11.1028000000
P3	8.1935000000	2.3292000000	12.3132000000
P4	6.0463000000	5.7032000000	12.4590000000
O5	7.5334000000	4.5119000000	9.8776000000
O6	7.0834000000	2.1421000000	11.3541000000
O7	5.4703000000	4.5324000000	11.7408000000
O8	9.0844000000	3.4799000000	12.0545000000
O9	7.5404000000	5.8805000000	12.4109000000
O10	7.5355000000	2.4170000000	13.7529000000
O11	9.0194000000	1.0013000000	12.4348000000
O12	5.3148000000	6.9741000000	11.8450000000
O13	5.6767000000	5.6507000000	13.9908000000
N14	6.2789000000	2.1031000000	8.5696000000
N15	4.3255000000	2.0928000000	10.6356000000
N16	4.6681000000	4.3847000000	8.9222000000
N17	5.1951000000	1.6332000000	7.8484000000
N18	3.4889000000	1.7317000000	9.6408000000
N19	3.8154000000	3.7014000000	8.1406000000
N20	10.4515000000	4.6863000000	9.7566000000
N21	10.4563000000	6.0672000000	12.2753000000
N22	8.9229000000	7.0931000000	10.1356000000
N23	11.4369000000	5.5747000000	9.4592000000
N24	11.4730000000	6.7443000000	11.6384000000
N25	10.1212000000	7.6409000000	9.7329000000
C26	7.3293000000	1.4917000000	8.0748000000
C27	6.9578000000	0.6012000000	7.0562000000
C28	5.6159000000	0.7366000000	6.9588000000
C29	3.8535000000	1.5614000000	11.7595000000
C30	2.7054000000	0.8679000000	11.5489000000
C31	2.4709000000	0.9869000000	10.1750000000
C32	4.4622000000	5.6753000000	8.6669000000
C33	3.4610000000	5.8271000000	7.7458000000
C34	3.0655000000	4.5242000000	7.3957000000
C35	10.6660000000	3.6132000000	9.0380000000
C36	11.7825000000	3.7774000000	8.2748000000
C37	12.2368000000	5.0290000000	8.5432000000
C38	10.7579000000	6.0405000000	13.5518000000
C39	11.9544000000	6.6889000000	13.7966000000
C40	12.3826000000	7.0951000000	12.5622000000
C41	7.9671000000	7.8707000000	9.6013000000
C42	8.5016000000	8.8966000000	8.8722000000

C43	9.8656000000	8.7366000000	8.9828000000
C44	8.3126000000	2.5812000000	14.9230000000
C45	8.3236000000	3.8553000000	15.5205000000
C46	9.0154000000	4.0605000000	16.6601000000
C47	9.6143000000	2.9690000000	17.2918000000
C48	9.5988000000	1.7481000000	16.7285000000
C49	8.9321000000	1.5450000000	15.5152000000
C50	9.6873000000	0.4370000000	11.3226000000
C51	9.0479000000	-0.4186000000	10.5093000000
C52	9.6567000000	-1.0403000000	9.4881000000
C53	10.9675000000	-0.7920000000	9.2749000000
C54	11.6652000000	0.0328000000	10.0171000000
C55	11.0399000000	0.6976000000	11.1199000000
C56	5.2414000000	8.2647000000	12.3832000000
C57	4.4380000000	9.1100000000	11.7489000000
C58	4.2572000000	10.4129000000	12.2516000000
C59	4.9287000000	10.8171000000	13.3465000000
C60	5.7994000000	9.9471000000	13.9992000000
C61	5.9319000000	8.6299000000	13.4781000000
C62	4.3986000000	5.2157000000	14.3914000000
C63	4.1603000000	3.8800000000	14.5546000000
C64	2.9001000000	3.4470000000	14.9178000000
C65	1.9065000000	4.3601000000	15.1231000000
C66	2.1248000000	5.7102000000	14.9467000000
C67	3.4253000000	6.1780000000	14.5914000000
B68	3.7737000000	2.1380000000	8.1800000000
B69	11.4452000000	6.9453000000	10.1171000000
H70	7.5306000000	4.7397000000	9.2381000000
H71	8.2197000000	1.6230000000	8.3669000000
H72	7.5263000000	0.0390000000	6.5430000000
H73	5.0597000000	0.2626000000	6.3508000000
H74	4.2678000000	1.6579000000	12.6096000000
H75	2.1753000000	0.4063000000	12.1858000000
H76	1.7429000000	0.6114000000	9.6934000000
H77	4.9402000000	6.3893000000	9.0670000000
H78	3.0856000000	6.6417000000	7.4168000000
H79	2.4053000000	4.2780000000	6.7641000000
H80	10.1232000000	2.8315000000	9.0512000000
H81	12.1649000000	3.1454000000	7.6694000000
H82	12.9930000000	5.4475000000	8.1485000000
H83	10.2212000000	5.6301000000	14.2230000000
H84	12.3868000000	6.8181000000	14.6335000000
H85	13.1926000000	7.5609000000	12.3885000000
H86	7.0385000000	7.7332000000	9.7171000000
H87	8.0374000000	9.5675000000	8.3932000000
H88	10.5210000000	9.3008000000	8.5933000000
H89	7.8449000000	4.5714000000	15.1152000000
H90	9.0896000000	4.9387000000	17.0339000000
H91	10.0467000000	3.0756000000	18.1287000000
H92	10.0410000000	1.0177000000	17.1444000000
H93	8.9175000000	0.6853000000	15.1152000000
H94	8.1233000000	-0.5848000000	10.6593000000
H95	9.1752000000	-1.6476000000	8.9354000000
H96	11.3921000000	-1.2475000000	8.5538000000
H97	12.5814000000	0.1888000000	9.8171000000
H98	11.5280000000	1.2783000000	11.6963000000
H99	3.9963000000	8.8371000000	10.9567000000
H100	3.6498000000	11.0038000000	11.8200000000
H101	4.8120000000	11.6953000000	13.6808000000
H102	6.2852000000	10.2159000000	14.7678000000
H103	6.5180000000	8.0143000000	13.8940000000
H104	4.8615000000	3.2542000000	14.4177000000
H105	2.7210000000	2.5155000000	15.0231000000
H106	1.0405000000	4.0646000000	15.3836000000
H107	1.4114000000	6.3257000000	15.0652000000
H108	3.6137000000	7.1054000000	14.4993000000

H109 3.1223000000 1.7974000000 7.5800000000
H110 12.1924000000 7.4603000000 9.8408000000

17. ZOCPEM

Fe1 1.3330000000 12.1700000000 2.6960000000
Fe2 2.7530000000 11.8050000000 -0.0590000000
N3 1.3060000000 12.7600000000 4.8880000000
N4 -0.6270000000 13.1300000000 2.8640000000
N5 0.1430000000 10.5270000000 3.5610000000
N6 2.5310000000 9.9540000000 -1.1850000000
N7 1.8260000000 12.5860000000 -1.9090000000
N8 4.5370000000 11.9420000000 -1.4740000000
O9 1.2920000000 11.6840000000 0.9650000000
O10 3.0780000000 11.2770000000 3.2030000000
O11 4.0460000000 10.9280000000 1.2410000000
O12 2.1960000000 13.9800000000 2.4070000000
O13 3.2930000000 13.6730000000 0.4880000000
C14 0.0930000000 13.6210000000 5.1500000000
C15 -0.5030000000 14.1450000000 3.9060000000
C16 -1.6720000000 12.1060000000 3.1380000000
C17 -1.1980000000 10.7340000000 2.9620000000
C18 0.1450000000 10.5680000000 5.0520000000
C19 1.1980000000 11.4670000000 5.5980000000
C20 2.5180000000 13.4230000000 5.3400000000
C21 -0.9750000000 13.7960000000 1.6140000000
C22 0.6700000000 9.2050000000 3.1440000000
C23 1.6420000000 10.2040000000 -2.3570000000
C24 0.9820000000 11.4970000000 -2.3320000000
C25 2.8120000000 12.9450000000 -2.9370000000
C26 4.1910000000 12.9960000000 -2.4180000000
C27 4.7020000000 10.6430000000 -2.1670000000
C28 3.8830000000 9.5440000000 -1.6020000000
C29 1.9330000000 8.9130000000 -0.3310000000
C30 0.9800000000 13.7290000000 -1.6390000000
C31 5.7930000000 12.3060000000 -0.7910000000
C32 4.0150000000 10.8440000000 2.4850000000
C33 5.2010000000 10.1790000000 3.2010000000
C34 6.2480000000 11.2710000000 3.3830000000
C35 5.6800000000 8.9880000000 2.3800000000
C36 4.7980000000 9.6770000000 4.6140000000
C37 2.9420000000 14.3670000000 1.4820000000
C38 3.4610000000 15.8000000000 1.5490000000
C39 4.6970000000 15.7240000000 2.3910000000
C40 2.4010000000 16.6830000000 2.1540000000
C41 3.8590000000 16.3210000000 0.1650000000
H42 0.3560000000 14.3620000000 5.7010000000
H43 -0.5640000000 13.0960000000 5.6110000000
H44 0.0490000000 14.8580000000 3.5760000000
H45 -1.3780000000 14.4850000000 4.1050000000
H46 -2.4060000000 12.2530000000 2.5370000000
H47 -1.9730000000 12.2130000000 4.0420000000
H48 -1.8190000000 10.1360000000 3.3850000000
H49 -1.1530000000 10.5390000000 2.0240000000
H50 -0.7120000000 10.8820000000 5.3490000000
H51 0.2950000000 9.6800000000 5.3820000000
H52 2.0450000000 11.0180000000 5.5350000000
H53 0.9990000000 11.6440000000 6.5190000000
H54 2.5310000000 14.2710000000 4.8900000000
H55 3.2850000000 12.9100000000 5.0790000000
H56 2.5370000000 13.5650000000 6.2890000000
H57 -1.0920000000 13.1590000000 0.9090000000
H58 -0.2800000000 14.4130000000 1.3750000000
H59 -1.7960000000 14.2760000000 1.7520000000
H60 0.5760000000 9.2580000000 2.1920000000
H61 0.1450000000 8.4750000000 3.4790000000
H62 1.5930000000 9.0650000000 3.3680000000

H63	0.9680000000	9.5210000000	-2.3780000000
H64	2.1750000000	10.1520000000	-3.1550000000
H65	0.2350000000	11.4420000000	-1.7310000000
H66	0.6650000000	11.6890000000	-3.2180000000
H67	2.7750000000	12.2910000000	-3.6410000000
H68	2.5830000000	13.8070000000	-3.2930000000
H69	4.3100000000	13.8390000000	-1.9760000000
H70	4.7940000000	12.9390000000	-3.1650000000
H71	4.4560000000	10.7580000000	-3.0880000000
H72	5.6260000000	10.3890000000	-2.1120000000
H73	4.3400000000	9.1910000000	-0.8330000000
H74	3.7990000000	8.8570000000	-2.2670000000
H75	1.0510000000	9.1830000000	-0.0670000000
H76	2.4530000000	8.7110000000	0.4500000000
H77	1.8760000000	8.1340000000	-0.8880000000
H78	1.5620000000	14.4040000000	-1.2810000000
H79	0.3400000000	13.4730000000	-0.9710000000
H80	0.5190000000	14.0780000000	-2.4050000000
H81	6.1110000000	11.6200000000	-0.1990000000
H82	5.5930000000	13.0980000000	-0.2850000000
H83	6.4680000000	12.5050000000	-1.4420000000
H84	5.6589000000	9.2117000000	5.0941000000
H85	4.4582000000	10.5196000000	5.2162000000
H86	3.9936000000	8.9468000000	4.5250000000
H87	7.1204000000	10.8579000000	3.8893000000
H88	6.5438000000	11.6577000000	2.4078000000
H89	5.8298000000	12.0797000000	3.9823000000
H90	6.5215000000	8.5132000000	2.8845000000
H91	4.8678000000	8.2688000000	2.2741000000
H92	5.9938000000	9.3288000000	1.3934000000
H93	5.1328000000	16.7184000000	2.4881000000
H94	4.4411000000	15.3419000000	3.3792000000
H95	5.4180000000	15.0563000000	1.9194000000
H96	4.2238000000	17.3444000000	0.2525000000
H97	4.6452000000	15.6898000000	-0.2491000000
H98	2.9917000000	16.3001000000	-0.4949000000
H99	2.7669000000	17.7085000000	2.2042000000
H100	1.5028000000	16.6480000000	1.5374000000
H101	2.1652000000	16.3323000000	3.1587000000

18. YOCHKAC

Fe1	5.7990000000	0.5660000000	0.9280000000
O2	6.3870000000	-1.1970000000	0.4580000000
N3	4.5810000000	-0.3560000000	2.5010000000
N4	3.7540000000	0.2320000000	-0.0030000000
N5	4.8640000000	2.3850000000	1.8640000000
N6	7.0980000000	0.6640000000	2.7660000000
C7	3.7080000000	-1.3540000000	1.8260000000
C8	3.0540000000	-0.7280000000	0.6310000000
C9	1.8470000000	-1.2120000000	0.1570000000
C10	1.3340000000	-0.7160000000	-1.0280000000
C11	2.0520000000	0.2770000000	-1.6650000000
C12	3.2450000000	0.7580000000	-1.1410000000
C13	3.9650000000	1.8900000000	-1.7900000000
C14	3.7830000000	0.6570000000	3.2500000000
C15	4.0320000000	2.0840000000	2.8680000000
C16	3.3530000000	3.0570000000	3.5900000000
C17	3.5560000000	4.3860000000	3.2580000000
C18	4.4180000000	4.6980000000	2.2330000000
C19	5.0750000000	3.6860000000	1.5350000000
C20	5.9440000000	4.0600000000	0.3830000000
C21	5.5430000000	-1.0810000000	3.3970000000
C22	6.7420000000	-0.2550000000	3.7010000000
C23	7.4810000000	-0.4800000000	4.8530000000
C24	8.6540000000	0.2280000000	5.0220000000
C25	9.0400000000	1.1670000000	4.1000000000

C26	8.2270000000	1.3980000000	2.9750000000
C27	8.5900000000	2.4640000000	2.0090000000
H28	4.2360000000	-2.0950000000	1.5460000000
H29	3.0410000000	-1.6520000000	2.4330000000
H30	1.3760000000	-1.8800000000	0.6410000000
H31	0.5200000000	-1.0450000000	-1.3880000000
H32	1.7220000000	0.6400000000	-2.4780000000
H33	4.8560000000	1.6270000000	-1.9880000000
H34	3.5210000000	2.1280000000	-2.5970000000
H35	3.9770000000	2.6370000000	-1.2040000000
H36	2.8620000000	0.4710000000	3.1020000000
H37	3.9810000000	0.5610000000	4.1740000000
H38	2.7640000000	2.8170000000	4.2940000000
H39	3.1040000000	5.0740000000	3.7340000000
H40	4.5660000000	5.6070000000	1.9990000000
H41	6.8260000000	3.7360000000	0.5340000000
H42	5.5990000000	3.6730000000	-0.4140000000
H43	5.9640000000	5.0050000000	0.2940000000
H44	5.1020000000	-1.2980000000	4.2120000000
H45	5.8210000000	-1.8810000000	2.9670000000
H46	7.1880000000	-1.1020000000	5.5070000000
H47	9.1980000000	0.0630000000	5.7850000000
H48	9.8460000000	1.6570000000	4.2190000000
H49	9.4030000000	2.8740000000	2.2810000000
H50	8.6980000000	2.0850000000	1.1460000000
H51	7.8990000000	3.1160000000	1.9830000000
Fe52	7.4230000000	-0.5660000000	-0.9280000000
O53	6.8350000000	1.1970000000	-0.4580000000
N54	8.6410000000	0.3560000000	-2.5010000000
C55	9.5140000000	1.3540000000	-1.8260000000
C56	10.1680000000	0.7280000000	-0.6310000000
N57	9.4680000000	-0.2320000000	0.0030000000
N58	8.3580000000	-2.3850000000	-1.8640000000
C59	9.1900000000	-2.0840000000	-2.8680000000
C60	9.4390000000	-0.6570000000	-3.2500000000
C61	7.6790000000	1.0810000000	-3.3970000000
C62	6.4800000000	0.2550000000	-3.7010000000
N63	6.1240000000	-0.6640000000	-2.7660000000
C64	4.9950000000	-1.3980000000	-2.9750000000
C65	4.1820000000	-1.1670000000	-4.1000000000
C66	4.5680000000	-0.2280000000	-5.0220000000
C67	5.7410000000	0.4800000000	-4.8530000000
H68	6.0340000000	1.1020000000	-5.5070000000
H69	4.0240000000	-0.0630000000	-5.7850000000
H70	3.3760000000	-1.6570000000	-4.2190000000
C71	4.6320000000	-2.4640000000	-2.0090000000
H72	3.8190000000	-2.8740000000	-2.2810000000
H73	4.5240000000	-2.0850000000	-1.1460000000
H74	5.3230000000	-3.1160000000	-1.9830000000
H75	8.1200000000	1.2980000000	-4.2120000000
H76	7.4010000000	1.8810000000	-2.9670000000
H77	10.3600000000	-0.4710000000	-3.1020000000
H78	9.2410000000	-0.5610000000	-4.1740000000
C79	9.8690000000	-3.0570000000	-3.5900000000
C80	9.6660000000	-4.3860000000	-3.2580000000
C81	8.8040000000	-4.6980000000	-2.2330000000
C82	8.1470000000	-3.6860000000	-1.5350000000
C83	7.2780000000	-4.0600000000	-0.3830000000
H84	6.3960000000	-3.7360000000	-0.5340000000
H85	7.6230000000	-3.6730000000	0.4140000000
H86	7.2580000000	-5.0050000000	-0.2940000000
H87	8.6560000000	-5.6070000000	-1.9990000000
H88	10.1180000000	-5.0740000000	-3.7340000000
H89	10.4580000000	-2.8170000000	-4.2940000000
C90	9.9770000000	-0.7580000000	1.1410000000
C91	11.1700000000	-0.2770000000	1.6650000000

C92	11.8880000000	0.7160000000	1.0280000000
C93	11.3750000000	1.2120000000	-0.1570000000
H94	11.8460000000	1.8800000000	-0.6410000000
H95	12.7020000000	1.0450000000	1.3880000000
H96	11.5000000000	-0.6400000000	2.4780000000
C97	9.2570000000	-1.8900000000	1.7900000000
H98	8.3660000000	-1.6270000000	1.9880000000
H99	9.7010000000	-2.1280000000	2.5970000000
H100	9.2450000000	-2.6370000000	1.2040000000
H101	8.9860000000	2.0950000000	-1.5460000000
H102	10.1810000000	1.6520000000	-2.4330000000

19. RABHAD

Fe1	8.2078000000	3.9605000000	11.8650000000
Fe2	8.1222000000	6.0402000000	9.1216000000
O3	7.5164000000	4.3454000000	10.0092000000
O4	10.0005000000	5.0286000000	9.0820000000
O5	10.0365000000	3.6205000000	10.8559000000
O6	8.7433000000	8.1225000000	11.0289000000
O7	8.9535000000	6.3377000000	13.3112000000
N8	7.5925000000	1.8563000000	11.2049000000
N9	7.5631000000	4.7859000000	7.2990000000
N10	8.8292000000	7.1630000000	7.4765000000
N11	9.3336000000	7.3261000000	5.3157000000
N12	6.1082000000	6.6447000000	8.7512000000
N13	4.3394000000	6.6795000000	7.4158000000
N14	8.9261000000	2.6820000000	13.3946000000
N15	9.4249000000	0.6431000000	14.1200000000
N16	6.2160000000	3.8287000000	12.5706000000
N17	4.3873000000	2.5966000000	12.9667000000
N18	8.5056000000	7.1992000000	10.3764000000
N19	8.6202000000	5.4878000000	12.6101000000
C20	7.6254000000	1.9315000000	9.7330000000
C21	7.1615000000	3.2643000000	9.1731000000
C22	7.6573000000	3.3881000000	7.7664000000
C23	8.5441000000	5.0835000000	6.2398000000
C24	8.8902000000	6.5340000000	6.3172000000
C25	9.2644000000	8.4633000000	7.2398000000
C26	9.4305000000	9.5541000000	8.0865000000
C27	9.8665000000	10.7382000000	7.5221000000
C28	10.1682000000	10.8223000000	6.1427000000
C29	10.0352000000	9.7674000000	5.3050000000
C30	9.5741000000	8.5736000000	5.8786000000
C31	9.5077000000	6.9865000000	3.9044000000
C32	8.4341000000	7.5449000000	3.0334000000
C33	6.1868000000	5.1286000000	6.7906000000
C34	5.5476000000	6.1676000000	7.6435000000
C35	5.1859000000	7.5285000000	9.2671000000
C36	5.1953000000	8.2996000000	10.4143000000
C37	4.1160000000	9.1134000000	10.7102000000
C38	3.0207000000	9.1586000000	9.8104000000
C39	2.9744000000	8.3845000000	8.6890000000
C40	4.0743000000	7.5687000000	8.4371000000
C41	3.4581000000	6.3919000000	6.2701000000
C42	2.4427000000	5.3149000000	6.6328000000
C43	8.6061000000	0.9120000000	11.7315000000
C44	8.9702000000	1.3896000000	13.0927000000
C45	9.3848000000	2.7727000000	14.7163000000
C46	9.5635000000	3.8675000000	15.5479000000
C47	10.0352000000	3.6663000000	16.8135000000
C48	10.3403000000	2.3726000000	17.2444000000
C49	10.1839000000	1.2798000000	16.4417000000
C50	9.6938000000	1.5086000000	15.1610000000
C51	9.6430000000	-0.8106000000	14.1534000000
C52	8.5162000000	-1.5263000000	14.8499000000
C53	6.2593000000	1.5099000000	11.6966000000

C54	5.6253000000	2.6593000000	12.4159000000
C55	5.2924000000	4.6260000000	13.2414000000
C56	5.3470000000	5.9399000000	13.6526000000
C57	4.2442000000	6.4373000000	14.3430000000
C58	3.1364000000	5.6654000000	14.6040000000
C59	3.0612000000	4.3672000000	14.1837000000
C60	4.1507000000	3.8506000000	13.5130000000
C61	3.4733000000	1.4633000000	12.9728000000
C62	2.4569000000	1.5427000000	11.8696000000
C63	10.4579000000	4.0650000000	9.7664000000
C64	11.7046000000	3.3703000000	9.1913000000
C65	12.3097000000	2.3416000000	9.8756000000
C66	13.4082000000	1.6930000000	9.3278000000
C67	13.8944000000	2.0770000000	8.1002000000
C68	13.2818000000	3.1081000000	7.3870000000
C69	12.1870000000	3.7541000000	7.9363000000
H70	8.5196000000	1.7830000000	9.4473000000
H71	7.0644000000	1.2493000000	9.3863000000
H72	6.2121000000	3.2381000000	9.1351000000
H73	7.1318000000	2.8347000000	7.2019000000
H74	8.5640000000	3.1084000000	7.7315000000
H75	9.3264000000	4.5599000000	6.3688000000
H76	8.1689000000	4.8888000000	5.3900000000
H77	9.2510000000	9.4891000000	9.0168000000
H78	9.9647000000	11.5080000000	8.0699000000
H79	10.4761000000	11.6509000000	5.7921000000
H80	10.2447000000	9.8323000000	4.3809000000
H81	10.3440000000	7.3301000000	3.6116000000
H82	9.5057000000	6.0408000000	3.8179000000
H83	8.4282000000	8.4934000000	3.1062000000
H84	8.5966000000	7.2969000000	2.1305000000
H85	7.5913000000	7.2019000000	3.3096000000
H86	6.2572000000	5.4569000000	5.9014000000
H87	5.6485000000	4.3469000000	6.7967000000
H88	5.9430000000	8.2712000000	11.0001000000
H89	4.1098000000	9.6357000000	11.5054000000
H90	2.2974000000	9.7452000000	9.9955000000
H91	2.2250000000	8.4002000000	8.1063000000
H92	2.9968000000	7.1849000000	6.0243000000
H93	3.9839000000	6.0922000000	5.5387000000
H94	1.9101000000	5.6136000000	7.3597000000
H95	1.8855000000	5.1411000000	5.8832000000
H96	2.8990000000	4.5189000000	6.8787000000
H97	8.2424000000	0.0349000000	11.7800000000
H98	9.3722000000	0.9074000000	11.1700000000
H99	9.3612000000	4.7444000000	15.2414000000
H100	10.1547000000	4.4047000000	17.3992000000
H101	10.6687000000	2.2498000000	18.1276000000
H102	10.3979000000	0.4048000000	16.7437000000
H103	9.7091000000	-1.1327000000	13.2626000000
H104	10.4534000000	-0.9909000000	14.6147000000
H105	8.4494000000	-1.2149000000	15.7452000000
H106	7.7014000000	-1.3541000000	14.3916000000
H107	8.6863000000	-2.4600000000	14.8499000000
H108	5.7119000000	1.2679000000	10.9591000000
H109	6.3318000000	0.7747000000	12.2930000000
H110	6.1052000000	6.4834000000	13.4735000000
H111	4.2575000000	7.3378000000	14.6435000000
H112	2.4100000000	6.0409000000	15.0866000000
H113	2.2860000000	3.8403000000	14.3446000000
H114	3.9762000000	0.6642000000	12.8681000000
H115	3.0180000000	1.4418000000	13.8074000000
H116	1.9409000000	2.3334000000	11.9697000000
H117	2.9028000000	1.5587000000	11.0304000000
H118	1.8864000000	0.7851000000	11.9106000000
H119	11.9764000000	2.0751000000	10.7239000000

H120	13.8244000000	0.9835000000	9.8013000000
H121	14.6521000000	1.6361000000	7.7345000000
H122	13.6121000000	3.3633000000	6.5342000000
H123	11.7644000000	4.4585000000	7.4598000000

20. GIDKIN02

Fe1	4.9301000000	1.3525000000	2.7045000000
S2	6.6466000000	0.0000000000	2.1554000000
O3	4.4293000000	3.0205000000	0.4825000000
N4	4.6067000000	2.2288000000	1.3230000000
C5	8.0502000000	0.0000000000	3.3887000000
C6	8.8531000000	-1.2569000000	3.0804000000
H7	8.3651000000	-2.0094000000	3.2616000000
H8	9.6306000000	-1.3073000000	3.6727000000
H9	9.1364000000	-1.2633000000	2.1420000000
C10	7.5981000000	0.0000000000	4.8362000000
H11	8.4281000000	0.0000000000	5.4415000000
H12	7.1302000000	-0.7675000000	5.0412000000
Fe13	4.9301000000	-1.3525000000	2.7045000000
S14	3.2137000000	0.0000000000	3.2536000000
O15	5.4310000000	3.0205000000	4.9265000000
O16	4.4293000000	-3.0205000000	0.4825000000
O17	5.4310000000	-3.0205000000	4.9265000000
N18	5.2536000000	2.2288000000	4.0860000000
N19	4.6067000000	-2.2288000000	1.3230000000
N20	5.2536000000	-2.2288000000	4.0860000000
C21	1.8101000000	0.0000000000	2.0203000000
C22	1.0072000000	-1.2569000000	2.3286000000
C23	1.0072000000	1.2569000000	2.3286000000
C24	8.8531000000	1.2569000000	3.0804000000
H25	1.4952000000	-2.0094000000	2.1474000000
H26	1.4952000000	2.0094000000	2.1474000000
H27	8.3651000000	2.0094000000	3.2616000000
H28	0.2297000000	-1.3073000000	1.7363000000
H29	0.2297000000	1.3073000000	1.7363000000
H30	9.6306000000	1.3073000000	3.6727000000
H31	0.7239000000	-1.2633000000	3.2670000000
H32	0.7239000000	1.2633000000	3.2670000000
H33	9.1364000000	1.2633000000	2.1420000000
C34	2.2622000000	0.0000000000	0.5728000000
H35	1.4322000000	0.0000000000	-0.0325000000
H36	2.7301000000	-0.7675000000	0.3678000000
H37	2.7301000000	0.7675000000	0.3678000000
H38	7.1302000000	0.7675000000	5.0412000000

21. YOYMOX

Fe1	0.5238000000	-0.0290000000	1.7253000000
C12	2.6159000000	6.3325000000	1.2050000000
C13	-0.0423000000	4.8487000000	1.9864000000
C14	5.2221000000	4.6746000000	0.7447000000
C15	5.0820000000	1.5342000000	0.7949000000
O6	0.0000000000	0.0000000000	0.0000000000
O7	0.2813000000	1.8963000000	2.1933000000
O8	2.4385000000	0.5072000000	1.5995000000
N9	-1.3623000000	-0.8592000000	2.4893000000
N10	1.0763000000	-2.1840000000	1.8007000000
N11	0.9533000000	-0.4227000000	4.0327000000
C12	-1.3705000000	-2.2370000000	1.9303000000
C13	-0.1459000000	-2.9246000000	1.8123000000
C14	1.8648000000	-2.4187000000	2.9825000000
C15	1.6494000000	-1.7071000000	4.1372000000
C16	-0.3522000000	-0.4101000000	4.6536000000
C17	-1.4149000000	-0.8416000000	3.9399000000
C18	-2.5144000000	-0.1110000000	1.9071000000
C19	1.8708000000	-2.5184000000	0.6035000000
C20	1.7752000000	0.6485000000	4.6072000000

C21	2.5325000000	1.8269000000	1.5589000000
C22	1.3678000000	2.5777000000	1.8587000000
C23	1.4185000000	3.9567000000	1.7311000000
C24	2.6008000000	4.5951000000	1.3752000000
C25	3.7317000000	3.8747000000	1.1450000000
C26	3.6873000000	2.4843000000	1.2030000000
H27	-1.7470000000	-2.1865000000	1.0502000000
H28	-1.9443000000	-2.7619000000	2.4951000000
H29	-0.0940000000	-3.5227000000	2.5608000000
H30	-0.1784000000	-3.4318000000	0.9980000000
H31	2.7749000000	-2.2446000000	2.7349000000
H32	1.7637000000	-3.3486000000	3.2010000000
H33	1.1235000000	-2.2685000000	4.7116000000
H34	2.5016000000	-1.5405000000	4.5453000000
H35	-0.5388000000	0.4984000000	4.9012000000
H36	-0.2933000000	-0.9513000000	5.4447000000
H37	-1.5709000000	-1.7487000000	4.2107000000
H38	-2.1677000000	-0.2990000000	4.1875000000
H39	1.4330000000	-2.3278000000	-0.2302000000
H40	2.0644000000	-3.4571000000	0.6537000000
H41	2.6894000000	-2.0200000000	0.6557000000
H42	2.6248000000	0.7406000000	4.1700000000
H43	1.9137000000	0.5034000000	5.5472000000
H44	1.2597000000	1.4484000000	4.4795000000
Fe45	-0.5238000000	0.0290000000	-1.7253000000
O46	-0.2813000000	-1.8963000000	-2.1933000000
O47	-2.4385000000	-0.5072000000	-1.5995000000
N48	1.3623000000	0.8592000000	-2.4893000000
N49	-1.0763000000	2.1840000000	-1.8007000000
N50	-0.9533000000	0.4227000000	-4.0327000000
C51	-1.3678000000	-2.5777000000	-1.8587000000
C52	-2.5325000000	-1.8269000000	-1.5589000000
C53	1.3705000000	2.2370000000	-1.9303000000
C54	1.4149000000	0.8416000000	-3.9399000000
C55	2.5144000000	0.1110000000	-1.9071000000
C56	0.1459000000	2.9246000000	-1.8123000000
C57	-1.8648000000	2.4187000000	-2.9825000000
C58	-1.8708000000	2.5184000000	-0.6035000000
C59	-1.6494000000	1.7071000000	-4.1372000000
C60	0.3522000000	0.4101000000	-4.6536000000
C61	-1.7752000000	-0.6485000000	-4.6072000000
C62	-1.4185000000	-3.9567000000	-1.7311000000
C63	-3.6873000000	-2.4843000000	-1.2030000000
H64	1.7470000000	2.1865000000	-1.0502000000
H65	1.9443000000	2.7619000000	-2.4951000000
H66	1.5709000000	1.7487000000	-4.2107000000
H67	2.1677000000	0.2990000000	-4.1875000000
H68	0.0940000000	3.5227000000	-2.5608000000
H69	0.1784000000	3.4318000000	-0.9980000000
H70	-2.7749000000	2.2446000000	-2.7349000000
H71	-1.7637000000	3.3486000000	-3.2010000000
H72	-1.4330000000	2.3278000000	0.2302000000
H73	-2.0644000000	3.4571000000	-0.6537000000
H74	-2.6894000000	2.0200000000	-0.6557000000
H75	-1.1235000000	2.2685000000	-4.7116000000
H76	-2.5016000000	1.5405000000	-4.5453000000
H77	0.5388000000	-0.4984000000	-4.9012000000
H78	0.2933000000	0.9513000000	-5.4447000000
H79	-2.6248000000	-0.7406000000	-4.1700000000
H80	-1.9137000000	-0.5034000000	-5.5472000000
H81	-1.2597000000	-1.4484000000	-4.4795000000
C182	0.0423000000	-4.8487000000	-1.9864000000
C83	-2.6008000000	-4.5951000000	-1.3752000000
C184	-5.0820000000	-1.5342000000	-0.7949000000
C85	-3.7317000000	-3.8747000000	-1.1450000000
C186	-2.6159000000	-6.3325000000	-1.2050000000

C187	-5.2221000000	-4.6746000000	-0.7447000000
H88	-3.4476000000	-0.5257000000	2.2884000000
H89	-2.4438000000	0.9403000000	2.1861000000
H90	-2.4947000000	-0.2003000000	0.8209000000
H91	3.4476000000	0.5257000000	-2.2884000000
H92	2.4947000000	0.2003000000	-0.8209000000
H93	2.4438000000	-0.9403000000	-2.1861000000

22. JIGNUI

Fe1	2.6760000000	4.6740000000	6.1500000000
Fe2	0.6580000000	6.9650000000	5.3480000000
O3	1.7210000000	6.1420000000	6.5470000000
O4	1.1680000000	3.6940000000	5.1570000000
O5	-0.2970000000	5.3050000000	4.6620000000
C6	0.0760000000	4.0940000000	4.6770000000
C7	-0.8510000000	3.0940000000	4.0890000000
O8	3.4920000000	5.3920000000	4.4230000000
O9	1.9800000000	6.9370000000	3.7960000000
C10	3.0870000000	6.3600000000	3.7050000000
C11	4.0700000000	6.8470000000	2.6550000000
P12	4.8350000000	2.6220000000	8.2600000000
N13	3.7400000000	2.8120000000	5.6980000000
C14	4.5030000000	2.1190000000	6.5420000000
N15	4.9570000000	0.9980000000	5.9690000000
C16	3.7200000000	2.0930000000	4.5330000000
C17	4.4660000000	0.9720000000	4.6890000000
C18	5.8180000000	-0.0230000000	6.5450000000
N19	2.2270000000	3.6480000000	8.0080000000
C20	3.1110000000	2.9680000000	8.7390000000
C21	1.0940000000	3.7690000000	8.7670000000
C22	1.2920000000	3.1500000000	9.9630000000
N23	2.5680000000	2.6420000000	9.9360000000
C24	3.2210000000	1.9450000000	11.0400000000
N25	4.5260000000	5.1870000000	7.1580000000
C26	5.2230000000	4.3790000000	7.9440000000
C27	5.1170000000	6.4210000000	7.2510000000
C28	6.1420000000	6.3520000000	8.1210000000
N29	6.2240000000	5.0640000000	8.5580000000
C30	7.1620000000	4.5480000000	9.5160000000
P31	-1.2810000000	10.0150000000	5.7850000000
N32	-0.6960000000	7.9760000000	3.9650000000
C33	-1.3580000000	9.1120000000	4.2090000000
C34	-1.0490000000	7.6120000000	2.6950000000
C35	-1.8840000000	8.5250000000	2.1850000000
N36	-2.0910000000	9.4560000000	3.1260000000
C37	-2.9910000000	10.5950000000	3.0150000000
C38	-1.5560000000	8.5610000000	6.8460000000
N39	-0.9530000000	7.3810000000	6.7150000000
C40	-1.4720000000	6.5700000000	7.6890000000
C41	-2.3860000000	7.2680000000	8.4160000000
N42	-2.4210000000	8.5170000000	7.8780000000
C43	-3.2210000000	9.6360000000	8.3950000000
C44	0.5370000000	10.0200000000	5.9400000000
N45	1.3130000000	8.9530000000	5.7560000000
C46	2.5980000000	9.3770000000	5.9540000000
C47	2.5920000000	10.7050000000	6.2560000000
N48	1.2910000000	11.0900000000	6.2260000000
C49	0.7980000000	12.4290000000	6.5610000000
H50	-0.4630000000	2.2190000000	4.1580000000
H51	-1.0020000000	3.3040000000	3.1640000000
H52	-1.6850000000	3.1140000000	4.5620000000
H53	3.6800000000	7.5730000000	2.1640000000
H54	4.2790000000	6.1290000000	2.0530000000
H55	4.8740000000	7.1470000000	3.0860000000
H56	3.2500000000	2.3420000000	3.7340000000
H57	4.6210000000	0.2900000000	4.0290000000

H58	6.0360000000	0.2130000000	7.4480000000
H59	6.6230000000	-0.0920000000	6.0280000000
H60	5.3590000000	-0.8670000000	6.5370000000
H61	0.2880000000	4.2180000000	8.4980000000
H62	0.6630000000	3.0840000000	10.6850000000
H63	4.1090000000	1.6930000000	10.7780000000
H64	2.7170000000	1.1600000000	11.2660000000
H65	3.2670000000	2.5270000000	11.8020000000
H66	4.8430000000	7.2090000000	6.7720000000
H67	6.7120000000	7.0750000000	8.3870000000
H68	7.7590000000	5.2510000000	9.7870000000
H69	7.6680000000	3.8350000000	9.1210000000
H70	6.6890000000	4.2200000000	10.2840000000
H71	-0.7460000000	6.8210000000	2.2390000000
H72	-2.2660000000	8.5170000000	1.3040000000
H73	-2.9610000000	11.1080000000	3.8250000000
H74	-3.8860000000	10.2820000000	2.8680000000
H75	-2.7180000000	11.1470000000	2.2780000000
H76	-1.2290000000	5.6520000000	7.8360000000
H77	-2.9000000000	6.9470000000	9.1580000000
H78	-3.7500000000	9.3330000000	9.1380000000
H79	-3.8010000000	9.9640000000	7.7040000000
H80	-2.6380000000	10.3410000000	8.6860000000
H81	3.3810000000	8.8250000000	5.8880000000
H82	3.3540000000	11.2600000000	6.4540000000
H83	1.5430000000	13.0120000000	6.7210000000
H84	0.2530000000	12.3810000000	7.3500000000
H85	0.2760000000	12.7710000000	5.8320000000

23. VOFLOR

Fe1	0.0000000000	0.0000000000	0.0000000000
N2	-0.1970000000	1.9624000000	-0.3596000000
N3	-1.8606000000	-0.0292000000	0.7304000000
N4	-0.7280000000	-0.3992000000	-1.8137000000
N5	-2.2389000000	-1.2186000000	-5.6461000000
C6	0.7310000000	2.7694000000	-0.9698000000
C7	-1.2963000000	2.7607000000	-0.1414000000
C8	-2.7515000000	1.0295000000	0.8306000000
C9	-2.5454000000	-1.1237000000	1.1880000000
C10	0.1859000000	4.0932000000	-1.1780000000
C11	-1.0619000000	4.0843000000	-0.6480000000
C12	-4.0286000000	0.5718000000	1.3550000000
C13	-3.9035000000	-0.7625000000	1.5510000000
C14	2.0254000000	2.3898000000	-1.3161000000
C15	-2.4765000000	2.3290000000	0.4498000000
C16	0.8619000000	5.1919000000	-1.9540000000
C17	-2.0774000000	5.1895000000	-0.6458000000
C18	-5.2366000000	1.4400000000	1.6044000000
C19	-4.9475000000	-1.7380000000	2.0487000000
C20	0.6123000000	5.0212000000	-3.4583000000
C21	-3.1345000000	5.0241000000	-1.7503000000
C22	-5.2621000000	2.0309000000	3.0185000000
C23	-4.8941000000	-1.9756000000	3.5440000000
C24	-1.7038000000	0.3461000000	-2.3771000000
C25	-2.2268000000	0.1106000000	-3.6297000000
C26	-1.7625000000	-0.9716000000	-4.4058000000
C27	-0.7480000000	-1.7561000000	-3.8123000000
C28	-0.2818000000	-1.4329000000	-2.5642000000
C29	-1.8687000000	-2.4280000000	-6.3598000000
C30	-3.2681000000	-0.3775000000	-6.2396000000
H31	-2.0523000000	1.0789000000	-1.8806000000
H32	-2.9064000000	0.6844000000	-3.9738000000
H33	-0.3885000000	-2.5056000000	-4.2744000000
H34	0.4100000000	-1.9785000000	-2.1979000000
H35	-2.2942000000	-2.4360000000	-7.2105000000
H36	-2.1495000000	-3.1877000000	-5.8610000000

H37	-0.9194000000	-2.4553000000	-6.4745000000
H38	-3.4787000000	-0.6983000000	-7.1080000000
H39	-2.9462000000	0.5145000000	-6.3008000000
H40	-4.0540000000	-0.3958000000	-5.6973000000
H41	1.8021000000	5.1643000000	-1.7870000000
H42	0.5089000000	6.0305000000	-1.6735000000
H43	1.0449000000	5.7223000000	-3.9326000000
H44	-0.3279000000	5.0503000000	-3.6308000000
H45	0.9645000000	4.1852000000	-3.7444000000
H46	-1.6222000000	6.0143000000	-0.7783000000
H47	-2.5210000000	5.1987000000	0.1948000000
H48	-3.7559000000	5.7463000000	-1.7113000000
H49	-3.6005000000	4.2050000000	-1.6256000000
H50	-2.7018000000	5.0196000000	-2.5976000000
H51	-6.0242000000	0.9166000000	1.4820000000
H52	-5.2286000000	2.1545000000	0.9787000000
H53	-6.0444000000	2.5695000000	3.1231000000
H54	-4.4826000000	2.5628000000	3.1532000000
H55	-5.2778000000	1.3269000000	3.6564000000
H56	-4.8100000000	-2.5693000000	1.6089000000
H57	-5.8128000000	-1.3978000000	1.8304000000
H58	-5.5739000000	-2.5961000000	3.7901000000
H59	-5.0382000000	-1.1554000000	4.0005000000
H60	-4.0373000000	-2.3259000000	3.7789000000
H61	2.5804000000	3.0681000000	-1.6868000000
H62	-3.1420000000	2.9964000000	0.5990000000
N63	0.1970000000	-1.9624000000	0.3596000000
C64	-0.7310000000	-2.7694000000	0.9698000000
C65	-0.1859000000	-4.0932000000	1.1780000000
C66	1.0619000000	-4.0843000000	0.6480000000
C67	1.2963000000	-2.7607000000	0.1414000000
C68	2.4765000000	-2.3290000000	-0.4498000000
C69	2.7515000000	-1.0295000000	-0.8306000000
N70	1.8606000000	0.0292000000	-0.7304000000
N71	0.7280000000	0.3992000000	1.8137000000
C72	1.7038000000	-0.3461000000	2.3771000000
C73	2.2268000000	-0.1106000000	3.6297000000
C74	1.7625000000	0.9716000000	4.4058000000
N75	2.2389000000	1.2186000000	5.6461000000
C76	1.8687000000	2.4280000000	6.3598000000
H77	2.2942000000	2.4360000000	7.2105000000
H78	2.1495000000	3.1877000000	5.8610000000
H79	0.9194000000	2.4553000000	6.4745000000
C80	3.2681000000	0.3775000000	6.2396000000
H81	3.4787000000	0.6983000000	7.1080000000
H82	2.9462000000	-0.5145000000	6.3008000000
H83	4.0540000000	0.3958000000	5.6973000000
C84	0.7480000000	1.7561000000	3.8123000000
C85	0.2818000000	1.4329000000	2.5642000000
H86	-0.4100000000	1.9785000000	2.1979000000
H87	0.3885000000	2.5056000000	4.2744000000
H88	2.9064000000	-0.6844000000	3.9738000000
H89	2.0523000000	-1.0789000000	1.8806000000
C90	2.5454000000	1.1237000000	-1.1880000000
C91	3.9035000000	0.7625000000	-1.5510000000
C92	4.0286000000	-0.5718000000	-1.3550000000
C93	5.2366000000	-1.4400000000	-1.6044000000
C94	5.2621000000	-2.0309000000	-3.0185000000
H95	6.0444000000	-2.5695000000	-3.1231000000
H96	4.4826000000	-2.5628000000	-3.1532000000
H97	5.2778000000	-1.3269000000	-3.6564000000
H98	6.0242000000	-0.9166000000	-1.4820000000
H99	5.2286000000	-2.1545000000	-0.9787000000
C100	4.9475000000	1.7380000000	-2.0487000000
C101	4.8941000000	1.9756000000	-3.5440000000
H102	5.5739000000	2.5961000000	-3.7901000000

H103	5.0382000000	1.1554000000	-4.0005000000
H104	4.0373000000	2.3259000000	-3.7789000000
H105	4.8100000000	2.5693000000	-1.6089000000
H106	5.8128000000	1.3978000000	-1.8304000000
H107	3.1420000000	-2.9964000000	-0.5990000000
C108	2.0774000000	-5.1895000000	0.6458000000
C109	3.1345000000	-5.0241000000	1.7503000000
H110	3.7559000000	-5.7463000000	1.7113000000
H111	3.6005000000	-4.2050000000	1.6256000000
H112	2.7018000000	-5.0196000000	2.5976000000
H113	1.6222000000	-6.0143000000	0.7783000000
H114	2.5210000000	-5.1987000000	-0.1948000000
C115	-0.8619000000	-5.1919000000	1.9540000000
C116	-0.6123000000	-5.0212000000	3.4583000000
H117	-1.0449000000	-5.7223000000	3.9326000000
H118	0.3279000000	-5.0503000000	3.6308000000
H119	-0.9645000000	-4.1852000000	3.7444000000
H120	-1.8021000000	-5.1643000000	1.7870000000
H121	-0.5089000000	-6.0305000000	1.6735000000
C122	-2.0254000000	-2.3898000000	1.3161000000
H123	-2.5804000000	-3.0681000000	1.6868000000

24. WEDXAF

Fe1	5.8847000000	3.6244000000	9.6840000000
S2	6.4382000000	1.4597000000	9.1890000000
S3	6.3896000000	4.3298000000	11.7751000000
S4	6.9797000000	5.0405000000	8.2905000000
O5	3.0237000000	3.7452000000	9.4249000000
N6	4.1866000000	3.6514000000	9.4754000000
C7	4.9278000000	2.2615000000	12.8838000000
H8	4.2393000000	1.9463000000	13.5690000000
H9	5.7984000000	1.8658000000	13.1156000000
H10	4.6238000000	2.0071000000	12.0098000000
C11	5.6628000000	4.1103000000	14.3851000000
H12	5.0377000000	3.8139000000	15.0509000000
H13	5.7621000000	5.0643000000	14.4415000000
H14	6.5134000000	3.6904000000	14.5351000000
C15	3.8461000000	4.4949000000	12.7928000000
H16	3.1926000000	4.1931000000	13.4278000000
H17	3.5239000000	4.3344000000	11.9028000000
H18	3.9999000000	5.4346000000	12.9120000000
C19	5.1504000000	3.7348000000	13.0067000000
C20	8.5091000000	1.2592000000	11.0156000000
H21	9.4236000000	1.0519000000	11.1640000000
H22	8.0057000000	0.5957000000	11.5252000000
H23	8.3066000000	2.1252000000	11.3662000000
C24	9.0868000000	2.0928000000	8.7368000000
H25	9.9965000000	1.9195000000	8.9345000000
H26	8.9220000000	3.0178000000	8.9954000000
H27	8.9055000000	2.0035000000	7.8123000000
C28	8.4873000000	-0.3034000000	9.0796000000
H29	9.4198000000	-0.4830000000	9.1961000000
H30	8.3032000000	-0.4293000000	8.1348000000
H31	7.9764000000	-0.8980000000	9.6182000000
C32	8.2278000000	1.1268000000	9.5325000000
C33	7.1202000000	7.7369000000	8.4410000000
H34	6.7151000000	8.6027000000	8.3519000000
H35	7.8777000000	7.6760000000	7.8554000000
H36	7.4060000000	7.6116000000	9.3492000000
C37	4.9006000000	6.8335000000	8.9360000000
H38	4.5062000000	7.6904000000	8.7532000000
H39	5.1679000000	6.7941000000	9.8560000000
H40	4.2590000000	6.1430000000	8.7576000000
C41	5.7827000000	6.8353000000	6.5979000000
H42	5.3167000000	7.6635000000	6.4731000000
H43	5.2352000000	6.1108000000	6.2873000000

H44	6.6038000000	6.8514000000	6.1015000000
C45	6.0854000000	6.6419000000	8.0686000000

25. VOCBAQ

Fe1	5.3897000000	2.9179000000	3.3439000000
C12	7.0882000000	1.4535000000	4.1314000000
C13	3.7609000000	1.4064000000	4.1734000000
C14	3.6737000000	4.5069000000	2.9302000000
C15	7.0474000000	4.4650000000	2.7828000000
C16	5.3231000000	2.0080000000	1.2007000000
O7	5.4927000000	3.7637000000	5.3506000000
H8	5.3019000000	3.2697000000	6.1216000000
H9	4.9612000000	4.5148000000	5.4634000000

26. CANDAW10

Fe1	0.0000000000	-5.2990000000	-9.4410000000
S2	1.4110000000	-6.5040000000	-10.7480000000
C3	1.8620000000	-5.3910000000	-12.0920000000
C4	2.9890000000	-5.2870000000	-11.6850000000
S5	1.2050000000	-3.8880000000	-8.1340000000
S6	-1.4110000000	-4.0940000000	-10.7480000000
S7	-1.2050000000	-6.7100000000	-8.1340000000
C8	-1.8620000000	-5.2070000000	-12.0920000000
C9	-0.0920000000	-7.1610000000	-6.7900000000
C10	-2.9890000000	-5.3110000000	-11.6850000000
C11	0.0120000000	-8.2880000000	-7.1970000000
H12	1.7194000000	-5.8970000000	-13.0468000000
H13	1.2325000000	-4.5020000000	-12.0550000000
H14	3.5530000000	-4.6238000000	-12.3409000000
H15	2.9749000000	-4.8739000000	-10.6764000000
H16	3.4619000000	-6.2689000000	-11.6683000000
H17	-1.7194000000	-4.7010000000	-13.0468000000
H18	-1.2325000000	-6.0960000000	-12.0550000000
H19	-3.5530000000	-5.9742000000	-12.3409000000
H20	-2.9749000000	-5.7241000000	-10.6764000000
H21	-3.4619000000	-4.3291000000	-11.6683000000
H22	0.6752000000	-8.8520000000	-6.5411000000
H23	-0.9699000000	-8.7609000000	-7.2137000000
H24	0.4251000000	-8.2739000000	-8.2056000000
H25	0.7970000000	-6.5315000000	-6.8270000000
H26	-0.5980000000	-7.0184000000	-5.8352000000
C27	0.0873000000	-3.4351000000	-6.7843000000
H28	0.6099000000	-2.7334000000	-6.0869000000
H29	-0.2174000000	-4.3564000000	-6.2273000000
C30	-1.1522000000	-2.7537000000	-7.3572000000
H31	-1.6747000000	-3.4555000000	-8.0547000000
H32	-1.8431000000	-2.4738000000	-6.5229000000
H33	-0.8474000000	-1.8324000000	-7.9142000000

27. SONMUE

Fe1	7.2080000000	4.6763000000	6.8119000000
S2	7.1500000000	5.8941000000	4.8228000000
N3	7.3899000000	5.6977000000	8.1707000000
S4	9.1079000000	3.3275000000	6.9531000000
N5	5.7572000000	3.7517000000	6.7628000000
C6	8.0933000000	7.4160000000	5.0219000000
C7	9.0925000000	2.2024000000	5.5449000000
C8	9.1639000000	7.5408000000	5.9456000000
H9	9.3998000000	6.8006000000	6.4920000000
C10	9.8818000000	8.7494000000	6.0635000000
H11	10.5864000000	8.8089000000	6.6979000000
O12	7.3453000000	6.3195000000	9.1911000000
C13	9.2213000000	0.4197000000	3.2688000000
C14	7.7830000000	8.5477000000	4.2146000000
H15	7.0696000000	8.4931000000	3.5901000000
O16	4.6759000000	3.2718000000	6.9591000000

C17	8.1084000000	2.2392000000	4.5282000000
H18	7.3899000000	2.8576000000	4.5920000000
C19	9.5803000000	9.8771000000	5.2605000000
C20	8.5204000000	9.7536000000	4.3275000000
H21	8.3011000000	10.4891000000	3.7687000000
C22	10.2039000000	0.3805000000	4.2879000000
H23	10.9167000000	-0.2453000000	4.2227000000
C24	10.1481000000	1.2510000000	5.4010000000
H25	10.8255000000	1.2019000000	6.0652000000
C26	8.1818000000	1.3669000000	3.4180000000
H27	7.5089000000	1.4196000000	2.7496000000
C28	10.3798000000	11.1833000000	5.4045000000
H29	10.6286000000	11.3139000000	6.3437000000
H30	9.8311000000	11.9363000000	5.1046000000
H31	11.1910000000	11.1330000000	4.8564000000
C32	9.2574000000	-0.5123000000	2.0516000000
H33	8.6215000000	-1.2448000000	2.1835000000
H34	10.1610000000	-0.8769000000	1.9464000000
H35	9.0141000000	-0.0092000000	1.2471000000

28. CELVEU

Fe1	5.4388000000	1.5280000000	2.9971000000
C12	5.3827000000	3.3488000000	1.7261000000
S3	7.6890000000	0.7352000000	3.1554000000
S4	3.1670000000	1.1505000000	3.6277000000
O5	5.2954000000	0.0535000000	1.7360000000
O6	5.5788000000	2.0831000000	4.8568000000
C7	7.5085000000	-0.5354000000	2.0228000000
C8	8.6453000000	-1.4606000000	1.7953000000
C9	9.9063000000	-0.9655000000	1.5233000000
C10	10.9787000000	-1.8183000000	1.3749000000
C11	10.8088000000	-3.1778000000	1.5085000000
C12	9.5693000000	-3.6695000000	1.8077000000
C13	8.4798000000	-2.8282000000	1.9437000000
N14	6.3601000000	-0.7064000000	1.4170000000
C15	6.0630000000	-1.6349000000	0.3215000000
C16	3.2941000000	1.9088000000	5.1461000000
C17	2.0651000000	2.0749000000	5.9696000000
C18	0.9496000000	2.6827000000	5.4033000000
C19	-0.2395000000	2.7641000000	6.1155000000
C20	-0.3058000000	2.2443000000	7.3816000000
C21	0.7889000000	1.6390000000	7.9503000000
C22	1.9671000000	1.5626000000	7.2530000000
N23	4.4624000000	2.2912000000	5.5912000000
C24	4.7669000000	2.9656000000	6.8499000000
H25	9.9760000000	-0.0987000000	1.4590000000
H26	11.8435000000	-1.5214000000	1.1870000000
H27	11.4682000000	-3.7090000000	1.4343000000
H28	9.3883000000	-4.5150000000	1.9536000000
H29	7.6538000000	-3.1333000000	2.1761000000
H30	5.4827000000	-2.2780000000	0.5935000000
H31	5.6109000000	-1.1185000000	-0.3462000000
H32	6.8934000000	-2.0231000000	-0.0742000000
H33	1.0409000000	2.9853000000	4.5007000000
H34	-1.0027000000	3.2156000000	5.6629000000
H35	-1.1218000000	2.3274000000	7.8885000000
H36	0.7401000000	1.2994000000	8.8035000000
H37	2.7267000000	1.1596000000	7.5918000000
H38	5.2772000000	2.2698000000	7.3939000000
H39	5.2821000000	3.6679000000	6.6768000000
H40	4.0044000000	3.2567000000	7.2950000000

29. KAJBIH

Fe1	5.4779000000	9.7198000000	15.5570000000
O2	6.2435000000	9.2935000000	17.0466000000
O3	3.2767000000	12.9222000000	16.3920000000

O4	1.8739000000	8.0083000000	16.3011000000
O5	5.1932000000	6.1163000000	13.7032000000
O6	8.4053000000	10.0245000000	12.8895000000
N7	4.9955000000	11.5176000000	15.7783000000
N8	3.6371000000	9.3898000000	15.8693000000
N9	5.7095000000	8.2152000000	14.4146000000
N10	6.7823000000	10.4922000000	14.4532000000
C11	5.9261000000	12.4583000000	15.3465000000
C12	6.9725000000	11.8589000000	14.6010000000
C13	7.9999000000	12.6614000000	14.0896000000
C14	7.9584000000	14.0206000000	14.3078000000
C15	6.9205000000	14.6074000000	15.0033000000
C16	5.9036000000	13.8475000000	15.5260000000
C17	3.7234000000	11.8037000000	16.2193000000
C18	2.8814000000	10.5424000000	16.4170000000
C19	2.6352000000	10.3718000000	17.9126000000
C20	1.5585000000	10.7806000000	15.6647000000
C21	3.0413000000	8.1927000000	15.8897000000
C22	3.8352000000	6.9338000000	15.4647000000
C23	4.4710000000	6.4072000000	16.7534000000
C24	2.8359000000	5.8780000000	14.9487000000
C25	4.9732000000	7.0968000000	14.4305000000
C26	6.8091000000	8.3030000000	13.4282000000
C27	7.9211000000	7.2824000000	13.6782000000
C28	6.2943000000	8.2278000000	11.9917000000
C29	7.4418000000	9.6847000000	13.5645000000
H30	8.6285000000	12.2125000000	13.5464000000
H31	8.7351000000	14.5697000000	14.0237000000
H32	6.9220000000	15.6230000000	15.1601000000
H33	5.2001000000	14.2187000000	16.0238000000
H34	3.5105000000	10.1311000000	18.3421000000
H35	1.9911000000	9.6546000000	18.0694000000
H36	2.3534000000	11.2345000000	18.2512000000
H37	1.6819000000	10.8082000000	14.7283000000
H38	0.8734000000	10.1060000000	16.0238000000
H39	1.2313000000	11.6107000000	15.9329000000
H40	5.1606000000	7.2473000000	17.1830000000
H41	5.0162000000	5.5922000000	16.6148000000
H42	3.8698000000	6.1940000000	17.4103000000
H43	3.4578000000	5.0405000000	14.6828000000
H44	2.0436000000	5.8680000000	15.7283000000
H45	2.4952000000	6.1188000000	14.0919000000
H46	7.5214000000	6.4448000000	13.5918000000
H47	8.2774000000	7.3476000000	14.6373000000
H48	8.7010000000	7.4479000000	13.0236000000
H49	6.9960000000	8.6014000000	11.3871000000
H50	5.9022000000	7.3726000000	11.8417000000
H51	5.5868000000	8.7519000000	11.8872000000
Fe52	7.0091000000	9.7198000000	18.5362000000
O53	9.2103000000	12.9222000000	17.7012000000
O54	10.6131000000	8.0083000000	17.7921000000
O55	7.2938000000	6.1163000000	20.3900000000
O56	4.0818000000	10.0245000000	21.2037000000
N57	7.4915000000	11.5176000000	18.3149000000
N58	8.8499000000	9.3898000000	18.2240000000
N59	6.7776000000	8.2152000000	19.6786000000
N60	5.7047000000	10.4922000000	19.6400000000
C61	6.5609000000	12.4583000000	18.7467000000
C62	5.5146000000	11.8589000000	19.4922000000
C63	4.4871000000	12.6614000000	20.0036000000
C64	4.5287000000	14.0206000000	19.7854000000
C65	5.5665000000	14.6074000000	19.0899000000
C66	6.5834000000	13.8475000000	18.5672000000
C67	8.7636000000	11.8037000000	17.8739000000
C68	9.6056000000	10.5424000000	17.6762000000
C69	9.8518000000	10.3718000000	16.1806000000

C70	10.9285000000	10.7806000000	18.4285000000
C71	9.4457000000	8.1927000000	18.2035000000
C72	8.6519000000	6.9338000000	18.6285000000
C73	8.0161000000	6.4072000000	17.3398000000
C74	9.6511000000	5.8780000000	19.1445000000
C75	7.5138000000	7.0968000000	19.6627000000
C76	5.6780000000	8.3030000000	20.6650000000
C77	4.5659000000	7.2824000000	20.4150000000
C78	6.1927000000	8.2278000000	22.1015000000
C79	5.0452000000	9.6847000000	20.5287000000
H80	3.8585000000	12.2125000000	20.5468000000
H81	3.7519000000	14.5697000000	20.0695000000
H82	5.5650000000	15.6230000000	18.9331000000
H83	7.2869000000	14.2187000000	18.0694000000
H84	8.9765000000	10.1311000000	15.7511000000
H85	10.4959000000	9.6546000000	16.0238000000
H86	10.1336000000	11.2345000000	15.8420000000
H87	10.8052000000	10.8082000000	19.3649000000
H88	11.6137000000	10.1060000000	18.0694000000
H89	11.2557000000	11.6107000000	18.1603000000
H90	7.3264000000	7.2473000000	16.9102000000
H91	7.4709000000	5.5922000000	17.4784000000
H92	8.6172000000	6.1940000000	16.6829000000
H93	9.0292000000	5.0405000000	19.4104000000
H94	10.4434000000	5.8680000000	18.3649000000
H95	9.9918000000	6.1188000000	20.0013000000
H96	4.9656000000	6.4448000000	20.5014000000
H97	4.2096000000	7.3476000000	19.4559000000
H98	3.7861000000	7.4479000000	21.0696000000
H99	5.4910000000	8.6014000000	22.7061000000
H100	6.5848000000	7.3726000000	22.2515000000
H101	6.9003000000	8.7519000000	22.2060000000

30. SOCVUB

Fe1	3.5328000000	2.5587000000	6.7795000000
S2	4.4897000000	1.1543000000	8.3195000000
S3	5.2577000000	3.8982000000	6.9878000000
S4	1.6232000000	1.3371000000	6.3656000000
S5	2.8250000000	4.0749000000	5.3637000000
C6	6.2852000000	3.2284000000	8.2224000000
C7	7.4310000000	3.9126000000	8.6231000000
C8	8.2177000000	3.3848000000	9.6583000000
C9	7.8482000000	2.1992000000	10.2699000000
C10	6.7481000000	1.4741000000	9.8560000000
C11	5.9344000000	2.0152000000	8.8270000000
C12	1.2869000000	3.5230000000	4.7539000000
C13	0.5687000000	4.3274000000	3.8299000000
C14	-0.6227000000	3.8537000000	3.2918000000
C15	-1.1126000000	2.5948000000	3.6890000000
C16	-0.4484000000	1.8385000000	4.6174000000
C17	0.7763000000	2.2822000000	5.1721000000
P18	2.3331000000	3.3138000000	8.6266000000
C19	3.3606000000	4.1819000000	9.8464000000
C20	1.4820000000	2.0477000000	9.5944000000
C21	1.0648000000	4.5355000000	8.2338000000
P22	4.4711000000	1.0906000000	5.2404000000
C23	4.2033000000	-0.6625000000	5.5230000000
C24	3.8546000000	1.3022000000	3.5438000000
C25	6.2645000000	1.2024000000	5.0881000000
H26	7.6780000000	4.7387000000	8.1988000000
H27	9.0127000000	3.8453000000	9.9409000000
H28	8.3754000000	1.8685000000	11.0031000000
H29	6.5385000000	0.6265000000	10.2576000000
H30	0.9009000000	5.1932000000	3.5779000000
H31	-1.1043000000	4.3803000000	2.6486000000
H32	-1.9325000000	2.2665000000	3.3093000000

H33	-0.8137000000	0.9944000000	4.8930000000
H34	4.0788000000	3.6084000000	10.1264000000
H35	2.8230000000	4.4164000000	10.6068000000
H36	3.7217000000	4.9791000000	9.4509000000
H37	0.9112000000	1.5355000000	9.0169000000
H38	0.9527000000	2.4673000000	10.2778000000
H39	2.1297000000	1.4669000000	10.0021000000
H40	0.4608000000	4.1687000000	7.5845000000
H41	1.4800000000	5.3254000000	7.8750000000
H42	0.5812000000	4.7627000000	9.0309000000
H43	4.4980000000	-0.8946000000	6.4076000000
H44	4.6994000000	-1.1687000000	4.8764000000
H45	3.2672000000	-0.8621000000	5.4364000000
H46	3.9480000000	2.2208000000	3.2830000000
H47	2.9267000000	1.0521000000	3.5070000000
H48	4.3610000000	0.7455000000	2.9470000000
H49	6.5156000000	2.1162000000	4.9341000000
H50	6.5571000000	0.6613000000	4.3505000000
H51	6.6775000000	0.8886000000	5.8975000000

31. SOCWAI

Fe1	0.5432000000	-0.2506000000	9.0522000000
P2	0.2290000000	-2.4362000000	9.4319000000
C3	-0.7191000000	-2.6977000000	10.9451000000
C4	1.6620000000	-3.5081000000	9.6237000000
C5	-0.7231000000	-3.1873000000	8.1202000000
S6	-0.8547000000	0.8008000000	10.3639000000
S7	2.0232000000	-0.2777000000	10.6564000000
S8	2.0534000000	-0.8578000000	7.5951000000
S9	-0.8437000000	0.2163000000	7.4266000000
C10	-0.0746000000	-0.3741000000	5.9715000000
C11	-0.7236000000	-0.3485000000	4.7373000000
C12	-0.0864000000	-0.7782000000	3.6057000000
C13	1.2344000000	-1.2458000000	3.6871000000
C14	1.8780000000	-1.2787000000	4.8942000000
C15	1.2383000000	-0.8454000000	6.0451000000
C16	1.2170000000	0.3537000000	12.0805000000
C17	1.8166000000	0.3259000000	13.3457000000
C18	1.1564000000	0.8783000000	14.4191000000
C19	-0.1121000000	1.4124000000	14.2757000000
C20	-0.7348000000	1.3949000000	13.0532000000
C21	-0.0847000000	0.8505000000	11.9430000000
H22	-1.5093000000	-2.1534000000	10.9238000000
H23	-0.1840000000	-2.4544000000	11.7046000000
H24	-0.9690000000	-3.6221000000	11.0129000000
H25	2.2291000000	-3.1690000000	10.3193000000
H26	2.1503000000	-3.5329000000	8.7964000000
H27	1.3719000000	-4.3952000000	9.8504000000
H28	-1.5131000000	-2.6649000000	7.9633000000
H29	-0.9745000000	-4.0795000000	8.3721000000
H30	-0.1961000000	-3.2173000000	7.3181000000
H31	-1.6333000000	-0.0453000000	4.6830000000
H32	-0.5403000000	-0.7760000000	2.7610000000
H33	1.6976000000	-1.5323000000	2.8966000000
H34	2.7775000000	-1.6090000000	4.9504000000
H35	2.6861000000	-0.0658000000	13.4581000000
H36	1.5761000000	0.8893000000	15.2833000000
H37	-0.5585000000	1.7990000000	15.0333000000
H38	-1.6184000000	1.7566000000	12.9582000000

The isomer shifts and quadrupole splittings
For each compound, the order of the isomer shift or quadrupole splitting
values coincides with the order of the iron atoms given in the
Cartesian coordinates section. When the compound has two atoms that produce
one signal in the experiment the theoretical values are averaged and
the averaged value is shown. Only the absolute values of the quadrupole
splitting are shown in any case.

B3LYP/Partridge-1

Isomer shift, mm/s

+2, MUE = 0.0272 (17 points)

FATBOR	0.99	0.06
YUZKAF10	1.36	1.07
XIGDIA	1.11	
VUNMIA	1.13	
JOHCEP	0.53	
SISKOU	1.28	1.17
VUPJOF	1.27	
VUPJUL	1.28	1.28
PTHPFE10	0.70	
DEDWUE	0.67	
BUYKUB10	0.63	
YEQPOA	0.25	
PTSQFE10	0.69	

+3, +4, MUE = 0.0238 (18 points)

VOCBAQ	0.55	
YOCKAC	0.48	
ZOCPEM	0.46	
SOCWAI	0.11	
CACZIP10	0.50	
WEDXAF	0.25	
GIDKIN02	0.14	
SOCVUB	0.17	
SONMUE	0.26	
CELVEU	0.43	
KAJBIH	-0.09	
COCJIN10	0.48	
PIMTAG	0.49	
YOHMOX	0.45	
CANDAW10	0.23	
VOFLOR	0.27	
RABHAD	0.61	
JIGNUI	0.50	

all, MUE = 0.0296 (35 points)

VOCBAQ	0.60	
FATBOR	0.97	0.04
YUZKAF10	1.35	1.06
YOCKAC	0.51	
XIGDIA	1.10	
ZOCPEM	0.48	
SOCWAI	0.09	
VUNMIA	1.12	
CACZIP10	0.54	
WEDXAF	0.25	
GIDKIN02	0.12	
SOCVUB	0.16	
JOHCEP	0.51	
SISKOU	1.27	1.15
SONMUE	0.26	
VUPJOF	1.26	
VUPJUL	1.27	1.26
CELVEU	0.45	

PTHPFE10	0.68
DEDWUE	0.65
BUYKUB10	0.62
KAJBIH	-0.15
COCJIN10	0.51
PIMTAG	0.52
YOHMOX	0.48
YEQPOA	0.23
CANDAW10	0.23
PTSQFE10	0.67
VOFLOR	0.27
RABHAD	0.67
JIGNUI	0.54

|Quadrupole splitting|, mm/s

VOCBAQ	0.58	
FATBOR	3.24	0.19
YUZKAF10	3.69	3.04
YOCKAC	1.81	
XIGDIA	3.25	
ZOCPEM	1.48	
SOCWAI	3.17	
VUNMIA	3.38	
CACZIP10	1.67	
WEDXAF	0.37	
GIDKIN02	0.97	
SOCVUB	1.83	
JOHCEP	0.25	
SISKOU	3.58	4.28
SONMUE	0.58	
VUPJOF	3.58	
VUPJUL	3.79	3.61
CELVEU	0.85	
PTHPFE10	3.31	
DEDWUE	2.98	
BUYKUB10	2.78	
KAJBIH	3.71	
COCJIN10	0.25	
PIMTAG	0.21	
YOHMOX	1.41	
YEQPOA	1.78	
CANDAW10	0.43	
PTSQFE10	2.92	
VOFLOR	2.44	
RABHAD	1.51	
JIGNUI	1.56	

BPW91/Partridge-1

Isomer shift, mm/s

+2, MUE = 0.0349 (17 points)		
FATBOR	1.00	0.09
YUZKAF10	1.37	1.08
XIGDIA	1.09	
VUNMIA	1.09	
JOHCEP	0.53	
SISKOU	1.29	1.18
VUPJOF	1.27	
VUPJUL	1.28	1.28
PTHPFE10	0.75	
DEDWUE	0.63	
BUYKUB10	0.53	
YEQPOA	0.28	
PTSQFE10	0.72	

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+3, +4, MUE = 0.0253 (18 points)

VOCBAQ	0.56
YOCKAC	0.47
ZOCPEM	0.48
SOCWAI	0.11
CACZIP10	0.52
WEDXAF	0.25
GIDKIN02	0.08
SOCVUB	0.18
SONMUE	0.22
CELVEU	0.42
KAJBIH	-0.05
COCJIN10	0.49
PIMTAG	0.49
YOHMOX	0.45
CANDAW10	0.26
VOFLOR	0.26
RABHAD	0.57
JIGNUI	0.52

all, MUE = 0.0733 (35 points)

VOCBAQ	0.69	
FATBOR	0.94	-0.03
YUZKAF10	1.34	1.02
YOCKAC	0.58	
XIGDIA	1.04	
ZOCPEM	0.58	
SOCWAI	0.09	
VUNMIA	1.04	
CACZIP10	0.63	
WEDXAF	0.28	
GIDKIN02	0.05	
SOCVUB	0.19	
JOHCEP	0.43	
SISKOU	1.26	1.13
SONMUE	0.24	
VUPJOF	1.23	
VUPJUL	1.25	1.25
CELVEU	0.51	
PTHPFE10	0.68	
DEDWUE	0.54	
BUYKUB10	0.44	
KAJBIH	-0.12	
COCJIN10	0.59	
PIMTAG	0.60	
YOHMOX	0.55	
YEQPOA	0.16	
CANDAW10	0.29	
PTSQFE10	0.64	
VOFLOR	0.29	
RABHAD	0.71	
JIGNUI	0.63	

|Quadrupole splittings|, mm/s

VOCBAQ	0.49	
FATBOR	2.58	0.29
YUZKAF10	3.32	2.87
YOCKAC	1.77	
XIGDIA	2.87	
ZOCPEM	1.54	
SOCWAI	2.73	
VUNMIA	2.85	
CACZIP10	1.58	
WEDXAF	0.28	

GIDKIN02	0.65	
SOCVUB	1.38	
JOHCEP	0.24	
SISKOU	3.33	3.93
SONMUE	0.19	
VUPJOF	2.90	
VUPJUL	3.08	3.04
CELVEU	0.98	
PTHPF10	2.76	
DEDWUE	1.85	
BUYKUB10	1.18	
KAJBIH	3.44	
COCJIN10	0.29	
PIMTAG	0.16	
YOHMOX	1.45	
YEQPOA	1.95	
CANDAW10	0.43	
PTSQFE10	2.46	
VOFLOR	2.34	
RABHAD	1.27	
JIGNUI	1.49	

M06/Partridge-1

Isomer shift, mm/s

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+2, MUE = 0.0524 (17 points)
FATBOR      0.93  0.1
YUZKAF10    1.52  1.23
XIGDIA      1.08
VUNMIA      1.08
JOHCEP      0.58
SISKOU      1.23  1.12
VUPJOF      1.22
VUPJUL      1.23  1.23
PTHPF10     0.67
DEDWUE      0.66
BUYKUB10    0.63
YEQPOA      0.30
PTSQFE10    0.65

+3, +4, MUE = 0.0344 (18 points)
VOCBAQ      0.53
YOCKAC      0.47
ZOCPEM      0.44
SOCWAI      0.14
CACZIP10    0.50
WEDXAF      0.24
GIDKIN02    0.14
SOCVUB      0.21
SONMUE      0.26
CELVEU      0.41
KAJBIH     -0.11
COCJIN10    0.46
PIMTAG      0.48
YOHMOX      0.44
CANDAW10    0.19
VOFLOR      0.34
RABHAD      0.65
JIGNUI      0.50

all, MUE = 0.0450 (35 points)
VOCBAQ      0.52
FATBOR      0.93  0.11
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YUZKAF10	1.52	1.23
YOCKAC	0.46	
XIGDIA	1.08	
ZOCPEM	0.43	
SOCWAI	0.15	
VUNMIA	1.08	
CACZIP10	0.49	
WEDXAF	0.24	
GIDKIN02	0.15	
SOCVUB	0.21	
JOHCEP	0.58	
SISKOU	1.23	1.13
SONMUE	0.26	
VUPJOF	1.23	
VUPJUL	1.24	1.23
CELVEU	0.40	
PTHPFE10	0.67	
DEDWUE	0.67	
BUYKUB10	0.64	
KAJBIH	-0.09	
COCJIN10	0.45	
PIMTAG	0.47	
YOHMOX	0.43	
YEQPOA	0.31	
CANDAW10	0.19	
PTSQFE10	0.66	
VOFLOR	0.33	
RABHAD	0.63	
JIGNUI	0.49	

|Quadrupole splitting|, mm/s

VOCBAQ	0.56	
FATBOR	2.97	0.18
YUZKAF10	3.46	2.87
YUZKAF10	3.46	2.86
YOCKAC	1.81	
XIGDIA	3.08	
ZOCPEM	1.52	
SOCWAI	3.23	
VUNMIA	3.18	
CACZIP10	1.71	
WEDXAF	0.41	
GIDKIN02	1.17	
SOCVUB	1.98	
JOHCEP	0.24	
SISKOU	3.34	4.03
SONMUE	0.72	
VUPJOF	3.33	
VUPJUL	3.53	3.36
CELVEU	0.85	
PTHPFE10	3.17	
DEDWUE	2.93	
BUYKUB10	2.74	
KAJBIH	3.23	
COCJIN10	0.26	
PIMTAG	0.21	
YOHMOX	1.40	
YEQPOA	1.66	
CANDAW10	0.42	
PTSQFE10	2.69	
VOFLOR	2.92	
RABHAD	1.51	
JIGNUI	1.60	

M06-2X/Partridge-1

Isomer shift, mm/s

+2, MUE = 0.0581 (17 points)

FATBOR	1.01	0.06
YUZKAF10	1.29	1.03
XIGDIA	1.40	
VUNMIA	1.12	
JOHCEP	0.58	
SISKOU	1.23	1.13
VUPJOF	1.21	
VUPJUL	1.22	1.22
PTHPFE10	0.73	
DEDWUE	0.65	
BUYKUB10	0.61	
YEQPOA	0.26	
PTSQFE10	0.72	

+3, +4, MUE = 0.0345 (18 points)

VOCBAQ	0.48	
YOCKAC	0.48	
ZOCPEM	0.45	
SOCWAI	0.09	
CACZIP10	0.51	
WEDXAF	0.23	
GIDKIN02	0.24	
SOCVUB	0.14	
SONMUE	0.25	
CELVEU	0.40	
KAJBIH	-0.05	
COCJIN10	0.50	
PIMTAG	0.51	
YOHMOX	0.44	
CANDAW10	0.17	
VOFLOR	0.29	
RABHAD	0.65	
JIGNUI	0.51	

all, MUE = 0.0564 (35 points)

VOCBAQ	0.45	
FATBOR	1.02	0.12
YUZKAF10	1.29	1.04
YOCKAC	0.44	
XIGDIA	1.39	
ZOCPEM	0.42	
SOCWAI	0.11	
VUNMIA	1.13	
CACZIP10	0.47	
WEDXAF	0.23	
GIDKIN02	0.24	
SOCVUB	0.16	
JOHCEP	0.61	
SISKOU	1.23	1.14
SONMUE	0.25	
VUPJOF	1.22	
VUPJUL	1.22	1.22
CELVEU	0.37	
PTHPFE10	0.75	
DEDWUE	0.68	
BUYKUB10	0.65	
KAJBIH	-0.01	
COCJIN10	0.46	
PIMTAG	0.47	
YOHMOX	0.41	

YEQPOA	0.31
CANDAW10	0.18
PTSQFE10	0.75
VOFLOR	0.28
RABHAD	0.59
JIGNUI	0.47

|Quadrupole splitting|, mm/s

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VOCBAQ	0.60	
FATBOR	3.55	0.09
YUZKAF10	3.78	2.99
YOCKAC	1.97	
XIGDIA	3.19	
ZOCPEM	1.57	
SOCWAI	3.86	
VUNMIA	3.54	
CACZIP10	1.77	
WEDXAF	0.62	
GIDKIN02	1.96	
SOCVUB	2.80	
JOHCEP	0.35	
SISKOU	3.61	4.22
SONMUE	1.07	
VUPJOF	3.56	
VUPJUL	3.80	3.61
CELVEU	0.83	
PTHPFE10	3.64	
DEDWUE	3.79	
BUYKUB10	3.58	
KAJBIH	1.81	
COCJIN10	0.29	
PIMTAG	0.24	
YOHMOX	1.29	
YEQPOA	1.67	
CANDAW10	0.38	
PTSQFE10	3.20	
VOFLOR	2.53	
RABHAD	1.54	
JIGNUI	1.67	

OLYP/Partridge-1

Isomer shift, mm/s

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+2, MUE = 0.0372 (17 points)

FATBOR	0.99	0.06
YUZKAF10	1.36	1.08
XIGDIA	1.09	
VUNMIA	1.09	
JOHCEP	0.50	
SISKOU	1.29	1.17
VUPJOF	1.27	
VUPJUL	1.28	1.27
PTHPFE10	0.75	
DEDWUE	0.70	
BUYKUB10	0.56	
YEQPOA	0.26	
PTSQFE10	0.73	

+3, +4, MUE = 0.0269 (18 points)

VOCBAQ	0.56
YOCKAC	0.48
ZOCPEM	0.47

SOCWAI	0.10
CACZIP10	0.51
WEDXAF	0.26
GIDKIN02	0.08
SOCVUB	0.17
SONMUE	0.23
CELVEU	0.43
KAJBIH	-0.04
COCJIN10	0.49
PIMTAG	0.50
YOHMOX	0.46
CANDAW10	0.27
VOFLOR	0.26
RABHAD	0.57
JIGNUI	0.51

all, MUE = 0.0703 (35 points)

VOCBAQ	0.69	
FATBOR	0.94	-0.06
YUZKAF10	1.33	1.03
YOCKAC	0.58	
XIGDIA	1.05	
ZOCPPEM	0.57	
SOCWAI	0.08	
VUNMIA	1.04	
CACZIP10	0.62	
WEDXAF	0.28	
GIDKIN02	0.05	
SOCVUB	0.16	
JOHCEP	0.41	
SISKOU	1.25	1.13
SONMUE	0.25	
VUPJOF	1.23	
VUPJUL	1.25	1.24
CELVEU	0.51	
PTHPFE10	0.68	
DEDWUE	0.63	
BUYKUB10	0.48	
KAJBIH	-0.11	
COCJIN10	0.59	
PIMTAG	0.60	
YOHMOX	0.55	
YEQPOA	0.15	
CANDAW10	0.30	
PTSQFE10	0.65	
VOFLOR	0.28	
RABHAD	0.70	
JIGNUI	0.62	

|Quadrupole splitting|, mm/s

VOCBAQ	0.50	
FATBOR	2.53	0.29
YUZKAF10	3.32	2.83
YOCKAC	1.74	
XIGDIA	2.88	
ZOCPPEM	1.43	
SOCWAI	2.78	
VUNMIA	2.82	
CACZIP10	1.52	
WEDXAF	0.26	
GIDKIN02	0.64	
SOCVUB	1.44	
JOHCEP	0.23	
SISKOU	3.32	3.89

SONMUE	0.28	
VUPJOF	2.55	
VUPJUL	2.65	2.64
CELVEU	0.96	
PTHPFE10	2.82	
DEDWUE	2.00	
BUYKUB10	1.27	
KAJBIH	3.42	
COCJIN10	0.23	
PIMTAG	0.16	
YOHMOX	1.47	
YEQPOA	1.95	
CANDAW10	0.40	
PTSQFE10	2.45	
VOFLOR	2.37	
RABHAD	1.32	
JIGNUI	1.42	

O3LYP/Partridge-1

Isomer shift, mm/s

+2, MUE = 0.0285 (17 points)
FATBOR 0.99 0.05
YUZKAF10 1.35 1.07
XIGDIA 1.12
VUNMIA 1.11
JOHCEP 0.50
SISKOU 1.28 1.17
VUPJOF 1.27
VUPJUL 1.28 1.28
PTHPFE10 0.73
DEDWUE 0.67
BUYKUB10 0.64
YEQPOA 0.25
PTSQFE10 0.71

+3, +4, MUE = 0.0227 (18 points)
VOCBAQ 0.56
YOCKAC 0.48
ZOCPEM 0.46
SOCWAI 0.10
CACZIP10 0.50
WEDXAF 0.26
GIDKIN02 0.11
SOCVUB 0.16
SONMUE 0.25
CELVEU 0.43
KAJBIH -0.07
COCJIN10 0.48
PIMTAG 0.49
YOHMOX 0.46
CANDAW10 0.25
VOFLOR 0.26
RABHAD 0.59
JIGNUI 0.50

all, MUE = 0.0420 (35 points)
VOCBAQ 0.63
FATBOR 0.96 -0.02
YUZKAF10 1.34 1.05
YOCKAC 0.54
XIGDIA 1.10
ZOCPEM 0.51

SOCWAI	0.08	
VUNMIA	1.08	
CACZIP10	0.56	
WEDXAF	0.27	
GIDKIN02	0.09	
SOCVUB	0.15	
JOHCEP	0.45	
SISKOU	1.26	1.15
SONMUE	0.26	
VUPJOF	1.25	
VUPJUL	1.26	1.26
CELVEU	0.48	
PTHPFE10	0.69	
DEDWUE	0.63	
BUYKUB10	0.60	
KAJBIH	-0.12	
COCJIN10	0.54	
PIMTAG	0.55	
YOHMOX	0.51	
YEQPOA	0.19	
CANDAW10	0.26	
PTSQFE10	0.67	
VOFLOR	0.27	
RABHAD	0.67	
JIGNUI	0.57	

|Quadrupole splitting|, mm/s

VOCBAQ	0.54	
FATBOR	3.01	0.22
YUZKAF10	3.56	2.94
YOCKAC	1.77	
XIGDIA	3.14	
ZOCPEM	1.44	
SOCWAI	3.04	
VUNMIA	3.16	
CACZIP10	1.60	
WEDXAF	0.32	
GIDKIN02	0.87	
SOCVUB	1.69	
JOHCEP	0.22	
SISKOU	3.47	4.14
SONMUE	0.52	
VUPJOF	3.49	
VUPJUL	3.69	3.52
CELVEU	0.89	
PTHPFE10	3.14	
DEDWUE	2.59	
BUYKUB10	2.42	
KAJBIH	3.58	
COCJIN10	0.24	
PIMTAG	0.20	
YOHMOX	1.43	
YEQPOA	1.86	
CANDAW10	0.40	
PTSQFE10	2.74	
VOFLOR	2.46	
RABHAD	1.46	
JIGNUI	1.50	

PBE/Partridge-1

Isomer shift, mm/s

+2, MUE = 0.0350 (17 points)

FATBOR	1.00	0.09
YUZKAF10	1.37	1.08
XIGDIA	1.09	
VUNMIA	1.09	
JOHCEP	0.52	
SISKOU	1.29	1.18
VUPJOF	1.27	
VUPJUL	1.28	1.28
PTHPFE10	0.75	
DEDWUE	0.64	
BUYKUB10	0.53	
YEQPOA	0.27	
PTSQFE10	0.72	

+3, +4, MUE = 0.0253 (18 points)

VOCBAQ	0.56	
YOCKAC	0.47	
ZOCPEM	0.48	
SOCWAI	0.11	
CACZIP10	0.52	
WEDXAF	0.25	
GIDKIN02	0.08	
SOCVUB	0.18	
SONMUE	0.22	
CELVEU	0.42	
KAJBIH	-0.05	
COCJIN10	0.49	
PIMTAG	0.50	
YOHMOX	0.45	
CANDAW10	0.26	
VOFLOR	0.26	
RABHAD	0.57	
JIGNUI	0.52	

all, MUE = 0.0746 (35 points)

VOCBAQ	0.69	
FATBOR	0.94	-0.04
YUZKAF10	1.34	1.02
YOCKAC	0.58	
XIGDIA	1.04	
ZOCPEM	0.59	
SOCWAI	0.09	
VUNMIA	1.04	
CACZIP10	0.64	
WEDXAF	0.28	
GIDKIN02	0.05	
SOCVUB	0.18	
JOHCEP	0.43	
SISKOU	1.26	1.13
SONMUE	0.24	
VUPJOF	1.23	
VUPJUL	1.25	1.24
CELVEU	0.51	
PTHPFE10	0.68	
DEDWUE	0.55	
BUYKUB10	0.43	
KAJBIH	-0.12	
COCJIN10	0.60	
PIMTAG	0.61	
YOHMOX	0.55	
YEQPOA	0.16	
CANDAW10	0.29	
PTSQFE10	0.64	
VOFLOR	0.29	
RABHAD	0.71	

JIGNUI 0.63

|Quadrupole splitting|, mm/s

VOCBAQ 0.49
FATBOR 2.53 0.3
YUZKAF10 3.29 2.84
YOCKAC 1.77
XIGDIA 2.85
ZOCPEM 1.52
SOCWAI 2.73
VUNMIA 2.82
CACZIP10 1.57
WEDXAF 0.28
GIDKIN02 0.66
SOCVUB 1.38
JOHCEP 0.25
SISKOU 3.31 3.91
SONMUE 0.19
VUPJOF 2.66
VUPJUL 2.77 2.76
CELVEU 0.98
PTHPFE10 2.74
DEDWUE 1.86
BUYKUB10 1.19
KAJBIH 3.43
COCJIN10 0.29
PIMTAG 0.16
YOHMOX 1.45
YEQPOA 1.95
CANDAW10 0.43
PTSQFE10 2.42
VOFLOR 2.34
RABHAD 1.27
JIGNUI 1.47

SVWN5/Partridge-1

Isomer shift, mm/s

+2, MUE = 0.0383 (17 points)

FATBOR 1.00 0.10
YUZKAF10 1.38 1.09
XIGDIA 1.07
VUNMIA 1.09
JOHCEP 0.53
SISKOU 1.30 1.18
VUPJOF 1.27
VUPJUL 1.28 1.26
PTHPFE10 0.77
DEDWUE 0.61
BUYKUB10 0.52
YEQPOA 0.28
PTSQFE10 0.72

+3, +4, MUE = 0.0274 (18 points)

VOCBAQ 0.56
YOCKAC 0.47
ZOCPEM 0.47
SOCWAI 0.12
CACZIP10 0.51
WEDXAF 0.26
GIDKIN02 0.08
SOCVUB 0.20

SONMUE	0.22
CELVEU	0.43
KAJBIH	-0.06
COCJIN10	0.49
PIMTAG	0.50
YOHMOX	0.45
CANDAW10	0.27
VOFLOR	0.25
RABHAD	0.57
JIGNUI	0.51

all, MUE = 0.0822 (35 points)

VOCBAQ	0.70	
FATBOR	0.94	-0.04
YUZKAF10	1.35	1.03
YOCKAC	0.58	
XIGDIA	1.01	
ZOCPEM	0.59	
SOCWAI	0.10	
VUNMIA	1.03	
CACZIP10	0.64	
WEDXAF	0.29	
GIDKIN02	0.05	
SOCVUB	0.21	
JOHCEP	0.42	
SISKOU	1.26	1.14
SONMUE	0.24	
VUPJOF	1.23	
VUPJUL	1.24	1.22
CELVEU	0.52	
PTHPFE10	0.69	
DEDWUE	0.51	
BUYKUB10	0.41	
KAJBIH	-0.14	
COCJIN10	0.61	
PIMTAG	0.62	
YOHMOX	0.55	
YEQPOA	0.15	
CANDAW10	0.30	
PTSQFE10	0.64	
VOFLOR	0.28	
RABHAD	0.71	
JIGNUI	0.64	

|Quadrupole splitting|, mm/s

VOCBAQ	0.48	
FATBOR	2.42	0.33
YUZKAF10	3.20	2.85
YOCKAC	1.80	
XIGDIA	2.80	
ZOCPEM	1.56	
SOCWAI	2.66	
VUNMIA	2.71	
CACZIP10	1.58	
WEDXAF	0.24	
GIDKIN02	0.65	
SOCVUB	1.31	
JOHCEP	0.27	
SISKOU	3.26	3.82
SONMUE	0.12	
VUPJOF	1.42	
VUPJUL	1.55	1.49
CELVEU	1.03	
PTHPFE10	2.64	
DEDWUE	2.23	

BUYKUB10	1.25
KAJBIH	3.44
COCJIN10	0.56
PIMTAG	0.30
YOHMOX	1.37
YEQPOA	1.97
CANDAW10	0.45
PTSQFE10	2.34
VOFLOR	2.37
RABHAD	1.22
JIGNUI	1.49

B3LYP/Wachters

Isomer shift, mm/s

+2, MUE = 0.0283 (17 points)

FATBOR	0.97	0.06
YUZKAF10	1.36	1.08
XIGDIA	1.11	
VUNMIA	1.12	
JOHCEP	0.52	
SISKOU	1.28	1.17
VUPJOF	1.27	
VUPJUL	1.28	1.27
PTHPE10	0.71	
DEWUE	0.67	
BUYKUB10	0.64	
YEQPOA	0.25	
PTSQFE10	0.7	

+3, +4, MUE = 0.0285 (18 points)

VOCBAQ	0.56
YOCKAC	0.47
ZOCPEM	0.45
SOCWAI	0.11
CACZIP10	0.50
WEDXAF	0.27
GIDKIN02	0.16
SOCVUB	0.16
SONMUE	0.28
CELVEU	0.44
KAJBIH	-0.10
COCJIN10	0.48
PIMTAG	0.48
YOHMOX	0.44
CANDAW10	0.24
VOFLOR	0.26
RABHAD	0.61
JIGNUI	0.50

all, MUE = 0.0324 (35 points)

VOCBAQ	0.62	
FATBOR	0.96	0.03
YUZKAF10	1.35	1.06
YOCKAC	0.50	
XIGDIA	1.10	
ZOCPEM	0.48	
SOCWAI	0.08	
VUNMIA	1.11	
CACZIP10	0.54	
WEDXAF	0.27	
GIDKIN02	0.14	
SOCVUB	0.14	

JOHCEP	0.49	
SISKOU	1.27	1.16
SONMUE	0.29	
VUPJOF	1.25	
VUPJUL	1.26	1.26
CELVEU	0.48	
PTHPFE10	0.69	
DEDWUE	0.65	
BUYKUB10	0.62	
KAJBIH	-0.16	
COCJIN10	0.52	
PIMTAG	0.53	
YOHMOX	0.47	
YEQPOA	0.22	
CANDAW10	0.24	
PTSQFE10	0.68	
VOFLOR	0.26	
RABHAD	0.67	
JIGNUI	0.54	

|Quadrupole splitting|, mm/s

VOCBAQ	0.60	
FATBOR	3.10	0.17
YUZKAF10	3.58	3.04
YOCKAC	1.70	
XIGDIA	3.19	
ZOCPEM	1.40	
SOCWAI	3.09	
VUNMIA	3.30	
CACZIP10	1.57	
WEDXAF	0.27	
GIDKIN02	0.78	
SOCVUB	1.82	
JOHCEP	0.26	
SISKOU	3.47	4.14
SONMUE	0.40	
VUPJOF	3.50	
VUPJUL	3.68	3.52
CELVEU	0.81	
PTHPFE10	3.18	
DEDWUE	3.29	
BUYKUB10	3.09	
KAJBIH	3.62	
COCJIN10	0.23	
PIMTAG	0.19	
YOHMOX	1.33	
YEQPOA	1.68	
CANDAW10	0.43	
PTSQFE10	2.86	
VOFLOR	2.37	
RABHAD	1.40	
JIGNUI	1.47	

BPW91/Wachters

Isomer shift, mm/s

+2, MUE = 0.0283 (17 points)		
FATBOR	0.99	0.08
YUZKAF10	1.37	1.09
XIGDIA	1.07	
VUNMIA	1.09	
JOHCEP	0.52	
SISKOU	1.29	1.18
VUPJOF	1.27	

VUPJUL	1.28	1.28
PTHPFE10	0.76	
DEDWUE	0.63	
BUYKUB10	0.54	
YEQPOA	0.27	
PTSQFE10	0.73	

+3, +4, MUE = 0.0289 (18 points)

VOCBAQ	0.57	
YOCKAC	0.46	
ZOCPEM	0.47	
SOCWAI	0.10	
CACZIP10	0.51	
WEDXAF	0.27	
GIDKIN02	0.10	
SOCVUB	0.17	
SONMUE	0.25	
CELVEU	0.44	
KAJBIH	-0.06	
COCJIN10	0.48	
PIMTAG	0.49	
YOHMOX	0.44	
CANDAW10	0.26	
VOFLOR	0.25	
RABHAD	0.57	
JIGNUI	0.51	

all, MUE = 0.0772 (35 points)

VOCBAQ	0.71	
FATBOR	0.92	-0.05
YUZKAF10	1.34	1.04
YOCKAC	0.56	
XIGDIA	1.02	
ZOCPEM	0.58	
SOCWAI	0.08	
VUNMIA	1.04	
CACZIP10	0.63	
WEDXAF	0.30	
GIDKIN02	0.08	
SOCVUB	0.17	
JOHCEP	0.42	
SISKOU	1.26	1.14
SONMUE	0.28	
VUPJOF	1.23	
VUPJUL	1.24	1.24
CELVEU	0.54	
PTHPFE10	0.68	
DEDWUE	0.54	
BUYKUB10	0.44	
KAJBIH	-0.14	
COCJIN10	0.59	
PIMTAG	0.61	
YOHMOX	0.53	
YEQPOA	0.15	
CANDAW10	0.30	
PTSQFE10	0.65	
VOFLOR	0.28	
RABHAD	0.71	
JIGNUI	0.63	

|Quadrupole splitting|, mm/s

VOCBAQ	0.52	
FATBOR	2.49	0.27
YUZKAF10	3.21	2.88
YOCKAC	1.65	

XIGDIA	2.83	
ZOCPEM	1.47	
SOCWAI	2.67	
VUNMIA	2.78	
CACZIP10	1.50	
WEDXAF	0.21	
GIDKIN02	0.49	
SOCVUB	1.38	
JOHCEP	0.23	
SISKOU	3.22	3.8
SONMUE	0.07	
VUPJOF	2.78	
VUPJUL	2.93	2.92
CELVEU	0.95	
PTHPFE10	2.64	
DEDWUE	1.57	
BUYKUB10	0.82	
KAJBIH	3.36	
COCJIN10	0.26	
PIMTAG	0.15	
YOHMOX	1.38	
YEQPOA	1.84	
CANDAW10	0.43	
PTSQFE10	2.38	
VOFLOR	2.27	
RABHAD	1.18	
JIGNUI	1.41	

M06/Wachters

Isomer shift, mm/s

+2, MUE = 0.0334 (17 points)

FATBOR	0.94	0.04
YUZKAF10	1.37	1.07
XIGDIA	1.12	
VUNMIA	1.11	
JOHCEP	0.59	
SISKOU	1.28	1.18
VUPJOF	1.27	
VUPJUL	1.28	1.28
PTHPFE10	0.68	
DEDWUE	0.67	
BUYKUB10	0.64	
YEQPOA	0.28	
PTSQFE10	0.66	

+3, +4, MUE = 0.0352 (18 points)

VOCBAQ	0.54	
YOCKAC	0.46	
ZOCPEM	0.43	
SOCWAI	0.13	
CACZIP10	0.50	
WEDXAF	0.25	
GIDKIN02	0.15	
SOCVUB	0.19	
SONMUE	0.28	
CELVEU	0.43	
KAJBIH	-0.10	
COCJIN10	0.47	
PIMTAG	0.48	
YOHMOX	0.42	
CANDAW10	0.19	
VOFLOR	0.35	

RABHAD	0.64	
JIGNUI	0.50	
all, MUE = 0.0370 (35 points)		
VOCBAQ	0.53	
FATBOR	0.95	0.08
YUZKAF10	1.36	1.08
YOCKAC	0.44	
XIGDIA	1.12	
ZOCPEM	0.42	
SOCWAI	0.12	
VUNMIA	1.11	
CACZIP10	0.48	
WEDXAF	0.24	
GIDKIN02	0.14	
SOCVUB	0.18	
JOHCEP	0.61	
SISKOU	1.28	1.18
SONMUE	0.27	
VUPJOF	1.27	
VUPJUL	1.28	1.28
CELVEU	0.41	
PTHPFE10	0.70	
DEDWUE	0.69	
BUYKUB10	0.66	
KAJBIH	-0.10	
COCJIN10	0.46	
PIMTAG	0.47	
YOHMOX	0.41	
YEQPOA	0.32	
CANDAW10	0.18	
PTSQFE10	0.68	
VOFLOR	0.34	
RABHAD	0.63	
JIGNUI	0.49	

|Quadrupole splitting|, mm/s

VOCBAQ	0.57	
FATBOR	2.87	0.16
YUZKAF10	3.33	2.85
YOCKAC	1.70	
XIGDIA	2.98	
ZOCPEM	1.43	
SOCWAI	3.13	
VUNMIA	3.07	
CACZIP10	1.60	
WEDXAF	0.29	
GIDKIN02	0.96	
SOCVUB	1.94	
JOHCEP	0.25	
SISKOU	3.22	3.88
SONMUE	0.52	
VUPJOF	3.22	
VUPJUL	3.41	3.25
CELVEU	0.82	
PTHPFE10	3.03	
DEDWUE	3.13	
BUYKUB10	2.99	
KAJBIH	3.11	
COCJIN10	0.24	
PIMTAG	0.19	
YOHMOX	1.32	
YEQPOA	1.55	
CANDAW10	0.42	
PTSQFE10	2.56	

VOFLOR	3.21
RABHAD	1.40
JIGNUI	1.50

M06-2X/Wachters

Isomer shift, mm/s

+2, MUE = 0.0380 (17 points)

FATBOR	1.02	0.01
YUZKAF10	1.33	1.07
XIGDIA	1.12	
VUNMIA	1.15	
JOHCEP	0.56	
SISKOU	1.26	1.16
VUPJOF	1.25	
VUPJUL	1.26	1.25
PTHPE10	0.74	
DEWUE	0.66	
BUYKUB10	0.63	
YEQPOA	0.23	
PTSQFE10	0.75	

+3, +4, MUE = 0.0342 (18 points)

VOCBAQ	0.54
YOCKAC	0.46
ZOCPEM	0.44
SOCWAI	0.09
CACZIP10	0.50
WEDXAF	0.25
GIDKIN02	0.18
SOCVUB	0.14
SONMUE	0.29
CELVEU	0.42
KAJBIH	-0.04
COCJIN10	0.49
PIMTAG	0.50
YOHMOX	0.43
CANDAW10	0.18
VOFLOR	0.25
RABHAD	0.64
JIGNUI	0.50

all, MUE = 0.0426 (35 points)

VOCBAQ	0.51	
FATBOR	1.03	0.09
YUZKAF10	1.32	1.08
YOCKAC	0.44	
XIGDIA	1.13	
ZOCPEM	0.42	
SOCWAI	0.10	
VUNMIA	1.15	
CACZIP10	0.47	
WEDXAF	0.24	
GIDKIN02	0.18	
SOCVUB	0.14	
JOHCEP	0.60	
SISKOU	1.25	1.17
SONMUE	0.28	
VUPJOF	1.25	
VUPJUL	1.25	1.25
CELVEU	0.40	
PTHPE10	0.77	
DEWUE	0.69	

BUYKUB10	0.66
KAJBIH	-0.03
COCJIN10	0.46
PIMTAG	0.47
YOHMOX	0.40
YEQPOA	0.30
CANDAW10	0.18
PTSQFE10	0.78
VOFLOR	0.24
RABHAD	0.60
JIGNUI	0.47

|Quadrupole splitting|, mm/s

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VOCBAQ	0.61	
FATBOR	3.40	0.08
YUZKAF10	3.65	2.98
YOCKAC	1.82	
XIGDIA	3.11	
ZOCPEM	1.45	
SOCWAI	3.71	
VUNMIA	3.43	
CACZIP10	1.64	
WEDXAF	0.48	
GIDKIN02	1.34	
SOCVUB	2.71	
JOHCEP	0.35	
SISKOU	3.47	4.07
SONMUE	0.86	
VUPJOF	3.45	
VUPJUL	3.66	3.48
CELVEU	0.74	
PTHPFE10	3.48	
DEDWUE	4.13	
BUYKUB10	3.92	
KAJBIH	1.69	
COCJIN10	0.27	
PIMTAG	0.22	
YOHMOX	1.18	
YEQPOA	1.56	
CANDAW10	0.37	
PTSQFE10	3.08	
VOFLOR	2.46	
RABHAD	1.41	
JIGNUI	1.54	

OLYP/Wachters

Isomer shift, mm/s

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+2, MUE = 0.0352 (17 points)

FATBOR	0.97	0.06
YUZKAF10	1.36	1.10
XIGDIA	1.07	
VUNMIA	1.09	
JOHCEP	0.50	
SISKOU	1.29	1.19
VUPJOF	1.27	
VUPJUL	1.28	1.27
PTHPFE10	0.77	
DEDWUE	0.66	
BUYKUB10	0.58	
YEQPOA	0.26	
PTSQFE10	0.74	

+3, +4, MUE = 0.0321 (18 points)

VOCBAQ	0.57
YOCKAC	0.47
ZOCPEM	0.46
SOCWAI	0.09
CACZIP10	0.50
WEDXAF	0.27
GIDKIN02	0.10
SOCVUB	0.15
SONMUE	0.26
CELVEU	0.45
KAJBIH	-0.05
COCJIN10	0.49
PIMTAG	0.49
YOHMOX	0.45
CANDAW10	0.27
VOFLOR	0.25
RABHAD	0.57
JIGNUI	0.51

all, MUE = 0.0756 (35 points)

VOCBAQ	0.71	
FATBOR	0.91	-0.07
YUZKAF10	1.34	1.05
YOCKAC	0.57	
XIGDIA	1.02	
ZOCPEM	0.56	
SOCWAI	0.07	
VUNMIA	1.04	
CACZIP10	0.62	
WEDXAF	0.30	
GIDKIN02	0.08	
SOCVUB	0.15	
JOHCEP	0.41	
SISKOU	1.25	1.14
SONMUE	0.29	
VUPJOF	1.23	
VUPJUL	1.24	1.23
CELVEU	0.54	
PTHPFE10	0.69	
DEDWUE	0.57	
BUYKUB10	0.49	
KAJBIH	-0.12	
COCJIN10	0.59	
PIMTAG	0.61	
YOHMOX	0.54	
YEQPOA	0.15	
CANDAW10	0.30	
PTSQFE10	0.66	
VOFLOR	0.27	
RABHAD	0.71	
JIGNUI	0.62	

|Quadrupole splitting|, mm/s

VOCBAQ	0.53	
FATBOR	2.44	0.28
YUZKAF10	3.20	2.83
YOCKAC	1.64	
XIGDIA	2.82	
ZOCPEM	1.37	
SOCWAI	2.73	
VUNMIA	2.74	
CACZIP10	1.45	

WEDXAF	0.19	
GIDKIN02	0.49	
SOCVUB	1.44	
JOHCEP	0.23	
SISKOU	3.21	3.77
SONMUE	0.13	
VUPJOF	2.45	
VUPJUL	2.47	2.48
CELVEU	0.93	
PTHPFE10	2.71	
DEDWUE	1.87	
BUYKUB10	1.05	
KAJBIH	3.35	
COCJIN10	0.21	
PIMTAG	0.15	
YOHMOX	1.41	
YEQPOA	1.83	
CANDAW10	0.40	
PTSQFE10	2.36	
VOFLOR	2.31	
RABHAD	1.24	
JIGNUI	1.36	

O3LYP/Wachters

Isomer shift, mm/s

+2, MUE = 0.0320 (17 points)
FATBOR 0.97 0.04
YUZKAF10 1.35 1.09
XIGDIA 1.10
VUNMIA 1.10
JOHCEP 0.50
SISKOU 1.28 1.17
VUPJOF 1.27
VUPJUL 1.28 1.28
PTHPFE10 0.73
DEDWUE 0.68
BUYKUB10 0.64
YEQPOA 0.25
PTSQFE10 0.72

+3, +4, MUE = 0.0291 (18 points)
VOCBAQ 0.57
YOCKAC 0.47
ZOCPEM 0.45
SOCWAI 0.10
CACZIP10 0.50
WEDXAF 0.27
GIDKIN02 0.13
SOCVUB 0.15
SONMUE 0.28
CELVEU 0.45
KAJBIH -0.07
COCJIN10 0.48
PIMTAG 0.49
YOHMOX 0.44
CANDAW10 0.25
VOFLOR 0.25
RABHAD 0.59
JIGNUI 0.50

all, MUE = 0.0461 (35 points)
VOCBAQ 0.65

FATBOR	0.94	-0.03
YUZKAF10	1.34	1.06
YOCKAC	0.52	
XIGDIA	1.07	
ZOCPEM	0.51	
SOCWAI	0.07	
VUNMIA	1.08	
CACZIP10	0.56	
WEDXAF	0.29	
GIDKIN02	0.12	
SOCVUB	0.13	
JOHCEP	0.44	
SISKOU	1.26	1.15
SONMUE	0.29	
VUPJOF	1.25	
VUPJUL	1.26	1.26
CELVEU	0.50	
PTHPF10	0.69	
DEDWUE	0.63	
BUYKUB10	0.60	
KAJBIH	-0.13	
COCJIN10	0.54	
PIMTAG	0.55	
YOHMOX	0.49	
YEQPOA	0.18	
CANDAW10	0.27	
PTSQFE10	0.68	
VOFLOR	0.26	
RABHAD	0.68	
JIGNUI	0.57	

|Quadrupole splitting|, mm/s

VOCBAQ	0.57	
FATBOR	2.90	0.21
YUZKAF10	3.43	2.95
YOCKAC	1.67	
XIGDIA	3.05	
ZOCPEM	1.37	
SOCWAI	2.98	
VUNMIA	3.07	
CACZIP10	1.52	
WEDXAF	0.23	
GIDKIN02	0.69	
SOCVUB	1.69	
JOHCEP	0.22	
SISKOU	3.36	4.01
SONMUE	0.34	
VUPJOF	3.42	
VUPJUL	3.58	3.43
CELVEU	0.86	
PTHPF10	3.01	
DEDWUE	2.84	
BUYKUB10	2.67	
KAJBIH	3.50	
COCJIN10	0.23	
PIMTAG	0.19	
YOHMOX	1.37	
YEQPOA	1.75	
CANDAW10	0.40	
PTSQFE10	2.65	
VOFLOR	2.39	
RABHAD	1.37	
JIGNUI	1.42	

PBE/Wachters

Isomer shift, mm/s

+2, MUE = 0.0355 (17 points)
FATBOR 0.99 0.08
YUZKAF10 1.37 1.09
XIGDIA 1.07
VUNMIA 1.09
JOHCEP 0.52
SISKOU 1.29 1.18
VUPJOF 1.27
VUPJUL 1.28 1.27
PTHPFE10 0.76
DEDWUE 0.63
BUYKUB10 0.54
YEQPOA 0.27
PTSQFE10 0.73

+3, +4, MUE = 0.0291 (18 points)
VOCBAQ 0.57
YOCKAC 0.46
ZOCPEM 0.47
SOCWAI 0.10
CACZIP10 0.51
WEDXAF 0.27
GIDKIN02 0.10
SOCVUB 0.17
SONMUE 0.25
CELVEU 0.44
KAJBIH -0.06
COCJIN10 0.49
PIMTAG 0.49
YOHMOX 0.44
CANDAW10 0.26
VOFLOR 0.25
RABHAD 0.57
JIGNUI 0.51

all, MUE = 0.0793 (35 points)
VOCBAQ 0.71
FATBOR 0.92 -0.06
YUZKAF10 1.34 1.04
YOCKAC 0.57
XIGDIA 1.02
ZOCPEM 0.58
SOCWAI 0.08
VUNMIA 1.03
CACZIP10 0.64
WEDXAF 0.30
GIDKIN02 0.08
SOCVUB 0.17
JOHCEP 0.42
SISKOU 1.26 1.14
SONMUE 0.28
VUPJOF 1.23
VUPJUL 1.24 1.23
CELVEU 0.54
PTHPFE10 0.68
DEDWUE 0.53
BUYKUB10 0.44
KAJBIH -0.13
COCJIN10 0.60
PIMTAG 0.61
YOHMOX 0.54

YEQPOA	0.15
CANDAW10	0.30
PTSQFE10	0.65
VOFLOR	0.28
RABHAD	0.71
JIGNUI	0.64

|Quadrupole splitting|, mm/s

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VOCBAQ	0.52	
FATBOR	2.46	0.28
YUZKAF10	3.17	2.86
YOCKAC	1.65	
XIGDIA	2.79	
ZOCPEM	1.45	
SOCWAI	2.67	
VUNMIA	2.74	
CACZIP10	1.49	
WEDXAF	0.21	
GIDKIN02	0.50	
SOCVUB	1.37	
JOHCEP	0.24	
SISKOU	3.19	3.77
SONMUE	0.07	
VUPJOF	2.59	
VUPJUL	2.58	2.6
CELVEU	0.95	
PTHPFE10	2.62	
DEDWUE	1.46	
BUYKUB10	0.81	
KAJBIH	3.36	
COCJIN10	0.26	
PIMTAG	0.15	
YOHMOX	1.37	
YEQPOA	1.84	
CANDAW10	0.43	
PTSQFE10	2.34	
VOFLOR	2.27	
RABHAD	1.18	
JIGNUI	1.40	

SVWN5/Wachters

Isomer shift, mm/s

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+2, MUE = 0.0355 (17 points)

FATBOR	0.99	0.09
YUZKAF10	1.38	1.1
XIGDIA	1.07	
VUNMIA	1.08	
JOHCEP	0.51	
SISKOU	1.29	1.19
VUPJOF	1.27	
VUPJUL	1.28	1.26
PTHPFE10	0.78	
DEDWUE	0.63	
BUYKUB10	0.53	
YEQPOA	0.27	
PTSQFE10	0.74	

+3, +4, MUE = 0.0318 (18 points)

VOCBAQ	0.57
YOCKAC	0.46
ZOCPEM	0.47

SOCWAI	0.11
CACZIP10	0.51
WEDXAF	0.27
GIDKIN02	0.10
SOCVUB	0.18
SONMUE	0.25
CELVEU	0.45
KAJBIH	-0.07
COCJIN10	0.49
PIMTAG	0.49
YOHMOX	0.44
CANDAW10	0.27
VOFLOR	0.24
RABHAD	0.57
JIGNUI	0.51

all, MUE = 0.0845 (35 points)

VOCBAQ	0.73	
FATBOR	0.92	-0.05
YUZKAF10	1.34	1.04
YOCKAC	0.57	
XIGDIA	1.01	
ZOCPEM	0.58	
SOCWAI	0.09	
VUNMIA	1.02	
CACZIP10	0.64	
WEDXAF	0.31	
GIDKIN02	0.08	
SOCVUB	0.20	
JOHCEP	0.40	
SISKOU	1.25	1.14
SONMUE	0.28	
VUPJOF	1.23	
VUPJUL	1.23	1.22
CELVEU	0.55	
PTHPFE10	0.69	
DEDWUE	0.53	
BUYKUB10	0.43	
KAJBIH	-0.15	
COCJIN10	0.61	
PIMTAG	0.62	
YOHMOX	0.54	
YEQPOA	0.14	
CANDAW10	0.31	
PTSQFE10	0.65	
VOFLOR	0.27	
RABHAD	0.71	
JIGNUI	0.64	

|Quadrupole splitting|, mm/s

VOCBAQ	0.51	
FATBOR	2.32	0.32
YUZKAF10	3.09	2.85
YOCKAC	1.69	
XIGDIA	2.72	
ZOCPEM	1.49	
SOCWAI	2.60	
VUNMIA	2.64	
CACZIP10	1.49	
WEDXAF	0.18	
GIDKIN02	0.48	
SOCVUB	1.30	
JOHCEP	0.25	
SISKOU	3.14	3.68
SONMUE	0.16	

VUPJOF	1.38	
VUPJUL	1.51	1.44
CELVEU	0.99	
PTHPFE10	2.52	
DEDWUE	2.04	
BUYKUB10	0.91	
KAJBIH	3.36	
COCJIN10	0.51	
PIMTAG	0.27	
YOHMOX	1.30	
YEQPOA	1.87	
CANDAW10	0.45	
PTSQFE10	2.26	
VOFLOR	2.29	
RABHAD	1.12	
JIGNUI	1.42	

The isomer shift calibrations

The equations $y = kx + b$ correlate density on atom (x) with the isomer shift (y). The densities are in atomic units, the resulting isomer shifts are in mm/s.

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B3LYP/Partridge-1

+2 eqn: $y = -0.415417 x + 4914.100608$
+3, +4 eqn: $y = -0.362076 x + 4283.128131$
all eqn: $y = -0.418388 x + 4949.219306$

BPW91/Partridge-1

+2 eqn: $y = -0.439211 x + 5198.627730$
+3, +4 eqn: $y = -0.354372 x + 4194.389259$
all eqn: $y = -0.473505 x + 5604.407662$

M06/Partridge-1

+2 eqn: $y = -0.423003 x + 4997.160442$
+3, +4 eqn: $y = -0.444197 x + 5247.533444$
all eqn: $y = -0.419420 x + 4954.837965$

M06-2X/Partridge-1

+2 eqn: $y = -0.370567 x + 4382.414799$
+3, +4 eqn: $y = -0.416372 x + 4924.142329$
all eqn: $y = -0.352767 x + 4171.970965$

OLYP/Partridge-1

+2 eqn: $y = -0.418834 x + 4951.190055$
+3, +4 eqn: $y = -0.336536 x + 3978.264936$
all eqn: $y = -0.448969 x + 5307.301759$

O3LYP/Partridge-1

+2 eqn: $y = -0.401759 x + 4748.279391$
+3, +4 eqn: $y = -0.348911 x + 4123.657739$
all eqn: $y = -0.420000 x + 4963.792615$

PBE/Partridge-1

+2 eqn: $y = -0.438096 x + 5184.513216$
+3, +4 eqn: $y = -0.351946 x + 4164.935453$
all eqn: $y = -0.472381 x + 5590.113424$

SVWN5/Partridge-1

+2 eqn: $y = -0.456209 x + 5372.977503$
+3, +4 eqn: $y = -0.364626 x + 4294.290051$
all eqn: $y = -0.495225 x + 5832.338399$

B3LYP/Wachters

+2 eqn: $y = -0.403244 x + 4683.331863$
+3, +4, eqn: $y = -0.347271 x + 4033.261027$
all, eqn: $y = -0.409087 x + 4751.159223$

BPW91/Wachters

+2 eqn: $y = -0.430143 x + 4997.158352$
+3, +4 eqn: $y = -0.346058 x + 4020.240840$
all eqn: $y = -0.465771 x + 5410.914106$

M06/Wachters

+2 eqn: $y = -0.444991 x + 5174.475932$
+3, +4 eqn: $y = -0.431490 x + 5017.531584$
all eqn: $y = -0.427390 x + 4969.849624$

M06-2X/Wachters

+2 eqn: $y = -0.382461 x + 4434.542519$
+3, +4 eqn: $y = -0.387962 x + 4498.403090$
all eqn: $y = -0.358582 x + 4157.743628$

OLYP/Wachters

+2 eqn: $y = -0.412265 x + 4787.456787$
+3, +4 eqn: $y = -0.332943 x + 3866.259545$
all eqn: $y = -0.445584 x + 5174.231901$

O3LYP/Wachters

+2 eqn: $y = -0.395380 x + 4590.578802$
+3, +4 eqn: $y = -0.341303 x + 3962.689897$
all eqn: $y = -0.415390 x + 4822.827968$

PBE/Wachters

+2 eqn: $y = -0.427967 x + 4971.467448$
+3, +4 eqn: $y = -0.343391 x + 3988.918681$
all eqn: $y = -0.464242 x + 5392.702744$

SVWN5/Wachters

+2 eqn: $y = -0.445356 x + 5149.087888$

+3, +4 eqn: $y = -0.355122 x + 4105.751957$
all eqn: $y = -0.484710 x + 5603.939113$