

Supporting Information for

Insight into Magnetically Induced Ring-Currents and Photophysics of Nanorings

Lenara I. Valiulina, Victor N. Cherepanov and Kirill Khoroshkin

Department of Optics and Spectroscopy, Tomsk State University, Tomsk, 634050, Russia.

Correspondence to: valiulina.lenara.01.01.1998@gmail.com

The Cartesian coordinates of the optimized molecular structures at the BHandHLYP/def2-SVP level of theory:

c-P6			c-P6²⁺				
C	-12.593488000000	2.790639000000	1.249501000000	C	-12.583610000000	2.789131000000	1.256685000000
C	-12.580595000000	3.460322000000	2.524201000000	C	-12.588615000000	3.460977000000	2.527627000000
C	-12.732090000000	2.500353000000	3.468377000000	C	-12.749609000000	2.500026000000	3.471295000000
C	-12.809575000000	1.243931000000	2.773679000000	C	-12.814262000000	1.246018000000	2.775578000000
N	-12.739831000000	1.459317000000	1.433550000000	N	-12.726928000000	1.460866000000	1.435069000000
H	-12.475913000000	4.525658000000	2.663649000000	H	-12.494379000000	4.526832000000	2.669918000000
H	-12.772934000000	2.622199000000	4.541812000000	H	-12.808586000000	2.623172000000	4.543594000000
C	-12.870342000000	0.000000000000	3.389917000000	C	-12.881595000000	0.000000000000	3.388296000000
C	-12.809575000000	-1.243931000000	2.773679000000	C	-12.814262000000	-1.246018000000	2.775578000000
C	-12.732090000000	-2.500353000000	3.468377000000	C	-12.749609000000	-2.500026000000	3.471295000000
N	-12.739831000000	-1.459317000000	1.433550000000	N	-12.726928000000	-1.460866000000	1.435069000000
C	-12.580595000000	-3.460322000000	2.524201000000	C	-12.588615000000	-3.460977000000	2.527627000000
H	-12.772934000000	-2.622199000000	4.541812000000	H	-12.808586000000	-2.623172000000	4.543594000000
C	-12.593488000000	-2.790639000000	1.249501000000	C	-12.583610000000	-2.789131000000	1.256685000000
H	-12.475913000000	-4.525658000000	2.663649000000	H	-12.494379000000	-4.526832000000	2.669918000000
C	-12.467162000000	-3.432366000000	0.000000000000	C	-12.445041000000	-3.430514000000	0.000000000000
C	-12.593488000000	-2.790639000000	-1.249501000000	C	-12.583610000000	-2.789131000000	-1.256685000000
C	-12.580595000000	-3.460322000000	-2.524201000000	C	-12.588615000000	-3.460977000000	-2.527627000000
N	-12.739831000000	-1.459317000000	-1.433550000000	N	-12.726928000000	-1.460866000000	-1.435069000000
C	-12.732090000000	-2.500353000000	-3.468377000000	C	-12.749609000000	-2.500026000000	-3.471295000000
H	-12.475913000000	-4.525658000000	-2.663649000000	H	-12.494379000000	-4.526832000000	-2.669918000000
C	-12.809575000000	-1.243931000000	-2.773679000000	C	-12.814262000000	-1.246018000000	-2.775578000000
H	-12.772934000000	-2.622199000000	-4.541812000000	H	-12.808586000000	-2.623172000000	-4.543594000000
C	-12.870342000000	0.000000000000	-3.389917000000	C	-12.881595000000	0.000000000000	-3.388296000000
C	-12.809575000000	1.243931000000	-2.773679000000	C	-12.814262000000	1.246018000000	-2.775578000000
C	-12.732090000000	2.500353000000	-3.468377000000	C	-12.749609000000	2.500026000000	-3.471295000000
N	-12.739831000000	1.459317000000	-1.433550000000	N	-12.726928000000	1.460866000000	-1.435069000000
C	-12.580595000000	3.460322000000	-2.524201000000	C	-12.588615000000	3.460977000000	-2.527627000000
H	-12.772934000000	2.622199000000	-4.541812000000	H	-12.808586000000	2.623172000000	-4.543594000000
C	-12.593488000000	2.790639000000	-1.249501000000	C	-12.583610000000	2.789131000000	-1.256685000000
H	-12.475913000000	4.525658000000	-2.663649000000	H	-12.494379000000	4.526832000000	-2.669918000000
C	-12.467162000000	3.432366000000	0.000000000000	C	-12.445041000000	3.430514000000	0.000000000000
Zn	-12.751320000000	0.000000000000	0.000000000000	Zn	-12.743192000000	0.000000000000	0.000000000000
C	-12.091855000000	4.802241000000	0.000000000000	C	-12.059864000000	4.782665000000	0.000000000000
C	-11.621585000000	5.919906000000	0.000000000000	C	-11.577088000000	5.900884000000	0.000000000000
C	-12.091855000000	-4.802241000000	0.000000000000	C	-12.059864000000	-4.782665000000	0.000000000000
C	-11.621585000000	-5.919906000000	0.000000000000	C	-11.577088000000	-5.900884000000	0.000000000000
C	-6.434913000000	-11.143962000000	-3.389945000000	C	-6.440222000000	-11.152640000000	-3.388352000000
C	-5.327162000000	-11.713065000000	-2.773698000000	C	-5.327375000000	-11.717045000000	-2.775612000000
C	-7.481973000000	-10.469685000000	-2.773700000000	C	-7.485855000000	-10.471741000000	-2.775633000000
C	-4.200160000000	-12.273847000000	-3.468383000000	C	-4.208823000000	-12.287625000000	-3.471314000000
N	-5.105785000000	-11.760344000000	-1.433563000000	N	-5.097720000000	-11.748876000000	-1.435092000000
C	-8.531473000000	-9.774586000000	-3.468383000000	C	-8.539718000000	-9.789020000000	-3.471330000000
N	-7.633695000000	-10.301692000000	-1.433566000000	N	-7.628359000000	-10.288842000000	-1.435108000000
C	-3.292978000000	-12.622406000000	-2.524200000000	C	-3.296059000000	-12.628457000000	-2.527624000000
H	-4.115016000000	-12.370088000000	-4.541820000000	H	-4.131571000000	-12.400143000000	-4.543620000000
C	-3.879501000000	-12.298919000000	-1.249503000000	C	-3.875581000000	-12.288505000000	-1.256688000000
Zn	-6.375493000000	-11.040966000000	0.000000000000	Zn	-6.371162000000	-11.032894000000	0.000000000000
C	-9.287235000000	-9.163612000000	-2.524198000000	C	-9.291657000000	-9.169438000000	-2.527640000000
H	-8.657401000000	-9.749019000000	-4.541821000000	H	-8.675803000000	-9.778474000000	-4.543635000000
C	-8.713657000000	-9.509534000000	-1.249502000000	C	-8.707254000000	-9.500942000000	-1.256699000000
H	-2.317907000000	-13.064152000000	-2.663641000000	H	-2.325728000000	-13.079443000000	-2.669901000000
C	-3.260508000000	-12.510256000000	0.000000000000	C	-3.250743000000	-12.489117000000	0.000000000000
N	-7.633695000000	-10.301692000000	1.433566000000	N	-7.628359000000	-10.288842000000	1.435108000000
N	-5.105785000000	-11.760344000000	1.433563000000	N	-5.097720000000	-11.748876000000	1.435092000000
H	-10.157638000000	-8.540475000000	-2.663641000000	H	-10.167777000000	-8.555154000000	-2.669912000000
C	-9.206385000000	-9.079380000000	0.000000000000	C	-9.193671000000	-9.060402000000	0.000000000000

C	-3.879501000000	-12.298919000000	1.249503000000	C	-3.875581000000	-12.288505000000	1.256688000000
C	-1.886475000000	-12.869820000000	0.000000000000	C	-1.887143000000	-12.831251000000	0.000000000000
C	-8.713657000000	-9.509534000000	1.249502000000	C	-8.707254000000	-9.500942000000	1.256699000000
C	-7.481973000000	-10.469685000000	2.773700000000	C	-7.485855000000	-10.471741000000	2.775633000000
C	-5.327162000000	-11.713065000000	2.773698000000	C	-5.327375000000	-11.717045000000	2.775612000000
C	-10.205187000000	-8.069577000000	0.000000000000	C	-10.172273000000	-8.051040000000	0.000000000000
C	-3.292978000000	-12.622406000000	2.524200000000	C	-3.296059000000	-12.628457000000	2.527624000000
C	-0.683406000000	-13.021394000000	0.000000000000	C	-0.677339000000	-12.972181000000	0.000000000000
C	-9.287235000000	-9.163612000000	2.524198000000	C	-9.291657000000	-9.169438000000	2.527640000000
C	-8.531473000000	-9.774586000000	3.468383000000	C	-8.539718000000	-9.789020000000	3.471330000000
C	-6.434913000000	-11.143962000000	3.389945000000	C	-6.440222000000	-11.152640000000	3.388352000000
C	-4.200160000000	-12.273847000000	3.468383000000	C	-4.208823000000	-12.287625000000	3.471314000000
C	-10.938082000000	-7.103559000000	0.000000000000	C	-10.899529000000	-7.074011000000	0.000000000000
H	-2.317907000000	-13.064152000000	2.663641000000	H	-2.325728000000	-13.079443000000	2.669901000000
H	-10.157638000000	-8.540475000000	2.663641000000	H	-10.167777000000	-8.555154000000	2.669912000000
H	-8.657401000000	-9.749019000000	4.541821000000	H	-8.675803000000	-9.778474000000	4.543635000000
H	-4.115016000000	-12.370088000000	4.541820000000	H	-4.131571000000	-12.400143000000	4.543620000000
C	10.938082000000	-7.103559000000	0.000000000000	C	10.899529000000	-7.074011000000	0.000000000000
C	11.621585000000	-5.919906000000	0.000000000000	C	11.577088000000	-5.900884000000	0.000000000000
C	10.205187000000	-8.069577000000	0.000000000000	C	10.172273000000	-8.051040000000	0.000000000000
C	12.091855000000	-4.802241000000	0.000000000000	C	12.059864000000	-4.782665000000	0.000000000000
C	9.206385000000	-9.079380000000	0.000000000000	C	9.193671000000	-9.060402000000	0.000000000000
C	12.467162000000	-3.432366000000	0.000000000000	C	12.445041000000	-3.430514000000	0.000000000000
C	8.713657000000	-9.509534000000	-1.249502000000	C	8.707254000000	-9.500942000000	-1.256699000000
C	8.713657000000	-9.509534000000	1.249502000000	C	8.707254000000	-9.500942000000	1.256699000000
C	12.593488000000	-2.790639000000	-1.249501000000	C	12.583610000000	-2.789131000000	-1.256685000000
C	12.593488000000	-2.790639000000	1.249501000000	C	12.583610000000	-2.789131000000	1.256685000000
C	9.287235000000	-9.163612000000	-2.524198000000	C	9.291657000000	-9.169438000000	-2.527640000000
N	7.633695000000	-10.301692000000	-1.433566000000	N	7.628359000000	-10.288842000000	-1.435108000000
C	9.287235000000	-9.163612000000	2.524198000000	C	9.291657000000	-9.169438000000	2.527640000000
N	7.633695000000	-10.301692000000	1.433566000000	N	7.628359000000	-10.288842000000	1.435108000000
N	12.739831000000	-1.459317000000	-1.433550000000	N	12.726928000000	-1.460866000000	-1.435069000000
C	12.580595000000	-3.460322000000	-2.524201000000	C	12.588615000000	-3.460977000000	-2.527627000000
N	12.739831000000	-1.459317000000	1.433550000000	N	12.726928000000	-1.460866000000	1.435069000000
C	12.580595000000	-3.460322000000	2.524201000000	C	12.588615000000	-3.460977000000	2.527627000000
C	8.531473000000	-9.774586000000	-3.468383000000	C	8.539718000000	-9.789020000000	-3.471330000000
H	10.157638000000	-8.540475000000	-2.663641000000	H	10.167777000000	-8.555154000000	-2.669912000000
C	7.481973000000	-10.469685000000	-2.773700000000	C	7.485855000000	-10.471741000000	-2.775633000000
Zn	6.375493000000	-11.040966000000	0.000000000000	Zn	6.371162000000	-11.032894000000	0.000000000000
C	8.531473000000	-9.774586000000	3.468383000000	C	8.539718000000	-9.789020000000	3.471330000000
H	10.157638000000	-8.540475000000	2.663641000000	H	10.167777000000	-8.555154000000	2.669912000000
C	7.481973000000	-10.469685000000	2.773700000000	C	7.485855000000	-10.471741000000	2.775633000000
C	12.809575000000	-1.243931000000	-2.773679000000	C	12.814262000000	-1.246018000000	-2.775578000000
Zn	12.751320000000	0.000000000000	0.000000000000	Zn	12.743192000000	0.000000000000	0.000000000000
C	12.732090000000	-2.500353000000	-3.468377000000	C	12.749609000000	-2.500026000000	-3.471295000000
H	12.475913000000	-4.525658000000	-2.663649000000	H	12.494379000000	-4.526832000000	-2.669918000000
C	12.809575000000	-1.243931000000	2.773679000000	C	12.814262000000	-1.246018000000	2.775578000000
C	12.732090000000	-2.500353000000	3.468377000000	C	12.749609000000	-2.500026000000	3.471295000000
H	12.475913000000	-4.525658000000	2.663649000000	H	12.494379000000	-4.526832000000	2.669918000000
H	8.657401000000	-9.749019000000	-4.541821000000	H	8.675803000000	-9.778474000000	-4.543635000000
C	6.434913000000	-11.143962000000	-3.389945000000	C	6.440222000000	-11.152640000000	-3.388352000000
N	5.105785000000	-11.760344000000	-1.433563000000	N	5.097720000000	-11.748876000000	-1.435092000000
N	5.105785000000	-11.760344000000	1.433563000000	N	5.097720000000	-11.748876000000	1.435092000000
H	8.657401000000	-9.749019000000	4.541821000000	H	8.675803000000	-9.778474000000	4.543635000000
C	6.434913000000	-11.143962000000	3.389945000000	C	6.440222000000	-11.152640000000	3.388352000000
C	12.870342000000	0.000000000000	-3.389917000000	C	12.881595000000	0.000000000000	-3.388296000000
N	12.739831000000	1.459317000000	-1.433550000000	N	12.726928000000	1.460866000000	-1.435069000000
N	12.739831000000	1.459317000000	1.433550000000	N	12.726928000000	1.460866000000	1.435069000000
H	12.772934000000	-2.622199000000	-4.541812000000	H	12.808586000000	-2.623172000000	-4.543594000000
C	12.870342000000	0.000000000000	3.389917000000	C	12.881595000000	0.000000000000	3.388296000000
H	12.772934000000	-2.622199000000	4.541812000000	H	12.808586000000	-2.623172000000	4.543594000000
C	5.327162000000	-11.713065000000	-2.773698000000	C	5.327375000000	-11.717045000000	-2.775612000000
C	3.879501000000	-12.298919000000	-1.249503000000	C	3.875581000000	-12.288505000000	-1.256688000000
C	5.327162000000	-11.713065000000	2.773698000000	C	5.327375000000	-11.717045000000	2.775612000000
C	3.879501000000	-12.298919000000	1.249503000000	C	3.875581000000	-12.288505000000	1.256688000000
C	12.809575000000	1.243931000000	-2.773679000000	C	12.814262000000	1.246018000000	-2.775578000000
C	12.593488000000	2.790639000000	-1.249501000000	C	12.583610000000	2.789131000000	-1.256685000000
C	12.593488000000	2.790639000000	1.249501000000	C	12.583610000000	2.789131000000	1.256685000000
C	12.809575000000	1.243931000000	2.773679000000	C	12.814262000000	1.246018000000	2.775578000000
C	4.200160000000	-12.273847000000	-3.468383000000	C	4.208823000000	-12.287625000000	-3.471314000000
C	3.292978000000	-12.622406000000	-2.524200000000	C	3.296059000000	-12.628457000000	-2.527624000000
C	3.260508000000	-12.510256000000	0.000000000000	C	3.250743000000	-12.489117000000	0.000000000000
C	4.200160000000	-12.273847000000	3.468383000000	C	4.208823000000	-12.287625000000	3.471314000000
C	3.292978000000	-12.622406000000	2.524200000000	C	3.296059000000	-12.628457000000	2.527624000000

C	12.732090000000	2.500353000000	-3.468377000000	C	12.749609000000	2.500026000000	-3.471295000000
C	12.580595000000	3.460322000000	-2.524201000000	C	12.588615000000	3.460977000000	-2.527627000000
C	12.467162000000	3.432366000000	0.000000000000	C	12.445041000000	3.430514000000	0.000000000000
C	12.580595000000	3.460322000000	2.524201000000	C	12.588615000000	3.460977000000	2.527627000000
C	12.732090000000	2.500353000000	3.468377000000	C	12.749609000000	2.500026000000	3.471295000000
H	4.115016000000	-12.370088000000	-4.541820000000	H	4.131571000000	-12.400143000000	-4.543620000000
H	2.317907000000	-13.064152000000	-2.663641000000	H	2.325728000000	-13.079443000000	-2.669901000000
C	1.886475000000	-12.869892000000	0.000000000000	C	1.887143000000	-12.831251000000	0.000000000000
H	4.115016000000	-12.370088000000	4.541820000000	H	4.131571000000	-12.400143000000	4.543620000000
H	2.317907000000	-13.064152000000	2.663641000000	H	2.325728000000	-13.079443000000	2.669901000000
H	12.772934000000	2.622199000000	-4.541812000000	H	12.808586000000	2.623172000000	-4.543594000000
H	12.475913000000	4.525658000000	-2.663649000000	H	12.494379000000	4.526832000000	-2.669918000000
C	12.091855000000	4.802241000000	0.000000000000	C	12.059864000000	4.782665000000	0.000000000000
H	12.475913000000	4.525658000000	2.663649000000	H	12.494379000000	4.526832000000	2.669918000000
H	12.772934000000	2.622199000000	4.541812000000	H	12.808586000000	2.623172000000	4.543594000000
C	0.683406000000	-13.021394000000	0.000000000000	C	0.677339000000	-12.972181000000	0.000000000000
C	11.621585000000	5.919906000000	0.000000000000	C	11.577088000000	5.900884000000	0.000000000000
C	10.938082000000	7.103559000000	0.000000000000	C	10.899529000000	7.074011000000	0.000000000000
C	10.205187000000	8.069577000000	0.000000000000	C	10.172273000000	8.051040000000	0.000000000000
C	9.206385000000	9.079380000000	0.000000000000	C	9.193671000000	9.060402000000	0.000000000000
C	8.713657000000	9.509534000000	1.249502000000	C	8.707254000000	9.500942000000	1.256699000000
C	8.713657000000	9.509534000000	-1.249502000000	C	8.707254000000	9.500942000000	-1.256699000000
C	9.287235000000	9.163612000000	2.524198000000	C	9.291657000000	9.169438000000	2.527640000000
N	7.633695000000	10.301692000000	1.433566000000	N	7.628359000000	10.288842000000	1.435108000000
N	7.633695000000	10.301692000000	-1.433566000000	N	7.628359000000	10.288842000000	-1.435108000000
C	9.287235000000	9.163612000000	-2.524198000000	C	9.291657000000	9.169438000000	-2.527640000000
C	8.531473000000	9.774586000000	3.468383000000	C	8.539718000000	9.789020000000	3.471330000000
H	10.157638000000	8.540475000000	2.663641000000	H	10.167777000000	8.555154000000	2.669912000000
C	7.481973000000	10.469685000000	2.773700000000	C	7.485855000000	10.471741000000	2.775633000000
Zn	6.375493000000	11.040966000000	0.000000000000	Zn	6.371162000000	11.032894000000	0.000000000000
C	7.481973000000	10.469685000000	-2.773700000000	C	7.485855000000	10.471741000000	-2.775633000000
C	8.531473000000	9.774586000000	-3.468383000000	C	8.539718000000	9.789020000000	-3.471330000000
H	10.157638000000	8.540475000000	-2.663641000000	H	10.167777000000	8.555154000000	-2.669912000000
H	8.657401000000	9.749019000000	4.541821000000	H	8.675803000000	9.778474000000	4.543635000000
C	6.434913000000	11.143962000000	3.389945000000	C	6.440222000000	11.152640000000	3.388352000000
N	5.105785000000	11.760344000000	1.433563000000	N	5.097720000000	11.748876000000	1.435092000000
N	5.105785000000	11.760344000000	-1.433563000000	N	5.097720000000	11.748876000000	-1.435092000000
C	6.434913000000	11.143962000000	-3.389945000000	C	6.440222000000	11.152640000000	-3.388352000000
H	8.657401000000	9.749019000000	-4.541821000000	H	8.675803000000	9.778474000000	-4.543635000000
C	5.327162000000	11.713065000000	2.773698000000	C	5.327375000000	11.717045000000	2.775612000000
C	3.879501000000	12.298919000000	1.249503000000	C	3.875581000000	12.288505000000	1.256688000000
C	3.879501000000	12.298919000000	-1.249503000000	C	3.875581000000	12.288505000000	-1.256688000000
C	5.327162000000	11.713065000000	-2.773698000000	C	5.327375000000	11.717045000000	-2.775612000000
C	4.200160000000	12.273847000000	3.468383000000	C	4.208823000000	12.287625000000	3.471314000000
C	3.292978000000	12.622406000000	2.524200000000	C	3.296059000000	12.628457000000	2.527624000000
C	3.260508000000	12.510256000000	0.000000000000	C	3.250743000000	12.489117000000	0.000000000000
C	3.292978000000	12.622406000000	-2.524200000000	C	3.296059000000	12.628457000000	-2.527624000000
C	4.200160000000	12.273847000000	-3.468383000000	C	4.208823000000	12.287625000000	-3.471314000000
H	4.115016000000	12.370088000000	4.541820000000	H	4.131571000000	12.400143000000	4.543620000000
H	2.317907000000	13.064152000000	2.663641000000	H	2.325728000000	13.079443000000	2.669901000000
C	1.886475000000	12.869892000000	0.000000000000	C	1.887143000000	12.831251000000	0.000000000000
H	2.317907000000	13.064152000000	-2.663641000000	H	2.325728000000	13.079443000000	-2.669901000000
H	4.115016000000	12.370088000000	-4.541820000000	H	4.131571000000	12.400143000000	-4.543620000000
C	0.683406000000	13.021394000000	0.000000000000	C	0.677339000000	12.972181000000	0.000000000000
C	-0.683406000000	13.021394000000	0.000000000000	C	-0.677339000000	12.972181000000	0.000000000000
C	-1.886475000000	12.869892000000	0.000000000000	C	-1.887143000000	12.831251000000	0.000000000000
C	-3.260508000000	12.510256000000	0.000000000000	C	-3.250743000000	12.489117000000	0.000000000000
C	-3.879501000000	12.298919000000	1.249503000000	C	-3.875581000000	12.288505000000	1.256688000000
C	-3.879501000000	12.298919000000	-1.249503000000	C	-3.875581000000	12.288505000000	-1.256688000000
C	-3.292978000000	12.622406000000	2.524200000000	C	-3.296059000000	12.628457000000	2.527624000000
N	-5.105785000000	11.760344000000	1.433563000000	N	-5.097720000000	11.748876000000	1.435092000000
N	-5.105785000000	11.760344000000	-1.433563000000	N	-5.097720000000	11.748876000000	-1.435092000000
C	-3.292978000000	12.622406000000	-2.524200000000	C	-3.296059000000	12.628457000000	-2.527624000000
C	-4.200160000000	12.273847000000	3.468383000000	C	-4.208823000000	12.287625000000	3.471314000000
H	-2.317907000000	13.064152000000	2.663641000000	H	-2.325728000000	13.079443000000	2.669901000000
C	-5.327162000000	11.713065000000	2.773698000000	C	-5.327375000000	11.717045000000	2.775612000000
Zn	-6.375493000000	11.040966000000	0.000000000000	Zn	-6.371162000000	11.032894000000	0.000000000000
C	-5.327162000000	11.713065000000	-2.773698000000	C	-5.327375000000	11.717045000000	-2.775612000000
C	-4.200160000000	12.273847000000	-3.468383000000	C	-4.208823000000	12.287625000000	-3.471314000000
H	-2.317907000000	13.064152000000	-2.663641000000	H	-2.325728000000	13.079443000000	-2.669901000000
H	-4.115016000000	12.370088000000	4.541820000000	H	-4.131571000000	12.400143000000	4.543620000000
C	-6.434913000000	11.143962000000	3.389945000000	C	-6.440222000000	11.152640000000	3.388352000000
N	-7.633695000000	10.301692000000	1.433566000000	N	-7.628359000000	10.288842000000	1.435108000000
N	-7.633695000000	10.301692000000	-1.433566000000	N	-7.628359000000	10.288842000000	-1.435108000000

C	-6.434913000000	11.143962000000	-3.389945000000	C	-6.440222000000	11.152640000000	-3.388352000000
H	-4.115016000000	12.370088000000	-4.541820000000	H	-4.131571000000	12.400143000000	-4.543620000000
C	-7.481973000000	10.469685000000	2.773700000000	C	-7.485855000000	10.471741000000	2.775633000000
C	-8.713657000000	9.509534000000	1.249502000000	C	-8.707254000000	9.500942000000	1.256699000000
C	-8.713657000000	9.509534000000	-1.249502000000	C	-8.707254000000	9.500942000000	-1.256699000000
C	-7.481973000000	10.469685000000	-2.773700000000	C	-7.485855000000	10.471741000000	-2.775633000000
C	-8.531473000000	9.774586000000	3.468383000000	C	-8.539718000000	9.789020000000	3.471330000000
C	-9.287235000000	9.163612000000	2.524198000000	C	-9.291657000000	9.169438000000	2.527640000000
C	-9.206385000000	9.079380000000	0.000000000000	C	-9.193671000000	9.060402000000	0.000000000000
C	-9.287235000000	9.163612000000	-2.524198000000	C	-9.291657000000	9.169438000000	-2.527640000000
C	-8.531473000000	9.774586000000	-3.468383000000	C	-8.539718000000	9.789020000000	-3.471330000000
H	-8.657401000000	9.749019000000	4.541821000000	H	-8.675803000000	9.778474000000	4.543635000000
H	-10.157638000000	8.540475000000	2.663641000000	H	-10.167777000000	8.555154000000	2.669912000000
C	-10.205187000000	8.069577000000	0.000000000000	C	-10.172273000000	8.051040000000	0.000000000000
H	-10.157638000000	8.540475000000	-2.663641000000	H	-10.167777000000	8.555154000000	-2.669912000000
H	-8.657401000000	9.749019000000	-4.541821000000	H	-8.675803000000	9.778474000000	-4.543635000000
C	-10.938082000000	7.103559000000	0.000000000000	C	-10.899529000000	7.074011000000	0.000000000000
H	-6.456196000000	-11.180850000000	-4.473044000000	H	-6.470866000000	-11.205779000000	-4.470644000000
H	6.456196000000	-11.180850000000	-4.473044000000	H	6.470866000000	-11.205779000000	-4.470644000000
H	12.913097000000	0.000000000000	-4.473019000000	H	12.943131000000	0.000000000000	-4.470605000000
H	6.456196000000	11.180850000000	-4.473044000000	H	6.470866000000	11.205779000000	-4.470644000000
H	-6.456196000000	11.180850000000	-4.473044000000	H	-6.470866000000	11.205779000000	-4.470644000000
H	-12.913097000000	0.000000000000	-4.473019000000	H	-12.943131000000	0.000000000000	-4.470605000000
H	6.456196000000	11.180850000000	4.473044000000	H	6.470866000000	11.205779000000	4.470644000000
H	12.913097000000	0.000000000000	4.473019000000	H	12.943131000000	0.000000000000	4.470605000000
H	6.456196000000	-11.180850000000	4.473044000000	H	6.470866000000	-11.205779000000	4.470644000000
H	-6.456196000000	-11.180850000000	4.473044000000	H	-6.470866000000	-11.205779000000	4.470644000000
H	-12.913097000000	0.000000000000	4.473019000000	H	-12.943131000000	0.000000000000	4.470605000000
H	-6.456196000000	11.180850000000	4.473044000000	H	-6.470866000000	11.205779000000	4.470644000000
c-P6⁴⁺				c-P6⁶⁺			
C	-13.165591000000	2.786868000000	1.271611000000	C	10.837819000000	-6.649518000000	1.256402000000
C	-13.217885000000	3.462359000000	2.530813000000	C	10.602696000000	-7.274376000000	2.522283000000
C	-13.419432000000	2.499277000000	3.472234000000	C	11.155455000000	-6.460187000000	3.464436000000
C	-13.458800000000	1.251407000000	2.776680000000	C	11.691813000000	-5.339217000000	2.761773000000
N	-13.317448000000	1.465507000000	1.436485000000	N	11.501217000000	-5.478589000000	1.434850000000
H	-13.134654000000	4.528596000000	2.677471000000	H	10.104988000000	-8.220155000000	2.674094000000
H	-13.524462000000	2.626647000000	4.540543000000	H	11.190121000000	-6.609402000000	4.534363000000
C	-13.550250000000	0.000572000000	3.379549000000	C	12.285481000000	-4.213945000000	3.380175000000
C	-13.458850000000	-1.250242000000	2.776655000000	C	12.694812000000	-3.046597000000	2.787737000000
C	-13.419537000000	-2.498136000000	3.472176000000	C	13.179308000000	-1.882191000000	3.479578000000
N	-13.317495000000	-1.464320000000	1.436449000000	N	12.635572000000	-2.777093000000	1.435446000000
C	-13.218023000000	-3.461201000000	2.530733000000	C	13.369411000000	-0.921548000000	2.542445000000
H	-13.524579000000	-2.625530000000	4.540481000000	H	13.346168000000	-1.812924000000	4.545625000000
C	-13.165693000000	-2.785676000000	1.271547000000	C	13.026603000000	-1.519887000000	1.280585000000
H	-13.134838000000	-4.527445000000	2.677363000000	H	13.730889000000	0.085561000000	2.685827000000
C	-12.969961000000	-3.426537000000	0.000158000000	C	13.082798000000	-0.840984000000	-0.001138000000
C	-13.165641000000	-2.785643000000	-1.271224000000	C	13.026454000000	-1.520061000000	-1.282765000000
C	-13.217921000000	-3.461138000000	-2.530428000000	C	13.369128000000	-0.921892000000	-2.544744000000
N	-13.317435000000	-1.464284000000	-1.436099000000	N	12.635402000000	-2.777285000000	-1.437411000000
C	-13.419396000000	-2.498050000000	-3.471855000000	C	13.178921000000	-1.882661000000	-3.481725000000
H	-13.134732000000	-4.527379000000	-2.677081000000	H	13.730592000000	0.085196000000	-2.688301000000
C	-13.458736000000	-1.250173000000	-2.776306000000	C	12.694496000000	-3.046973000000	-2.789673000000
H	-13.524395000000	-2.625417000000	-4.540168000000	H	13.345666000000	-1.813539000000	-4.547799000000
C	-13.550111000000	0.000657000000	-3.379172000000	C	12.285102000000	-4.214401000000	-3.381906000000
C	-13.458686000000	1.251476000000	-2.776268000000	C	11.691499000000	-5.339589000000	-2.763283000000
C	-13.419291000000	2.499364000000	-3.471788000000	C	11.155052000000	-6.460648000000	-3.465737000000
N	-13.317388000000	1.465543000000	-1.436061000000	N	11.501060000000	-5.478785000000	-1.436321000000
C	-13.217783000000	3.462423000000	-2.530335000000	C	10.602399000000	-7.274709000000	-2.523412000000
H	-13.524277000000	2.626762000000	-4.540098000000	H	11.189594000000	-6.610004000000	-4.535649000000
C	-13.165538000000	2.786899000000	-1.271148000000	C	10.837674000000	-6.649688000000	-1.257639000000
H	-13.134548000000	4.528663000000	-2.676962000000	H	10.104667000000	-8.220504000000	-2.675041000000
C	-12.969849000000	3.427751000000	0.000243000000	C	10.458925000000	-7.175317000000	-0.000562000000
Zn	-13.329759000000	0.000616000000	0.000193000000	Zn	12.082351000000	-4.148021000000	-0.000855000000
C	-12.509345000000	4.723327000000	0.000269000000	C	9.585255000000	-8.292837000000	-0.000433000000
C	-11.925962000000	5.809518000000	0.000274000000	C	8.733407000000	-9.156284000000	-0.000295000000
C	-12.509461000000	-4.722100000000	0.000150000000	C	13.117002000000	0.512707000000	-0.001234000000
C	-11.926091000000	-5.808308000000	0.000134000000	C	13.001225000000	1.755488000000	-0.001301000000
C	-6.547599000000	-10.754634000000	-3.388384000000	C	9.943482000000	8.354302000000	-3.382564000000
C	-5.385394000000	-11.247132000000	-2.768267000000	C	8.984547000000	9.190359000000	-2.764047000000
C	-7.622945000000	-10.143855000000	-2.786635000000	C	10.745739000000	7.412636000000	-2.790211000000
C	-4.242920000000	-11.750298000000	-3.467698000000	C	8.080441000000	10.042991000000	-3.466615000000
N	-5.159305000000	-11.257454000000	-1.436625000000	N	8.756735000000	9.251789000000	-1.437101000000
C	-8.732836000000	-9.544832000000	-3.480491000000	C	11.616979000000	6.500822000000	-3.482135000000
N	-7.773801000000	-9.946537000000	-1.435865000000	N	10.787667000000	7.139893000000	-1.437921000000

C	-3.307691000000	-12.036699000000	-2.523255000000	C	7.271707000000	10.603544000000	-2.524370000000
H	-4.162803000000	-11.863508000000	-4.539566000000	H	8.058913000000	10.194656000000	-4.536543000000
C	-3.901284000000	-11.729510000000	-1.254928000000	C	7.716215000000	10.105291000000	-1.258534000000
Zn	-6.470203000000	-10.623484000000	-0.000101000000	Zn	9.778130000000	8.219709000000	-0.001497000000
C	-9.516212000000	-8.967660000000	-2.539773000000	C	12.140340000000	5.673076000000	-2.545051000000
H	-8.881329000000	-9.562240000000	-4.551150000000	H	11.797495000000	6.496295000000	-4.548197000000
C	-8.894413000000	-9.241996000000	-1.268372000000	C	11.605179000000	6.107825000000	-1.283141000000
H	-2.315112000000	-12.434796000000	-2.669681000000	H	6.466801000000	11.306653000000	-2.676094000000
C	-3.275418000000	-11.898493000000	-0.000170000000	C	7.173568000000	10.459412000000	-0.001512000000
N	-7.773803000000	-9.946696000000	1.435737000000	N	10.787789000000	7.140049000000	1.434950000000
N	-5.159307000000	-11.257614000000	1.436355000000	N	8.756851000000	9.251941000000	1.434075000000
H	-10.437493000000	-8.423546000000	-2.682238000000	H	12.840209000000	4.863695000000	-2.688505000000
C	-9.405735000000	-8.815020000000	-0.000030000000	C	11.902198000000	5.494700000000	-0.001444000000
C	-3.901286000000	-11.729649000000	1.254606000000	C	7.716326000000	10.105431000000	1.255506000000
C	-1.889752000000	-12.199056000000	-0.000186000000	C	5.956124000000	11.187410000000	-0.001500000000
C	-8.894415000000	-9.242137000000	1.268320000000	C	11.605283000000	6.107956000000	1.280213000000
C	-7.622948000000	-10.144164000000	2.786485000000	C	10.745972000000	7.412931000000	2.787212000000
C	-5.385398000000	-11.247439000000	2.767997000000	C	8.984786000000	9.190661000000	2.761011000000
C	-10.403869000000	-7.863596000000	0.000490000000	C	12.421595000000	4.244149000000	-0.001406000000
C	-3.307694000000	-12.036981000000	2.522900000000	C	7.271938000000	10.603836000000	2.521324000000
C	-0.682600000000	-12.315001000000	-0.000184000000	C	4.850501000000	11.686185000000	-0.001462000000
C	-9.516215000000	-8.967941000000	2.539751000000	C	12.140539000000	5.673334000000	2.542125000000
C	-8.732840000000	-9.545218000000	3.480406000000	C	11.617256000000	6.501183000000	3.479162000000
C	-6.547603000000	-10.755010000000	3.388167000000	C	9.943767000000	8.354667000000	3.379532000000
C	-4.242925000000	-11.750685000000	3.467373000000	C	8.080753000000	10.043383000000	3.463561000000
C	-11.200628000000	-6.923152000000	0.000092000000	C	12.761253000000	3.043090000000	-0.001363000000
H	-2.315116000000	-12.435094000000	2.669282000000	H	6.467053000000	11.306970000000	2.673040000000
H	-10.437496000000	-8.423844000000	2.682276000000	H	12.840412000000	4.863963000000	2.685610000000
H	-8.881335000000	-9.562745000000	4.551063000000	H	11.797856000000	6.496765000000	4.545211000000
H	-4.162809000000	-11.864014000000	4.539229000000	H	8.059322000000	10.195172000000	4.533474000000
C	11.200085000000	-6.924099000000	0.000238000000	C	-8.020316000000	10.379792000000	-0.000264000000
C	11.925718000000	-5.809349000000	0.000222000000	C	-9.015695000000	9.528488000000	-0.000027000000
C	10.403190000000	-7.864415000000	0.000241000000	C	-7.001743000000	11.101187000000	-0.000468000000
C	12.509164000000	-4.723192000000	0.000206000000	C	-9.886314000000	8.634101000000	0.000196000000
C	9.404917000000	-8.815717000000	0.000176000000	C	-5.812264000000	11.748327000000	-0.000575000000
C	12.969729000000	-3.427637000000	0.000210000000	C	-10.709952000000	7.559265000000	0.000386000000
C	8.893569000000	-9.242627000000	-1.268192000000	C	-5.196244000000	12.039123000000	-1.282309000000
C	8.893523000000	-9.242754000000	1.268484000000	C	-5.196006000000	12.039114000000	1.281043000000
C	13.165537000000	-2.786799000000	-1.271170000000	C	-11.092849000000	6.995495000000	-1.281194000000
C	13.165397000000	-2.786755000000	1.271589000000	C	-11.092526000000	6.995700000000	1.282150000000
C	9.515404000000	-8.968337000000	-2.539587000000	C	-5.885847000000	12.036759000000	-2.544161000000
N	7.772891000000	-9.947069000000	-1.435710000000	N	-3.911992000000	12.329232000000	-1.437184000000
C	9.515312000000	-8.968591000000	2.539929000000	C	-5.885365000000	12.036728000000	2.543024000000
N	7.772839000000	-9.947212000000	1.435890000000	N	-3.911725000000	12.329239000000	1.435678000000
N	13.317456000000	-1.465449000000	-1.436078000000	N	-11.578269000000	5.771600000000	-1.435790000000
C	13.217849000000	-3.462330000000	-2.530350000000	C	-10.984053000000	7.676225000000	-2.543175000000
N	13.317298000000	-1.465400000000	1.436468000000	N	-11.577919000000	5.771830000000	1.437049000000
C	13.217569000000	-3.462243000000	2.530799000000	C	-10.983399000000	7.676623000000	2.543995000000
C	8.731985000000	-9.545427000000	-3.480319000000	C	-4.958908000000	12.352568000000	-3.481304000000
H	10.436735000000	-8.424304000000	-2.682038000000	H	-6.938745000000	11.846126000000	-2.687534000000
C	7.622034000000	-10.144359000000	-2.786478000000	C	-3.708267000000	12.515338000000	-2.789477000000
Zn	6.469212000000	-10.623892000000	0.000032000000	Zn	-2.448163000000	12.535919000000	-0.000882000000
C	8.731858000000	-9.545774000000	3.480574000000	C	-4.958249000000	12.352541000000	3.479994000000
H	10.436637000000	-8.424572000000	2.682468000000	H	-6.938234000000	11.846083000000	2.686597000000
C	7.621932000000	-10.144636000000	2.786633000000	C	-3.707746000000	12.515333000000	2.787931000000
C	13.458860000000	-1.251395000000	-2.776275000000	C	-11.793910000000	5.598902000000	-2.788004000000
Zn	13.329782000000	-0.000518000000	0.000171000000	Zn	-12.008643000000	4.357590000000	0.000807000000
C	13.419462000000	-2.499284000000	-3.471793000000	C	-11.439715000000	6.809185000000	-3.480088000000
H	13.134581000000	-4.528568000000	-2.676979000000	H	-10.632806000000	8.686916000000	-2.686778000000
C	13.458554000000	-1.251299000000	2.776674000000	C	-11.793215000000	5.599347000000	2.789353000000
C	13.419078000000	-2.499164000000	3.472231000000	C	-11.438831000000	6.809731000000	3.481160000000
H	13.134285000000	-4.528475000000	2.677455000000	H	-10.632103000000	8.687332000000	2.687353000000
H	8.880486000000	-9.562837000000	-4.550976000000	H	-5.102351000000	12.462445000000	-4.547345000000
C	6.546642000000	-10.755043000000	-3.388250000000	C	-2.492707000000	12.744771000000	-3.381932000000
N	5.158281000000	-11.257753000000	-1.436513000000	N	-1.005350000000	12.698296000000	-1.436609000000
N	5.158228000000	-11.257896000000	1.436466000000	N	-1.005080000000	12.698291000000	1.434562000000
H	8.880320000000	-9.563292000000	4.551235000000	H	-5.101491000000	12.462404000000	4.546065000000
C	6.546518000000	-10.755381000000	3.388305000000	C	-2.492072000000	12.744770000000	3.380161000000
C	13.550380000000	-0.000582000000	-3.379179000000	C	-12.208720000000	4.433364000000	-3.380193000000
N	13.317623000000	1.464377000000	-1.436129000000	N	-12.392396000000	2.957001000000	-1.434611000000
N	13.317465000000	1.464427000000	1.436418000000	N	-12.392040000000	2.957226000000	1.436534000000
H	13.524521000000	-2.626690000000	-4.540095000000	H	-11.526287000000	6.967743000000	-4.546137000000
C	13.550009000000	-0.000464000000	3.379544000000	C	-12.207886000000	4.433903000000	3.381833000000
H	13.524018000000	-2.626533000000	4.540549000000	H	-11.525127000000	6.968456000000	4.547206000000

C	5.384394000000	-11.247445000000	-2.768153000000	C	-1.221365000000	12.793567000000	-2.763530000000
C	3.900222000000	-11.729710000000	-1.254836000000	C	0.340410000000	12.709448000000	-1.258166000000
C	5.384292000000	-11.247721000000	2.768115000000	C	-1.220850000000	12.793578000000	2.761527000000
C	3.900176000000	-11.729836000000	1.254696000000	C	0.340641000000	12.709459000000	1.255872000000
C	13.459013000000	1.250254000000	-2.776325000000	C	-12.453405000000	3.184956000000	-2.761556000000
C	13.165864000000	2.785743000000	-1.271272000000	C	-12.611496000000	1.629188000000	-1.255924000000
C	13.165725000000	2.785788000000	1.271499000000	C	-12.611197000000	1.629392000000	1.258114000000
C	13.458709000000	1.250351000000	2.776637000000	C	-12.452734000000	3.185400000000	2.763460000000
C	4.241887000000	-11.750521000000	-3.467602000000	C	0.017580000000	12.889736000000	-3.466207000000
C	3.306623000000	-12.036852000000	-2.523176000000	C	0.999084000000	12.818330000000	-2.524057000000
C	3.274323000000	-11.898647000000	-0.000090000000	C	0.985221000000	12.644303000000	-0.001209000000
C	4.241759000000	-11.750867000000	3.467472000000	C	0.018226000000	12.889771000000	3.463968000000
C	3.306531000000	-12.037104000000	2.522984000000	C	0.999555000000	12.818368000000	2.521633000000
C	13.419775000000	2.498130000000	-3.471883000000	C	-12.740194000000	1.975685000000	-3.463984000000
C	13.218273000000	3.461231000000	-2.530475000000	C	-12.821218000000	0.995083000000	-2.521670000000
C	12.970108000000	3.426649000000	0.000091000000	C	-12.646671000000	0.982267000000	0.001148000000
C	13.217998000000	3.461319000000	2.530683000000	C	-12.820630000000	0.995493000000	2.524010000000
C	13.419396000000	2.498250000000	3.472147000000	C	-12.739374000000	1.976247000000	3.466149000000
H	4.161778000000	-11.863722000000	-4.539472000000	H	0.129451000000	12.994341000000	-4.536140000000
H	2.314016000000	-12.434871000000	-2.669617000000	H	2.066998000000	12.860364000000	-2.675881000000
C	1.888632000000	-12.199107000000	-0.000130000000	C	2.389864000000	12.446504000000	-0.001331000000
H	4.161611000000	-11.864174000000	4.539328000000	H	0.130299000000	12.994388000000	4.533878000000
H	2.313918000000	-12.435137000000	2.669349000000	H	2.067497000000	12.860417000000	2.673255000000
H	13.524859000000	2.625488000000	-4.540188000000	H	-12.861091000000	1.881182000000	-4.533874000000
H	13.135140000000	4.527474000000	-2.677138000000	H	-13.027947000000	-0.053503000000	-2.673289000000
C	12.509661000000	4.722231000000	0.000043000000	C	-12.668531000000	-0.436064000000	0.001264000000
H	13.134850000000	4.527567000000	2.677301000000	H	-13.027338000000	-0.053065000000	2.675847000000
H	13.524363000000	2.625646000000	4.540459000000	H	-12.860021000000	1.881917000000	4.536082000000
C	0.681477000000	-12.315015000000	-0.000155000000	C	3.563556000000	12.140513000000	-0.001400000000
C	11.926343000000	5.808467000000	0.000005000000	C	-12.547770100000	-1.642954000000	0.001349000000
C	11.200836000000	6.923281000000	-0.000037000000	C	-12.297768000000	-2.984657000000	0.001453000000
C	10.404022000000	7.863677000000	-0.000071000000	C	-11.975860000000	-4.154082000000	0.001533000000
C	9.405851000000	8.815061000000	-0.000116000000	C	-11.444688000000	-5.469378000000	0.001593000000
C	8.894505000000	9.242141000000	1.268208000000	C	-11.178627000000	-6.060164000000	1.258640000000
C	8.894524000000	9.242037000000	-1.268483000000	C	-11.178817000000	-6.060357000000	-1.255397000000
C	9.516307000000	8.967953000000	2.539640000000	C	-11.602377000000	-5.544092000000	2.524454000000
N	7.773865000000	9.946654000000	1.435626000000	N	-10.495968000000	-7.219945000000	1.437230000000
N	7.773887000000	9.946537000000	-1.435976000000	N	-10.496199000000	-7.220180000000	-1.433914000000
C	9.516346000000	8.967745000000	-2.539883000000	C	-11.602736000000	-5.544471000000	-2.521233000000
C	8.732900000000	9.545183000000	3.480297000000	C	-11.173420000000	-6.429668000000	3.466718000000
H	10.437608000000	8.423890000000	2.682164000000	H	-12.172851000000	-4.640321000000	2.676156000000
C	7.622993000000	10.144099000000	2.786375000000	C	-10.470505000000	-7.454528000000	2.764179000000
Zn	6.470250000000	10.623411000000	-0.000213000000	Zn	-9.633835000000	-8.388384000000	0.001689000000
C	7.623035000000	10.143869000000	-2.786744000000	C	-10.470927000000	-7.454960000000	-2.760826000000
C	8.732953000000	9.544897000000	-3.480600000000	C	-11.173926000000	-6.430196000000	-3.463423000000
H	10.437649000000	8.423671000000	-2.682348000000	H	-12.173215000000	-4.640713000000	-2.672992000000
H	8.881386000000	9.562700000000	4.550955000000	H	-11.320019000000	-6.385001000000	4.536636000000
C	6.547620000000	10.754896000000	3.388057000000	C	-9.792485000000	-8.531007000000	3.382710000000
N	5.159320000000	11.257473000000	1.436241000000	N	-8.722758000000	-9.552442000000	1.438115000000
N	5.159341000000	11.257353000000	-1.436739000000	N	-8.722971000000	-9.552659000000	-1.434707000000
C	6.547671000000	10.754616000000	-3.388493000000	C	-9.793007000000	-8.531544000000	-3.379297000000
H	8.881455000000	9.562325000000	-4.551257000000	H	-11.320674000000	-6.385689000000	-4.533327000000
C	5.385400000000	11.247289000000	2.767884000000	C	-8.985846000000	-9.468948000000	2.790388000000
C	3.901282000000	11.729463000000	1.254489000000	C	-7.829159000000	-10.519392000000	1.283381000000
C	3.901300000000	11.729358000000	-1.255045000000	C	-7.829361000000	-10.519592000000	-1.279958000000
C	5.385442000000	11.247060000000	-2.768378000000	C	-8.986279000000	-9.469388000000	-2.786953000000
C	4.242903000000	11.750483000000	3.467258000000	C	-8.219376000000	-10.470406000000	3.482357000000
C	3.307670000000	12.036759000000	2.522782000000	C	-7.482223000000	-11.115197000000	2.545314000000
C	3.275417000000	11.898299000000	-0.000290000000	C	-7.269221000000	-10.907516000000	0.001699000000
C	3.307708000000	12.036549000000	-2.523372000000	C	-7.482634000000	-11.115614000000	-2.541850000000
C	4.242955000000	11.750196000000	-3.467811000000	C	-8.219929000000	-10.470972000000	-3.478880000000
H	4.162776000000	11.863796000000	4.539115000000	H	-8.242804000000	-10.649450000000	4.548419000000
H	2.315076000000	12.434835000000	2.669162000000	H	-6.790509000000	-11.931550000000	2.688808000000
C	1.889741000000	12.198819000000	-0.000313000000	C	-6.113813000000	-11.613689000000	0.001657000000
H	2.315116000000	12.434613000000	-2.669800000000	H	-6.790953000000	-11.932000000000	-2.685318000000
H	4.162844000000	11.863420000000	-4.539678000000	H	-8.243532000000	-10.650193000000	-4.544908000000
C	0.682590000000	12.314763000000	-0.000326000000	C	-4.979591000000	-12.134692000000	0.001594000000
C	-0.681488000000	12.314819000000	-0.000312000000	C	-3.744515000000	-12.570679000000	0.001489000000
C	-1.888644000000	12.198924000000	-0.000295000000	C	-2.534549000000	-12.877085000000	0.001372000000
C	-3.274342000000	11.898495000000	-0.000245000000	C	-1.191872000000	-13.052756000000	0.001233000000
C	-3.900195000000	11.729717000000	1.254546000000	C	-0.512205000000	-13.102225000000	1.282829000000
C	-3.900254000000	11.729574000000	-1.254987000000	C	-0.512509000000	-13.102459000000	-1.280517000000
C	-3.306533000000	12.036977000000	2.522828000000	C	-1.156175000000	-13.348105000000	2.544838000000
N	-5.158262000000	11.257822000000	1.436326000000	N	0.790438000000	-12.910699000000	1.437410000000

N	-5.158330000000	11.257659000000	-1.436654000000	N	0.790093000000	-12.910953000000	-1.435446000000
C	-3.306652000000	12.036688000000	-2.523332000000	C	-1.156780000000	-13.348580000000	-2.542328000000
C	-4.241768000000	11.750782000000	3.467323000000	C	-0.177485000000	-13.309095000000	3.481767000000
H	-2.313906000000	12.434978000000	2.669185000000	H	-2.207099000000	-13.549170000000	2.688449000000
C	-5.384321000000	11.247668000000	2.767976000000	C	1.047780000000	-13.010891000000	2.789657000000
Zn	-6.469274000000	10.623851000000	-0.000097000000	Zn	2.230254000000	-12.576840000000	0.000784000000
C	-5.384452000000	11.247351000000	-2.768292000000	C	1.047115000000	-13.011395000000	-2.787737000000
C	-4.241931000000	11.750384000000	-3.467750000000	C	-0.178316000000	-13.309737000000	-3.479499000000
H	-2.314032000000	12.434671000000	-2.669782000000	H	-2.207737000000	-13.549677000000	-2.685649000000
H	-4.161611000000	11.864098000000	4.539177000000	H	-0.271545000000	-13.463151000000	4.547841000000
C	-6.546561000000	10.755374000000	3.388175000000	C	2.264586000000	-12.787372000000	3.381829000000
N	-7.772919000000	9.947231000000	1.435773000000	N	3.635091000000	-12.208785000000	1.436160000000
N	-7.772986000000	9.947066000000	-1.435827000000	N	3.634746000000	-12.209048000000	-1.435001000000
C	-6.546721000000	10.754985000000	-3.388379000000	C	2.263775000000	-12.787980000000	-3.380239000000
H	-4.161825000000	11.863575000000	-4.539622000000	H	-0.272629000000	-13.463992000000	-4.545521000000
C	-7.622000000000	10.144662000000	2.786513000000	C	3.468134000000	-12.375313000000	2.763136000000
C	-8.893630000000	9.242813000000	1.268377000000	C	4.894601000000	-11.734758000000	1.257405000000
C	-8.893689000000	9.242668000000	-1.268298000000	C	4.894298000000	-11.734977000000	-1.256633000000
C	-7.622131000000	10.144343000000	-2.786597000000	C	3.467471000000	-12.375802000000	-2.761905000000
C	-8.731945000000	9.545848000000	3.480464000000	C	4.658803000000	-12.019008000000	3.465519000000
C	-9.515423000000	8.968683000000	2.539827000000	C	5.548595000000	-11.599133000000	2.523137000000
C	-9.405045000000	8.815785000000	0.000076000000	C	5.472456000000	-11.441971000000	0.000288000000
C	-9.515542000000	8.968392000000	-2.539688000000	C	5.547981000000	-11.599561000000	-2.522547000000
C	-8.732109000000	9.545449000000	-3.480427000000	C	4.657965000000	-12.019604000000	-3.464640000000
H	-8.880403000000	9.563382000000	4.551125000000	H	4.801069000000	-12.076246000000	4.535423000000
H	-10.436767000000	8.424700000000	2.682375000000	H	6.560080000000	-11.253910000000	2.674710000000
C	-10.403354000000	7.864522000000	0.000154000000	C	6.711709000000	-10.751755000000	0.000078000000
H	-10.436893000000	8.424393000000	-2.682130000000	H	6.559427000000	-11.254353000000	-2.674425000000
H	-8.880616000000	9.562859000000	-4.551084000000	H	4.799971000000	-12.077024000000	-4.534569000000
C	-11.200294000000	6.924244000000	0.000216000000	C	7.696475000000	-10.043646000000	-0.000103000000
H	-6.576325000000	-10.826715000000	-4.469738000000	H	10.020772000000	8.442813000000	-4.460803000000
H	6.575377000000	-10.827116000000	-4.469605000000	H	-2.497402000000	12.862252000000	-4.460164000000
H	13.661637000000	-0.000609000000	-4.458176000000	H	-12.324276000000	4.456015000000	-4.458411000000
H	6.576404000000	10.826715000000	-4.469846000000	H	-9.892599000000	-8.594421000000	-4.457508000000
H	-6.575461000000	10.827055000000	-4.469734000000	H	2.301664000000	-12.899388000000	-4.458462000000
H	-13.661288000000	0.000675000000	-4.458178000000	H	12.389065000000	-4.269242000000	-4.460146000000
H	6.576337000000	10.827084000000	4.469405000000	H	-9.891905000000	-8.593715000000	4.460947000000
H	13.661147000000	-0.000455000000	4.458554000000	H	-12.323171000000	4.456730000000	4.460076000000
H	6.575214000000	-10.827562000000	4.469653000000	H	-2.496570000000	12.862246000000	4.458395000000
H	-6.576331000000	-10.827212000000	4.469513000000	H	10.021151000000	8.443292000000	4.457756000000
H	-13.661471000000	0.000563000000	4.458551000000	H	12.389561000000	-4.268637000000	4.458412000000
H	-6.575250000000	10.827568000000	4.469522000000	H	2.302730000000	-12.898586000000	4.460063000000
c-Iso6				c-Iso6²⁺			
C	-12.748002000000	2.861773000000	1.255885000000	C	-12.745891000000	2.853899000000	1.256923000000
C	-12.767369000000	3.480700000000	2.521566000000	C	-12.795519000000	3.475913000000	2.516573000000
C	-12.975255000000	2.476733000000	3.435255000000	C	-13.027865000000	2.475923000000	3.429277000000
C	-13.058430000000	1.270835000000	2.729649000000	C	-13.090809000000	2.269162000000	2.721874000000
O	-12.927014000000	1.549142000000	1.396406000000	O	-12.927264000000	1.540820000000	1.395532000000
H	-12.649442000000	4.538021000000	2.693929000000	H	-12.687088000000	4.534356000000	2.689819000000
H	-13.048738000000	2.567532000000	4.509950000000	H	-13.133151000000	2.570514000000	4.500790000000
C	-13.132372000000	0.000000000000	3.259525000000	C	-13.183252000000	0.000000000000	3.254589000000
C	-13.058430000000	-1.270835000000	2.729649000000	C	-13.090809000000	-1.269162000000	2.721874000000
C	-12.975255000000	-2.476733000000	3.435255000000	C	-13.027865000000	-2.475923000000	3.429277000000
O	-12.927014000000	-1.549142000000	1.396406000000	O	-12.927264000000	-1.540820000000	1.395532000000
C	-12.767369000000	-3.480700000000	2.521566000000	C	-12.795519000000	-3.475913000000	2.516573000000
H	-13.048738000000	-2.567532000000	4.509950000000	H	-13.133151000000	-2.570514000000	4.500790000000
C	-12.748002000000	-2.861773000000	1.255885000000	C	-12.745891000000	-2.853899000000	1.256923000000
H	-12.649442000000	-4.538021000000	2.693929000000	H	-12.687088000000	-4.534356000000	2.689819000000
C	-12.578022000000	-3.480734000000	0.000000000000	C	-12.552600000000	-3.470651000000	0.000000000000
C	-12.748002000000	-2.861773000000	-1.255885000000	C	-12.745891000000	-2.853899000000	-1.256923000000
C	-12.767369000000	-3.480700000000	-2.521566000000	C	-12.795519000000	-3.475913000000	-2.516573000000
O	-12.927014000000	-1.549142000000	-1.396406000000	O	-12.927264000000	-1.540820000000	-1.395532000000
C	-12.975255000000	-2.476733000000	-3.435255000000	C	-13.027865000000	-2.475923000000	-3.429277000000
H	-12.649442000000	-4.538021000000	-2.693929000000	H	-12.687088000000	-4.534356000000	-2.689819000000
C	-13.058430000000	-1.270835000000	-2.729649000000	C	-13.090809000000	-1.269162000000	-2.721874000000
H	-13.048738000000	-2.567532000000	-4.509950000000	H	-13.133151000000	-2.570514000000	-4.500790000000
C	-13.132372000000	0.000000000000	-3.259525000000	C	-13.183252000000	0.000000000000	-3.254589000000
C	-13.058430000000	1.270835000000	-2.729649000000	C	-13.090809000000	1.269162000000	-2.721874000000
C	-12.975255000000	2.476733000000	-3.435255000000	C	-13.027865000000	2.475923000000	-3.429277000000
O	-12.927014000000	1.549142000000	-1.396406000000	O	-12.927264000000	1.540820000000	-1.395532000000
C	-12.767369000000	3.480700000000	-2.521566000000	C	-12.795519000000	3.475913000000	-2.516573000000
H	-13.048738000000	2.567532000000	-4.509950000000	H	-13.133151000000	2.570514000000	-4.500790000000
C	-12.748002000000	2.861773000000	-1.255885000000	C	-12.745891000000	2.853899000000	-1.256923000000
H	-12.649442000000	4.538021000000	-2.693929000000	H	-12.687088000000	4.534356000000	-2.689819000000

C	-12.578022000000	3.480734000000	0.000000000000	C	-12.552600000000	3.470651000000	0.000000000000
C	-12.158189000000	4.834373000000	0.000000000000	C	-12.118040000000	4.810375000000	0.000000000000
C	-11.680268000000	5.949885000000	0.000000000000	C	-11.623409000000	5.921681000000	0.000000000000
C	-12.158189000000	-4.834373000000	0.000000000000	C	-12.118040000000	-4.810375000000	0.000000000000
C	-11.680268000000	-5.949885000000	0.000000000000	C	-11.623409000000	-5.921681000000	0.000000000000
C	-6.563780000000	-11.364104000000	-3.259705000000	C	-6.588961000000	-11.407732000000	-3.254786000000
C	-5.426044000000	-11.935087000000	-2.729797000000	C	-5.443448000000	-11.961830000000	-2.722051000000
C	-7.627931000000	-10.665517000000	-2.729782000000	C	-7.642460000000	-10.694023000000	-2.722038000000
C	-4.339743000000	-12.465254000000	-3.435380000000	C	-4.366537000000	-12.510044000000	-3.429428000000
O	-5.119608000000	-11.960825000000	-1.396507000000	O	-5.126725000000	-11.956483000000	-1.395625000000
C	-8.631013000000	-9.990999000000	-3.435355000000	C	-8.656527000000	-10.036811000000	-3.429406000000
O	-7.803679000000	-10.413160000000	-1.396495000000	O	-7.796425000000	-10.417138000000	-1.395634000000
C	-3.366441000000	-12.787253000000	-2.521604000000	C	-3.384472000000	-12.808894000000	-2.516631000000
H	-4.297565000000	-12.573830000000	-4.510111000000	H	-4.336971000000	-12.648047000000	-4.500955000000
C	-3.893149000000	-12.461692000000	-1.255905000000	C	-3.898744000000	-12.455601000000	-1.256934000000
C	-9.397259000000	-9.309928000000	-2.521574000000	C	-9.407168000000	-9.336573000000	-2.516605000000
H	-8.746149000000	-10.008924000000	-4.510081000000	H	-8.790860000000	-10.080466000000	-4.500956000000
C	-8.851572000000	-9.602616000000	-1.255893000000	C	-8.843636000000	-9.604472000000	-1.256943000000
H	-2.391603000000	-13.213321000000	-2.693934000000	H	-2.413427000000	-13.243797000000	-2.689837000000
C	-3.272268000000	-12.624147000000	0.000000000000	C	-3.268091000000	-12.596879000000	0.000000000000
O	-7.803679000000	-10.413160000000	1.396495000000	O	-7.796425000000	-10.417138000000	1.395634000000
O	-5.119608000000	-11.960825000000	1.396507000000	O	-5.126725000000	-11.956483000000	1.395625000000
H	-10.254376000000	-8.679690000000	-2.693893000000	H	-10.270107000000	-8.714154000000	-2.689812000000
C	-9.303157000000	-9.146585000000	0.000000000000	C	-9.281745000000	-9.129320000000	0.000000000000
C	-3.893149000000	-12.461692000000	1.255905000000	C	-3.898744000000	-12.455601000000	1.256934000000
C	-1.890074000000	-12.937528000000	0.000000000000	C	-1.890630000000	-12.890566000000	0.000000000000
C	-8.851572000000	-9.602616000000	1.255893000000	C	-8.843636000000	-9.604472000000	1.256943000000
C	-7.627931000000	-10.665517000000	2.729782000000	C	-7.642460000000	-10.694023000000	2.722038000000
C	-5.426044000000	-11.935087000000	2.729797000000	C	-5.443448000000	-11.961830000000	2.722051000000
C	-10.266558000000	-8.107111000000	0.000000000000	C	-10.225706000000	-8.084078000000	0.000000000000
C	-3.366441000000	-12.787253000000	2.521604000000	C	-3.384472000000	-12.808894000000	2.516631000000
C	-0.685098000000	-13.081736000000	0.000000000000	C	-0.680949000000	-13.018283000000	0.000000000000
C	-9.397259000000	-9.309928000000	2.521574000000	C	-9.407168000000	-9.336573000000	2.516605000000
C	-8.631013000000	-9.990999000000	3.435355000000	C	-8.656527000000	-10.036811000000	3.429406000000
C	-6.563780000000	-11.364104000000	3.259705000000	C	-6.588961000000	-11.407732000000	3.254786000000
C	-4.339743000000	-12.465254000000	3.435380000000	C	-4.366537000000	-12.510044000000	3.429428000000
C	-10.994610000000	-7.136176000000	0.000000000000	C	-10.941803000000	-7.100786000000	0.000000000000
H	-2.391603000000	-13.213321000000	2.693934000000	H	-2.413427000000	-13.243797000000	2.689837000000
H	-10.254376000000	-8.679690000000	2.693893000000	H	-10.270107000000	-8.714154000000	2.689812000000
H	-8.746149000000	-10.008924000000	4.510081000000	H	-8.790860000000	-10.080466000000	4.500956000000
H	-4.297565000000	-12.573830000000	4.510111000000	H	-4.336971000000	-12.648047000000	4.500955000000
C	10.994610000000	-7.136176000000	0.000000000000	C	10.941803000000	-7.100786000000	0.000000000000
C	11.680268000000	-5.949885000000	0.000000000000	C	11.623409000000	-5.921681000000	0.000000000000
C	10.266558000000	-8.107111000000	0.000000000000	C	10.225706000000	-8.084078000000	0.000000000000
C	12.158189000000	-4.834373000000	0.000000000000	C	12.118040000000	-4.810375000000	0.000000000000
C	9.303157000000	-9.146585000000	0.000000000000	C	9.281745000000	-9.129320000000	0.000000000000
C	12.578022000000	-3.480734000000	0.000000000000	C	12.552600000000	-3.470651000000	0.000000000000
C	8.851572000000	-9.602616000000	-1.255893000000	C	8.843636000000	-9.604472000000	-1.256943000000
C	8.851572000000	-9.602616000000	1.255893000000	C	8.843636000000	-9.604472000000	1.256943000000
C	12.748002000000	-2.861773000000	-1.255885000000	C	12.745891000000	-2.853899000000	-1.256923000000
C	12.748002000000	-2.861773000000	1.255885000000	C	12.745891000000	-2.853899000000	1.256923000000
C	9.397259000000	-9.309928000000	-2.521574000000	C	9.407168000000	-9.336573000000	-2.516605000000
O	7.803679000000	-10.413160000000	-1.396495000000	O	7.796425000000	-10.417138000000	-1.395634000000
C	9.397259000000	-9.309928000000	2.521574000000	C	9.407168000000	-9.336573000000	2.516605000000
O	7.803679000000	-10.413160000000	1.396495000000	O	7.796425000000	-10.417138000000	1.395634000000
O	12.927014000000	-1.549142000000	-1.396406000000	O	12.927264000000	-1.540820000000	-1.395532000000
C	12.767369000000	-3.480700000000	-2.521566000000	C	12.795519000000	-3.475913000000	-2.516573000000
O	12.927014000000	-1.549142000000	1.396406000000	O	12.927264000000	-1.540820000000	1.395532000000
C	12.767369000000	-3.480700000000	2.521566000000	C	12.795519000000	-3.475913000000	2.516573000000
C	8.631013000000	-9.990999000000	-3.435355000000	C	8.656527000000	-10.036811000000	-3.429406000000
H	10.254376000000	-8.679690000000	-2.693893000000	H	10.270107000000	-8.714154000000	-2.689812000000
C	7.627931000000	-10.665517000000	-2.729782000000	C	7.642460000000	-10.694023000000	-2.722038000000
C	8.631013000000	-9.990999000000	3.435355000000	C	8.656527000000	-10.036811000000	3.429406000000
H	10.254376000000	-8.679690000000	2.693893000000	H	10.270107000000	-8.714154000000	2.689812000000
C	7.627931000000	-10.665517000000	2.729782000000	C	7.642460000000	-10.694023000000	2.722038000000
C	13.058430000000	-1.270835000000	-2.729649000000	C	13.090809000000	-1.269162000000	-2.721874000000
C	12.975255000000	-2.476733000000	-3.435255000000	C	13.027865000000	-2.475923000000	-3.429277000000
H	12.649442000000	-4.538021000000	-2.693929000000	H	12.687088000000	-4.534356000000	-2.689819000000
C	13.058430000000	-1.270835000000	2.729649000000	C	13.090809000000	-1.269162000000	2.721874000000
C	12.975255000000	-2.476733000000	3.435255000000	C	13.027865000000	-2.475923000000	3.429277000000
H	12.649442000000	-4.538021000000	2.693929000000	H	12.687088000000	-4.534356000000	2.689819000000
H	8.746149000000	-10.008924000000	-4.510081000000	H	8.790860000000	-10.080466000000	-4.500956000000
C	6.563780000000	-11.364104000000	-3.259705000000	C	6.588961000000	-11.407732000000	-3.254786000000
O	5.119608000000	-11.960825000000	-1.396507000000	O	5.126725000000	-11.956483000000	-1.395625000000

O	5.119608000000	-11.960825000000	1.396507000000	O	5.126725000000	-11.956483000000	1.395625000000
H	8.746149000000	-10.008924000000	4.510081000000	H	8.790860000000	-10.080466000000	4.500956000000
C	6.563780000000	-11.364104000000	3.259705000000	C	6.588961000000	-11.407732000000	3.254786000000
C	13.132372000000	0.000000000000	-3.259525000000	C	13.183252000000	0.000000000000	-3.254589000000
O	12.927014000000	1.549142000000	-1.396406000000	O	12.927264000000	1.540820000000	-1.395532000000
O	12.927014000000	1.549142000000	1.396406000000	O	12.927264000000	1.540820000000	1.395532000000
H	13.048738000000	-2.567532000000	-4.509950000000	H	13.133151000000	-2.570514000000	-4.500790000000
C	13.132372000000	0.000000000000	3.259525000000	C	13.183252000000	0.000000000000	3.254589000000
H	13.048738000000	-2.567532000000	4.509950000000	H	13.133151000000	-2.570514000000	4.500790000000
C	5.426044000000	-11.935087000000	-2.729797000000	C	5.443448000000	-11.961830000000	-2.722051000000
C	3.893149000000	-12.461692000000	-1.255905000000	C	3.898744000000	-12.455601000000	-1.256934000000
C	5.426044000000	-11.935087000000	2.729797000000	C	5.443448000000	-11.961830000000	2.722051000000
C	3.893149000000	-12.461692000000	1.255905000000	C	3.898744000000	-12.455601000000	1.256934000000
C	13.058430000000	1.270835000000	-2.729649000000	C	13.090809000000	1.269162000000	-2.721874000000
C	12.748002000000	2.861773000000	-1.255885000000	C	12.745891000000	2.853899000000	-1.256923000000
C	12.748002000000	2.861773000000	1.255885000000	C	12.745891000000	2.853899000000	1.256923000000
C	13.058430000000	1.270835000000	2.729649000000	C	13.090809000000	1.269162000000	2.721874000000
C	4.339743000000	-12.465254000000	-3.435380000000	C	4.366537000000	-12.510044000000	-3.429428000000
C	3.366441000000	-12.787253000000	-2.521604000000	C	3.384472000000	-12.808894000000	-2.516631000000
C	3.272268000000	-12.624147000000	0.000000000000	C	3.268091000000	-12.596879000000	0.000000000000
C	4.339743000000	-12.465254000000	3.435380000000	C	4.366537000000	-12.510044000000	3.429428000000
C	3.366441000000	-12.787253000000	2.521604000000	C	3.384472000000	-12.808894000000	2.516631000000
C	12.975255000000	2.476733000000	-3.435255000000	C	13.027865000000	2.475923000000	-3.429277000000
C	12.767369000000	3.487000000000	0.000000000000	C	12.795519000000	3.475913000000	-2.516573000000
C	12.578022000000	3.480734000000	0.000000000000	C	12.552600000000	3.470651000000	0.000000000000
C	12.767369000000	3.480700000000	2.521566000000	C	12.795519000000	3.475913000000	2.516573000000
C	12.975255000000	2.476733000000	3.435255000000	C	13.027865000000	2.475923000000	3.429277000000
H	4.297565000000	-12.573830000000	-4.510111000000	H	4.336971000000	-12.648047000000	-4.500995000000
H	2.391603000000	-13.213321000000	-2.693934000000	H	2.413427000000	-13.243797000000	-2.689837000000
C	1.890074000000	-12.937528000000	0.000000000000	C	1.890630000000	-12.890566000000	0.000000000000
H	4.297565000000	-12.573830000000	4.510111000000	H	4.336971000000	-12.648047000000	4.500995000000
H	2.391603000000	-13.213321000000	2.693934000000	H	2.413427000000	-13.243797000000	2.689837000000
H	13.048738000000	2.567532000000	-4.509950000000	H	13.133151000000	2.570514000000	-4.500790000000
H	12.649442000000	4.538021000000	-2.693929000000	H	12.687088000000	4.534356000000	-2.689819000000
C	12.158189000000	4.834373000000	0.000000000000	C	12.118040000000	4.810375000000	0.000000000000
H	12.649442000000	4.538021000000	2.693929000000	H	12.687088000000	4.534356000000	2.689819000000
H	13.048738000000	2.567532000000	4.509950000000	H	13.133151000000	2.570514000000	4.500790000000
C	0.685098000000	-13.081736000000	0.000000000000	C	0.680949000000	-13.018283000000	0.000000000000
C	11.680268000000	5.949885000000	0.000000000000	C	11.623409000000	5.921681000000	0.000000000000
C	10.994610000000	7.136176000000	0.000000000000	C	10.941803000000	7.100786000000	0.000000000000
C	10.266558000000	8.107111000000	0.000000000000	C	10.225706000000	8.084078000000	0.000000000000
C	9.303157000000	9.146585000000	0.000000000000	C	9.281745000000	9.129320000000	0.000000000000
C	8.851572000000	9.602616000000	1.255893000000	C	8.843636000000	9.604472000000	1.256943000000
C	8.851572000000	9.602616000000	-1.255893000000	C	8.843636000000	9.604472000000	-1.256943000000
C	9.397259000000	9.309928000000	2.521574000000	C	9.407168000000	9.336573000000	2.516605000000
O	7.803679000000	10.413160000000	1.396495000000	O	7.796425000000	10.417138000000	1.395634000000
O	7.803679000000	10.413160000000	-1.396495000000	O	7.796425000000	10.417138000000	-1.395634000000
C	9.397259000000	9.309928000000	-2.521574000000	C	9.407168000000	9.336573000000	-2.516605000000
C	8.631013000000	9.990999000000	3.435355000000	C	8.656527000000	10.036811000000	3.429406000000
H	10.254376000000	8.679690000000	2.693893000000	H	10.270107000000	8.714154000000	2.689812000000
C	7.627931000000	10.665517000000	2.729782000000	C	7.642460000000	10.694023000000	2.722038000000
C	7.627931000000	10.665517000000	-2.729782000000	C	7.642460000000	10.694023000000	-2.722038000000
C	8.631013000000	9.990999000000	-3.435355000000	C	8.656527000000	10.036811000000	-3.429406000000
H	10.254376000000	8.679690000000	-2.693893000000	H	10.270107000000	8.714154000000	-2.689812000000
H	8.746149000000	10.008924000000	4.510081000000	H	8.790860000000	10.080466000000	4.500956000000
C	6.563780000000	11.364104000000	3.259705000000	C	6.588961000000	11.407732000000	3.254786000000
O	5.119608000000	11.960825000000	1.396507000000	O	5.126725000000	11.956483000000	1.395625000000
O	5.119608000000	11.960825000000	-1.396507000000	O	5.126725000000	11.956483000000	-1.395625000000
C	6.563780000000	11.364104000000	-3.259705000000	C	6.588961000000	11.407732000000	-3.254786000000
H	8.746149000000	10.008924000000	-4.510081000000	H	8.790860000000	10.080466000000	-4.500956000000
C	5.426044000000	11.935087000000	2.729797000000	C	5.443448000000	11.961830000000	2.722051000000
C	3.893149000000	12.461692000000	1.255905000000	C	3.898744000000	12.455601000000	1.256934000000
C	3.893149000000	12.461692000000	-1.255905000000	C	3.898744000000	12.455601000000	-1.256934000000
C	5.426044000000	11.935087000000	-2.729797000000	C	5.443448000000	11.961830000000	-2.722051000000
C	4.339743000000	12.465254000000	3.435380000000	C	4.366537000000	12.510044000000	3.429428000000
C	3.366441000000	12.787253000000	2.521604000000	C	3.384472000000	12.808894000000	2.516631000000
C	3.272268000000	12.624147000000	0.000000000000	C	3.268091000000	12.596879000000	0.000000000000
C	3.366441000000	12.787253000000	-2.521604000000	C	3.384472000000	12.808894000000	-2.516631000000
C	4.339743000000	12.465254000000	-3.435380000000	C	4.366537000000	12.510044000000	-3.429428000000
H	4.297565000000	12.573830000000	4.510111000000	H	4.336971000000	12.648047000000	4.500995000000
H	2.391603000000	13.213321000000	2.693934000000	H	2.413427000000	13.243797000000	2.689837000000
C	1.890074000000	12.937528000000	0.000000000000	C	1.890630000000	12.890566000000	0.000000000000
H	2.391603000000	13.213321000000	-2.693934000000	H	2.413427000000	13.243797000000	-2.689837000000
H	4.297565000000	12.573830000000	-4.510111000000	H	4.336971000000	12.648047000000	-4.500995000000

C	0.685098000000	13.081736000000	0.000000000000	C	0.680949000000	13.018283000000	0.000000000000
C	-0.685098000000	13.081736000000	0.000000000000	C	-0.680949000000	13.018283000000	0.000000000000
C	-1.890074000000	12.937528000000	0.000000000000	C	-1.890630000000	12.890566000000	0.000000000000
C	-3.272268000000	12.624147000000	0.000000000000	C	-3.268091000000	12.596879000000	0.000000000000
C	-3.893149000000	12.461692000000	1.255905000000	C	-3.898744000000	12.455601000000	1.256934000000
C	-3.893149000000	12.461692000000	-1.255905000000	C	-3.898744000000	12.455601000000	-1.256934000000
C	-3.366441000000	12.787253000000	2.521604000000	C	-3.384472000000	12.808894000000	2.516631000000
O	-5.119608000000	11.960825000000	1.396507000000	O	-5.126725000000	11.956483000000	1.395625000000
O	-5.119608000000	11.960825000000	-1.396507000000	O	-5.126725000000	11.956483000000	-1.395625000000
C	-3.366441000000	12.787253000000	-2.521604000000	C	-3.384472000000	12.808894000000	-2.516631000000
C	-4.339743000000	12.465254000000	3.435380000000	C	-4.366537000000	12.510044000000	3.429428000000
H	-2.391603000000	13.213321000000	2.693934000000	H	-2.413427000000	13.243797000000	2.689837000000
C	-5.426044000000	11.935087000000	2.729797000000	C	-5.443448000000	11.961830000000	2.722051000000
C	-5.426044000000	11.935087000000	-2.729797000000	C	-5.443448000000	11.961830000000	-2.722051000000
C	-4.339743000000	12.465254000000	-3.435380000000	C	-4.366537000000	12.510044000000	-3.429428000000
H	-2.391603000000	13.213321000000	-2.693934000000	H	-2.413427000000	13.243797000000	-2.689837000000
H	-4.297565000000	12.573830000000	4.510111000000	H	-4.336971000000	12.648047000000	4.500995000000
C	-6.563780000000	11.364104000000	3.259705000000	C	-6.588961000000	11.407732000000	3.254786000000
O	-7.803679000000	10.413160000000	1.396495000000	O	-7.796425000000	10.417138000000	1.395634000000
O	-7.803679000000	10.413160000000	-1.396495000000	O	-7.796425000000	10.417138000000	-1.395634000000
C	-6.563780000000	11.364104000000	-3.259705000000	C	-6.588961000000	11.407732000000	-3.254786000000
H	-4.297565000000	12.573830000000	-4.510111000000	H	-4.336971000000	12.648047000000	-4.500995000000
C	-7.627931000000	10.665517000000	2.729782000000	C	-7.642460000000	10.694023000000	2.722038000000
C	-8.851572000000	9.602616000000	1.255893000000	C	-8.843636000000	9.604472000000	1.256943000000
C	-8.851572000000	9.602616000000	-1.255893000000	C	-8.843636000000	9.604472000000	-1.256943000000
C	-7.627931000000	10.665517000000	-2.729782000000	C	-7.642460000000	10.694023000000	-2.722038000000
C	-8.631013000000	9.990999000000	3.435355000000	C	-8.656527000000	10.036811000000	3.429406000000
C	-9.397259000000	9.309928000000	2.521574000000	C	-9.407168000000	9.336573000000	2.516605000000
C	-9.303157000000	9.146585000000	0.000000000000	C	-9.281745000000	9.129320000000	0.000000000000
C	-9.397259000000	9.309928000000	-2.521574000000	C	-9.407168000000	9.336573000000	-2.516605000000
C	-8.631013000000	9.990999000000	-3.435355000000	C	-8.656527000000	10.036811000000	-3.429406000000
H	-8.746149000000	10.008924000000	4.510081000000	H	-8.790860000000	10.080466000000	4.500956000000
H	-10.254376000000	8.679690000000	2.693893000000	H	-10.270107000000	8.714154000000	2.689812000000
C	-10.266558000000	8.107111000000	0.000000000000	C	-10.225706000000	8.084078000000	0.000000000000
H	-10.254376000000	8.679690000000	-2.693893000000	H	-10.270107000000	8.714154000000	-2.689812000000
H	-8.746149000000	10.008924000000	-4.510081000000	H	-8.790860000000	10.080466000000	-4.500956000000
C	-10.994610000000	7.136176000000	0.000000000000	C	-10.941803000000	7.100786000000	0.000000000000
H	-6.605203000000	-11.435930000000	-4.341650000000	H	-6.645598000000	-11.505956000000	-4.333604000000
H	6.605203000000	-11.435930000000	-4.341650000000	H	6.645598000000	-11.505956000000	-4.333604000000
H	13.215668000000	0.000000000000	-4.341447000000	H	13.296957000000	0.000000000000	-4.333330000000
H	6.605203000000	11.435930000000	-4.341650000000	H	6.645598000000	11.505956000000	-4.333604000000
H	-6.605203000000	11.435930000000	-4.341650000000	H	-6.645598000000	11.505956000000	-4.333604000000
H	-13.215668000000	0.000000000000	-4.341447000000	H	-13.296957000000	0.000000000000	-4.333330000000
H	6.605203000000	11.435930000000	4.341650000000	H	6.645598000000	11.505956000000	4.333604000000
H	13.215668000000	0.000000000000	4.341447000000	H	13.296957000000	0.000000000000	4.333330000000
H	6.605203000000	-11.435930000000	4.341650000000	H	6.645598000000	-11.505956000000	4.333604000000
H	-6.605203000000	-11.435930000000	4.341650000000	H	-6.645598000000	-11.505956000000	4.333604000000
H	-13.215668000000	0.000000000000	4.341447000000	H	-13.296957000000	0.000000000000	4.333330000000
H	-6.605203000000	11.435930000000	4.341650000000	H	-6.645598000000	11.505956000000	4.333604000000
c-Iso6⁴⁺				c-Iso6⁶⁺			
C	2.832369000000	11.435226000000	1.308083000000	C	-12.766986000000	2.847726000000	1.255774000000
C	3.424216000000	11.399276000000	2.618863000000	C	-12.873100000000	3.470438000000	2.507245000000
C	2.428545000000	11.595516000000	3.502341000000	C	-13.158851000000	2.474436000000	3.409462000000
C	1.202837000000	11.705995000000	2.762771000000	C	-13.186272000000	1.268063000000	2.694898000000
O	1.509543000000	11.618123000000	1.432744000000	O	-12.958395000000	1.533726000000	1.384317000000
H	4.477606000000	11.270097000000	2.810757000000	H	-12.777559000000	4.529490000000	2.688210000000
H	2.496347000000	11.650841000000	4.579574000000	H	-13.326360000000	2.572252000000	4.472851000000
C	-0.035585000000	11.809865000000	3.280834000000	C	-13.313971000000	0.000000000000	3.227395000000
C	-1.340028000000	11.781079000000	2.712750000000	C	-13.186272000000	-1.268063000000	2.694898000000
C	-2.534410000000	11.853942000000	3.380230000000	C	-13.158851000000	-2.474436000000	3.409462000000
O	-1.570731000000	11.592079000000	1.394853000000	O	-12.958395000000	-1.533726000000	1.384317000000
C	-3.544391000000	11.692298000000	2.412209000000	C	-12.873100000000	-3.470438000000	2.507245000000
H	-2.655245000000	12.003101000000	4.443017000000	H	-13.326360000000	-2.572252000000	4.472851000000
C	-2.898193000000	11.534177000000	1.215086000000	C	-12.766986000000	-2.847726000000	1.255774000000
H	-4.612565000000	11.700424000000	2.559060000000	H	-12.777559000000	-4.529490000000	2.688210000000
C	-3.476135000000	11.332514000000	-0.100832000000	C	-12.534760000000	-3.462924000000	0.000000000000
C	-2.831097000000	11.435513000000	-1.308202000000	C	-12.766986000000	-2.847726000000	-1.255774000000
C	-3.422946000000	11.399750000000	-2.618987000000	C	-12.873100000000	-3.470438000000	-2.507245000000
O	-1.508262000000	11.618356000000	-1.432843000000	O	-12.958395000000	-1.533726000000	-1.384317000000
C	-2.427266000000	11.596047000000	-3.502442000000	C	-13.158851000000	-2.474436000000	-3.409462000000
H	-4.476343000000	11.270649000000	-2.810896000000	H	-12.777559000000	-4.529490000000	-2.688210000000
C	-1.201552000000	11.706376000000	-2.762859000000	C	-13.186272000000	-1.268063000000	-2.694898000000
H	-2.495067000000	11.651505000000	-4.579668000000	H	-13.326360000000	-2.572252000000	-4.472851000000
C	0.036874000000	11.810255000000	-3.280910000000	C	-13.313971000000	0.000000000000	-3.227395000000

C	1.341316000000	11.781353000000	-2.712828000000	C	-13.186272000000	1.268063000000	-2.694898000000
C	2.535702000000	11.854278000000	-3.380294000000	C	-13.158851000000	2.474436000000	-3.409462000000
O	1.572010000000	11.592164000000	-1.394956000000	O	-12.958395000000	1.533726000000	-1.384317000000
C	3.545676000000	11.692476000000	-2.412291000000	C	-12.873100000000	3.470438000000	-2.507245000000
H	2.656544000000	12.003581000000	-4.443060000000	H	-13.326360000000	2.572252000000	-4.472851000000
C	2.899469000000	11.534207000000	-1.215192000000	C	-12.766986000000	2.847726000000	-1.255774000000
H	4.613851000000	11.700598000000	-2.559136000000	H	-12.777559000000	4.529490000000	-2.688210000000
C	3.477402000000	11.332344000000	0.100700000000	C	-12.534760000000	3.462924000000	0.000000000000
C	4.845825000000	10.980032000000	0.127378000000	C	-12.068516000000	4.781557000000	0.000000000000
C	5.997618000000	10.595586000000	0.127425000000	C	-11.544740000000	5.884521000000	0.000000000000
C	-4.844576000000	10.980277000000	-0.127552000000	C	-12.068516000000	-4.781557000000	0.000000000000
C	-5.996396000000	10.595912000000	-0.127628000000	C	-11.544740000000	-5.884521000000	0.000000000000
C	-12.263634000000	6.469282000000	-3.312528000000	C	-6.656747000000	-11.529542000000	-3.227512000000
C	-12.967610000000	5.389485000000	-2.762527000000	C	-5.494715000000	-12.052929000000	-2.695001000000
C	-11.368531000000	7.353334000000	-2.788210000000	C	-7.691150000000	-10.785053000000	-2.694998000000
C	-13.732158000000	4.458796000000	-3.447790000000	C	-4.436226000000	-12.632377000000	-3.409519000000
O	-12.896345000000	5.034008000000	-1.460428000000	O	-5.150770000000	-11.988462000000	-1.384390000000
C	-10.568308000000	8.277144000000	-3.505545000000	C	-8.722375000000	-10.158349000000	-3.409489000000
O	-11.023817000000	7.423096000000	-1.472472000000	O	-7.807269000000	-10.454894000000	-1.384404000000
C	-14.111653000000	3.493305000000	-2.520820000000	C	-3.430857000000	-12.882989000000	-2.507250000000
H	-13.968554000000	4.493273000000	-4.501541000000	H	-4.435213000000	-12.826316000000	-4.472915000000
C	-13.570777000000	3.889841000000	-1.310963000000	C	-3.917141000000	-12.479752000000	-1.255790000000
C	-9.721489000000	8.858828000000	-2.612274000000	C	-9.442190000000	-9.413065000000	-2.507218000000
H	-10.632459000000	8.452660000000	-4.570249000000	H	-8.890896000000	-10.254559000000	-4.472865000000
C	-10.045676000000	8.318494000000	-1.344749000000	C	-8.849694000000	-9.632371000000	-1.255796000000
H	-14.721588000000	2.618081000000	-2.681241000000	H	-2.465932000000	-13.329817000000	-2.688168000000
C	-13.669159000000	3.232010000000	-0.033678000000	C	-3.268281000000	-12.586262000000	0.000000000000
O	-11.005555000000	7.445802000000	1.299295000000	O	-7.807269000000	-10.454894000000	1.384404000000
O	-12.880944000000	5.059375000000	1.351258000000	O	-5.150770000000	-11.988462000000	-1.384390000000
H	-8.964977000000	9.607276000000	-2.788406000000	H	-10.311764000000	-8.801030000000	-2.688110000000
C	-9.489895000000	8.679075000000	-0.106978000000	C	-9.266366000000	-9.123673000000	0.000000000000
C	-13.559875000000	3.914648000000	1.229688000000	C	-3.917141000000	-12.479752000000	1.255790000000
C	-13.931292000000	1.897272000000	-0.019486000000	C	-1.893192000000	-12.841830000000	0.000000000000
C	-10.027109000000	8.336468000000	1.144446000000	C	-8.849694000000	-9.632371000000	1.255796000000
C	-11.331884000000	7.397024000000	2.620668000000	C	-7.691150000000	-10.785053000000	2.694998000000
C	-12.937980000000	5.438906000000	2.647301000000	C	-5.494715000000	-12.052929000000	2.695001000000
C	-8.316315000000	9.475567000000	-0.120296000000	C	-10.175259000000	-8.060635000000	0.000000000000
C	-14.090365000000	3.542387000000	2.451812000000	C	-3.430857000000	-12.882989000000	2.507250000000
C	-14.034865000000	0.660330000000	-0.006537000000	C	-0.676120000000	-12.939764000000	0.000000000000
C	-9.682590000000	8.894022000000	2.398952000000	C	-9.442190000000	-9.413065000000	2.507218000000
C	-10.518461000000	8.328380000000	3.312735000000	C	-8.722375000000	-10.158349000000	3.409489000000
C	-12.223484000000	6.524937000000	3.170566000000	C	-6.656747000000	-11.529542000000	3.227512000000
C	-13.698770000000	4.523517000000	3.357024000000	C	-4.436226000000	-12.632377000000	3.409519000000
C	-7.242830000000	10.039831000000	-0.125705000000	C	-10.868614000000	-7.055581000000	0.000000000000
H	-14.700939000000	2.671965000000	2.634400000000	H	-2.465932000000	-13.329817000000	2.688168000000
H	-8.920633000000	9.641750000000	2.553490000000	H	-10.311764000000	-8.801030000000	2.688110000000
H	-10.566414000000	8.519653000000	4.375577000000	H	-8.890896000000	-10.254559000000	4.472865000000
H	-13.924456000000	4.578059000000	4.412279000000	H	-4.435213000000	-12.826316000000	4.472915000000
C	-7.243973000000	-10.039478000000	0.125458000000	C	10.868614000000	-7.055581000000	0.000000000000
C	-5.997608000000	-10.595711000000	0.127385000000	C	11.544740000000	-5.884521000000	0.000000000000
C	-8.317385000000	-9.475075000000	0.120074000000	C	10.175259000000	-8.060635000000	0.000000000000
C	-4.845819000000	-10.980166000000	0.127355000000	C	12.068516000000	-4.781557000000	0.000000000000
C	-9.490836000000	-8.678392000000	0.106802000000	C	9.266366000000	-9.123673000000	0.000000000000
C	-3.477404000000	-11.332499000000	0.100666000000	C	12.534760000000	-3.462924000000	0.000000000000
C	-10.027947000000	-8.335557000000	-1.144600000000	C	8.849694000000	-9.632371000000	-1.255796000000
C	-10.046577000000	-8.317827000000	1.344598000000	C	8.849694000000	-9.632371000000	1.255796000000
C	-2.899448000000	-11.534224000000	-1.215233000000	C	12.766986000000	-2.847726000000	-1.255774000000
C	-2.832397000000	-11.435529000000	1.308053000000	C	12.766986000000	-2.847726000000	1.255774000000
C	-9.683451000000	-8.893004000000	-2.399162000000	C	9.442190000000	-9.413065000000	-2.507218000000
O	-11.006252000000	-7.444724000000	-1.299384000000	O	7.807269000000	-10.454894000000	-1.384404000000
C	-9.722482000000	-8.858307000000	2.612083000000	C	9.442190000000	-9.413065000000	2.507218000000
O	-11.024578000000	-7.422286000000	1.472382000000	O	7.807269000000	-10.454894000000	1.384404000000
O	-1.571983000000	-11.592235000000	-1.394964000000	O	12.958395000000	-1.533726000000	-1.384317000000
C	-3.545619000000	-11.692316000000	-2.412374000000	C	12.873100000000	-3.470438000000	-2.507245000000
O	-1.509578000000	-11.618440000000	1.432726000000	O	12.958395000000	-1.533726000000	1.384317000000
C	-3.424283000000	-11.399739000000	2.618819000000	C	12.873100000000	-3.470438000000	2.507245000000
C	-10.519182000000	-8.327111000000	-3.312914000000	C	8.722375000000	-10.158349000000	-3.409489000000
H	-8.921600000000	-9.640828000000	-2.553756000000	H	10.311764000000	-8.801030000000	-2.688110000000
C	-11.332503000000	-7.395721000000	-2.620767000000	C	7.691150000000	-10.785053000000	-2.694998000000
C	-10.569206000000	-8.276546000000	3.505395000000	C	8.722375000000	-10.158349000000	3.409489000000
H	-8.966090000000	-9.606889000000	2.788162000000	H	10.311764000000	-8.801030000000	2.688110000000
C	-11.369282000000	-7.352561000000	2.788123000000	C	7.691150000000	-10.785053000000	2.694998000000
C	-1.341253000000	-11.781289000000	-2.712848000000	C	13.186272000000	-1.268063000000	-2.694898000000
C	-2.535622000000	-11.854075000000	-3.380359000000	C	13.158851000000	-2.474436000000	-3.409462000000

H	-4.613788000000	-11.700362000000	-2.559268000000	H	12.777559000000	-4.529490000000	-2.688210000000
C	-1.202910000000	-11.706471000000	2.762750000000	C	13.186272000000	-1.268063000000	2.694898000000
C	-2.428635000000	-11.596079000000	3.502302000000	C	13.158851000000	-2.474436000000	3.409462000000
H	-4.477680000000	-11.270582000000	2.810690000000	H	12.777559000000	-4.529490000000	2.688210000000
H	-10.567106000000	-8.518232000000	-4.375785000000	H	8.890896000000	-10.254559000000	-4.472865000000
C	-12.223941000000	-6.523433000000	-3.170603000000	C	6.656747000000	-11.529542000000	-3.227512000000
O	-12.881332000000	-5.058001000000	-1.351158000000	O	5.150770000000	-11.988462000000	-1.384390000000
O	-12.896805000000	-5.032911000000	1.460522000000	O	5.150770000000	-11.988462000000	-1.384390000000
H	-10.633384000000	-8.452123000000	4.570087000000	H	8.890896000000	-10.254559000000	4.472865000000
C	-12.264247000000	-6.468408000000	3.312507000000	C	6.656747000000	-11.529542000000	3.227512000000
C	-0.036800000000	-11.810193000000	-3.280896000000	C	13.313971000000	0.000000000000	-3.227395000000
O	1.508288000000	-11.618435000000	-1.432774000000	O	12.958395000000	1.533726000000	-1.384317000000
O	1.570695000000	-11.592399000000	1.394917000000	O	12.958395000000	1.533726000000	1.384317000000
H	-2.656447000000	-12.003255000000	-4.443145000000	H	13.326360000000	-2.572252000000	-4.472851000000
C	0.035500000000	-11.810394000000	3.280835000000	C	13.313971000000	0.000000000000	3.227395000000
H	-2.496456000000	-11.651535000000	4.579526000000	H	13.326360000000	-2.572252000000	4.472851000000
C	-12.938322000000	-5.437366000000	-2.647251000000	C	5.494715000000	-12.052929000000	-2.695001000000
C	-13.560122000000	-3.913199000000	-1.229499000000	C	3.917141000000	-12.479752000000	-1.255790000000
C	-12.968076000000	-5.388471000000	2.762598000000	C	5.494715000000	-12.052929000000	2.695001000000
C	-13.571077000000	-3.888637000000	1.311162000000	C	3.917141000000	-12.479752000000	1.255790000000
C	1.201616000000	-11.706369000000	-2.762803000000	C	13.186272000000	1.268063000000	-2.694898000000
C	2.831117000000	-11.435601000000	-1.308091000000	C	12.766986000000	2.847726000000	-1.255774000000
C	2.898164000000	-11.534452000000	1.215190000000	C	12.766986000000	2.847726000000	1.255774000000
C	1.339955000000	-11.781525000000	2.712789000000	C	13.186272000000	1.268063000000	2.694898000000
C	-13.698939000000	-4.521792000000	-3.356919000000	C	4.436226000000	-12.632377000000	-3.409519000000
C	-14.090474000000	-3.540721000000	-2.451616000000	C	3.430857000000	-12.882989000000	-2.507250000000
C	-13.669412000000	-3.230691000000	0.033936000000	C	3.268281000000	-12.586262000000	0.000000000000
C	-13.732471000000	-4.457721000000	3.447953000000	C	4.436226000000	-12.632377000000	3.409519000000
C	-14.111857000000	-3.492111000000	2.521068000000	C	3.430857000000	-12.882989000000	2.507250000000
C	2.427348000000	-11.595999000000	-3.502348000000	C	13.158851000000	2.474436000000	-3.409462000000
C	3.423005000000	-11.399763000000	-2.618854000000	C	12.873100000000	3.470438000000	-2.507245000000
C	3.476130000000	-11.332681000000	-0.100698000000	C	12.534760000000	3.462924000000	0.000000000000
C	3.544326000000	-11.692653000000	2.412321000000	C	12.873100000000	3.470438000000	2.507245000000
C	2.534320000000	-11.854418000000	3.380296000000	C	13.158851000000	2.474436000000	3.409462000000
H	-13.924510000000	-4.576175000000	-4.412198000000	H	4.435213000000	-12.826316000000	-4.474291500000
H	-14.700919000000	-2.670197000000	-2.634146000000	H	2.465932000000	-13.329817000000	-2.688168000000
C	-13.931465000000	-1.895933000000	0.019870000000	C	1.893192000000	-12.841830000000	0.000000000000
H	-13.968834000000	-4.492241000000	4.501711000000	H	4.435213000000	-12.826316000000	4.472915000000
H	-14.721658000000	-2.616809000000	2.681573000000	H	2.465932000000	-13.329817000000	2.688168000000
H	2.495166000000	-11.651395000000	-4.579576000000	H	13.326360000000	2.572252000000	-4.472851000000
H	4.476409000000	-11.270651000000	-2.810717000000	H	12.777559000000	4.529490000000	-2.688210000000
C	4.844566000000	-10.980426000000	-0.127367000000	C	12.068516000000	4.781557000000	0.000000000000
H	4.612494000000	-11.700766000000	2.559216000000	H	12.777559000000	4.529490000000	2.688210000000
H	2.655137000000	-12.003673000000	4.443072000000	H	13.326360000000	2.572252000000	4.472851000000
C	-14.034935000000	-0.658983000000	0.007021000000	C	0.676120000000	-12.939764000000	0.000000000000
C	5.996372000000	-10.596016000000	-0.127419000000	C	11.544740000000	5.884521000000	0.000000000000
C	7.242792000000	-10.039906000000	-0.125550000000	C	10.868614000000	7.055581000000	0.000000000000
C	8.316261000000	-9.475612000000	-0.120201000000	C	10.175259000000	8.060635000000	0.000000000000
C	9.489798000000	-8.679054000000	-0.106921000000	C	9.266366000000	9.123673000000	0.000000000000
C	10.026988000000	-8.336352000000	1.144484000000	C	8.849694000000	9.632371000000	1.255796000000
C	10.045560000000	-8.318511000000	-1.344713000000	C	8.849694000000	9.632371000000	-1.255796000000
C	9.682469000000	-8.893828000000	2.399025000000	C	9.442190000000	9.413065000000	2.507218000000
O	11.005409000000	-7.445648000000	1.299284000000	O	7.807269000000	10.454894000000	1.384404000000
O	11.023669000000	-7.423083000000	-1.472480000000	O	7.807269000000	10.454894000000	-1.384404000000
C	9.721385000000	-8.858909000000	-2.612211000000	C	9.442190000000	9.413065000000	-2.507218000000
C	10.518310000000	-8.328099000000	3.312779000000	C	8.722375000000	10.158349000000	3.409489000000
H	8.920531000000	-9.641567000000	2.553604000000	H	10.311764000000	8.801030000000	2.688110000000
C	11.331720000000	-7.396769000000	2.620657000000	C	7.691150000000	10.785053000000	2.694998000000
C	11.368368000000	-7.353362000000	-2.788221000000	C	7.691150000000	10.785053000000	-2.694998000000
C	10.568175000000	-8.277228000000	-3.505513000000	C	8.722375000000	10.158349000000	-3.409489000000
H	8.964900000000	-9.607395000000	-2.788306000000	H	10.311764000000	8.801030000000	-2.688110000000
H	10.566253000000	-8.519296000000	4.375635000000	H	8.890896000000	10.254559000000	4.472865000000
C	12.223292000000	-6.524628000000	3.170510000000	C	6.656747000000	11.529542000000	3.227512000000
O	12.880786000000	-5.059172000000	1.351122000000	O	5.150770000000	11.988462000000	1.384390000000
O	12.896190000000	-5.033949000000	-1.460556000000	O	5.150770000000	11.988462000000	-1.384390000000
C	12.263434000000	-6.469298000000	-3.312587000000	C	6.656747000000	11.529542000000	-3.227512000000
H	10.632323000000	-8.452189000000	-4.570210000000	H	8.890896000000	10.254559000000	-4.472865000000
C	12.937790000000	-5.438621000000	2.647190000000	C	5.494715000000	12.052929000000	2.695001000000
C	13.559723000000	-3.914453000000	1.229498000000	C	3.917141000000	12.479752000000	1.255790000000
C	13.570595000000	-3.889758000000	-1.311160000000	C	3.917141000000	12.479752000000	-1.255790000000
C	12.967394000000	-5.389462000000	-2.762648000000	C	5.494715000000	12.052929000000	-2.695001000000
C	13.698560000000	-4.523189000000	3.356876000000	C	4.436226000000	12.632377000000	3.409519000000
C	14.090182000000	-3.542117000000	2.451611000000	C	3.430857000000	12.882989000000	2.507250000000
C	13.669045000000	-3.231888000000	-0.033905000000	C	3.268281000000	12.586262000000	0.000000000000

C	14.111393000000	-3.493241000000	-2.521062000000	C	3.430857000000	12.882989000000	-2.507250000000
C	13.731877000000	-4.458768000000	-3.447980000000	C	4.436226000000	12.632377000000	-3.409519000000
H	13.924217000000	-4.577664000000	4.412140000000	H	4.435213000000	12.826316000000	4.472915000000
H	14.700752000000	-2.671684000000	2.634162000000	H	2.465932000000	13.329817000000	2.688168000000
C	13.931269000000	-1.897165000000	-0.019779000000	C	1.893192000000	12.841830000000	0.000000000000
H	14.721293000000	-2.618002000000	-2.681540000000	H	2.465932000000	13.329817000000	-2.688168000000
H	13.968216000000	-4.493271000000	-4.501744000000	H	4.435213000000	12.826316000000	-4.472915000000
C	14.034908000000	-0.660229000000	-0.006853000000	C	0.676120000000	12.939764000000	0.000000000000
C	14.035004000000	0.659083000000	0.006853000000	C	-0.676120000000	12.939764000000	0.000000000000
C	13.931552000000	1.896034000000	0.019819000000	C	-1.893192000000	12.841830000000	0.000000000000
C	13.669570000000	3.230804000000	0.033976000000	C	-3.268281000000	12.586262000000	0.000000000000
C	13.571160000000	3.888657000000	1.311248000000	C	-3.917141000000	12.479752000000	1.255790000000
C	13.560439000000	3.913438000000	-1.229408000000	C	-3.917141000000	12.479752000000	-1.255790000000
C	14.111890000000	3.492066000000	2.521153000000	C	-3.430857000000	12.882989000000	2.507250000000
O	12.896851000000	5.032904000000	1.460649000000	O	-5.150770000000	11.988462000000	1.384390000000
O	12.881629000000	5.058230000000	-1.351039000000	O	-5.150770000000	11.988462000000	-1.384390000000
C	14.090968000000	3.541104000000	-2.451491000000	C	-3.430857000000	12.882989000000	-2.507250000000
C	13.732426000000	4.457603000000	3.448085000000	C	-4.436226000000	12.632377000000	3.409519000000
H	14.721710000000	2.616772000000	2.681630000000	H	-2.465932000000	13.329817000000	2.688168000000
C	12.968047000000	5.388380000000	2.762752000000	C	-5.494715000000	12.052929000000	2.695001000000
C	12.938774000000	5.437728000000	-2.647087000000	C	-5.494715000000	12.052929000000	-2.695001000000
C	13.699514000000	4.522252000000	-3.356748000000	C	-4.436226000000	12.632377000000	-3.409519000000
H	14.701468000000	2.670620000000	-2.634028000000	H	-2.465932000000	13.329817000000	-2.688168000000
C	13.968735000000	4.492058000000	4.501857000000	H	-4.435213000000	12.826316000000	4.472915000000
C	12.264157000000	6.468264000000	3.312689000000	C	-6.656747000000	11.529542000000	3.227512000000
O	11.024586000000	7.422214000000	1.472537000000	O	-7.807269000000	10.454894000000	1.384404000000
O	11.006495000000	7.444874000000	-1.299230000000	O	-7.807269000000	10.454894000000	-1.384404000000
C	12.224412000000	6.523819000000	-3.170416000000	C	-6.656747000000	11.529542000000	-3.227512000000
H	13.925262000000	4.576748000000	-4.411992000000	H	-4.435213000000	12.826316000000	-4.472915000000
C	11.369201000000	7.352424000000	2.788299000000	C	-7.691150000000	10.785053000000	2.694998000000
C	10.046565000000	8.317731000000	1.344739000000	C	-8.849694000000	9.632371000000	1.255796000000
C	10.028137000000	8.335649000000	-1.144458000000	C	-8.849694000000	9.632371000000	-1.255796000000
C	11.332880000000	7.396016000000	-2.620588000000	C	-7.691150000000	10.785053000000	-2.694998000000
C	10.569046000000	8.276341000000	3.505569000000	C	-8.722375000000	10.158349000000	3.409489000000
C	9.722364000000	8.858127000000	2.612233000000	C	-9.442190000000	9.413065000000	2.507218000000
C	9.490899000000	8.678356000000	0.106927000000	C	-9.266366000000	9.123673000000	0.000000000000
C	9.683736000000	8.893200000000	-2.399000000000	C	-9.442190000000	9.413065000000	-2.507218000000
C	10.519585000000	8.327435000000	-3.312724000000	C	-8.722375000000	10.158349000000	-3.409489000000
H	10.633145000000	8.451860000000	4.570275000000	H	-8.890896000000	10.254559000000	4.472865000000
H	8.965937000000	9.606676000000	2.788304000000	H	-10.311764000000	8.801030000000	2.688110000000
C	8.317415000000	9.474990000000	0.120162000000	C	-10.175259000000	8.060635000000	0.000000000000
H	8.921867000000	9.641004000000	-2.553597000000	H	-10.311764000000	8.801030000000	-2.688110000000
H	10.567605000000	8.518663000000	-4.375571000000	H	-8.890896000000	10.254559000000	-4.472865000000
H	7.243994000000	10.039377000000	0.125525000000	C	-10.868614000000	7.055581000000	0.000000000000
H	-12.413119000000	6.579953000000	-4.380823000000	H	-6.744252000000	-11.681128000000	-4.297895000000
H	-12.359523000000	-6.652038000000	-4.238751000000	H	6.744252000000	-11.681128000000	-4.297895000000
H	-0.052083000000	-11.891644000000	-4.361902000000	H	13.489069000000	0.000000000000	-4.297776000000
H	12.412898000000	-6.580004000000	-4.380881000000	H	6.744252000000	11.681128000000	-4.297895000000
H	12.360102000000	6.652532000000	-4.238537000000	H	-6.744252000000	11.681128000000	-4.297895000000
H	0.052187000000	11.891778000000	-4.361910000000	H	-13.489069000000	0.000000000000	-4.297776000000
H	12.358904000000	-6.653316000000	4.238644000000	H	6.744252000000	11.681128000000	4.297895000000
H	0.050779000000	-11.891917000000	4.361836000000	H	13.489069000000	0.000000000000	4.297776000000
H	-12.413735000000	-6.579130000000	4.380796000000	H	6.744252000000	-11.681128000000	4.297895000000
H	-12.359116000000	6.653701000000	4.238688000000	H	-6.744252000000	-11.681128000000	4.297895000000
H	-0.050894000000	11.891256000000	4.361845000000	H	-13.489069000000	0.000000000000	4.297776000000
H	12.413570000000	6.578923000000	4.380995000000	H	-6.744252000000	11.681128000000	4.297895000000
c-P3Iso3				c-P3Iso3²⁺			
C	-8.682123000000	-9.713322000000	1.281183000000	C	-12.464219000000	-3.937086000000	1.287870000000
C	-9.165153000000	-9.344415000000	2.588443000000	C	-12.732409000000	-3.384536000000	2.577725000000
C	-8.426731000000	-10.017325000000	3.486000000000	C	-12.439294000000	-4.344998000000	3.482704000000
C	-7.433888000000	-10.769048000000	2.761674000000	C	-11.938034000000	-5.471996000000	2.762576000000
O	-7.651697000000	-10.571163000000	1.429074000000	O	-11.996825000000	-5.187465000000	1.434508000000
H	-9.986243000000	-8.666776000000	2.762815000000	H	-13.119744000000	-2.392659000000	2.750503000000
H	-8.509563000000	-10.000391000000	4.563301000000	H	-12.529710000000	-4.295548000000	4.558360000000
C	-6.419730000000	-11.471409000000	3.297105000000	C	-11.401710000000	-6.595494000000	3.301367000000
C	-5.263864000000	-12.092284000000	2.733643000000	C	-10.693168000000	-7.680908000000	2.744527000000
C	-4.247825000000	-12.719583000000	3.402346000000	C	-10.063134000000	-8.699818000000	3.430675000000
O	-4.970209000000	-12.034489000000	1.418073000000	O	-10.440634000000	-7.806605000000	1.424857000000
C	-3.274271000000	-13.047333000000	2.434360000000	C	-9.381208000000	-9.460445000000	2.478093000000
H	-4.209898000000	-12.901075000000	4.466186000000	H	-10.092650000000	-8.849827000000	4.499822000000
C	-3.766226000000	-12.602771000000	1.238732000000	C	-9.645505000000	-8.872759000000	1.258544000000
H	-2.328202000000	-13.543542000000	2.581620000000	H	-8.772223000000	-10.336646000000	2.633826000000
C	-3.149104000000	-12.679026000000	-0.073782000000	C	-9.188776000000	-9.290254000000	-0.039864000000
C	-3.752911000000	-12.471975000000	-1.280630000000	C	-9.654148000000	-8.841993000000	-1.253393000000

C	-3.185411000000	-12.690039000000	-2.587815000000	C	-9.345776000000	-9.372858000000	-2.547732000000
O	-5.022731000000	-12.041652000000	-1.428734000000	O	-10.520655000000	-7.821710000000	-1.394363000000
C	-4.144654000000	-12.411505000000	-3.485564000000	C	-10.067138000000	-8.667249000000	-3.442660000000
H	-2.178491000000	-13.035803000000	-2.762027000000	H	-8.675786000000	-10.199880000000	-2.724282000000
C	-5.304722000000	-11.958425000000	-2.761391000000	C	-10.782211000000	-7.658363000000	-2.718712000000
H	-4.086487000000	-12.472506000000	-4.562886000000	H	-10.103617000000	-8.792167000000	-4.515348000000
C	-6.433344000000	-11.460503000000	-3.296931000000	C	-11.516956000000	-6.656913000000	-3.255175000000
C	-7.567037000000	-10.800027000000	-2.733452000000	C	-12.102814000000	-5.493011000000	-2.700220000000
C	-8.632563000000	-10.261110000000	-3.402202000000	C	-12.716699000000	-4.467260000000	-3.385525000000
O	-7.671825000000	-10.520513000000	-1.417705000000	O	-12.037076000000	-5.182514000000	-1.389836000000
C	-9.421237000000	-9.603173000000	-2.434039000000	C	-13.015838000000	-3.479294000000	-2.440000000000
H	-8.806644000000	-10.322783000000	-4.466170000000	H	-12.905754000000	-4.444904000000	-4.448486000000
C	-8.785634000000	-9.791188000000	-1.238282000000	C	-12.579227000000	-3.965044000000	-1.228366000000
H	-10.338659000000	-9.055799000000	-2.581268000000	H	-13.496940000000	-2.527312000000	-2.599611000000
C	-9.173698000000	-9.305855000000	0.074426000000	C	-12.663642000000	-3.332403000000	0.062323000000
C	-10.132420000000	-8.259514000000	0.082367000000	C	-12.946183000000	-1.950153000000	0.065823000000
C	-10.848097000000	-7.280863000000	0.069393000000	C	-13.040159000000	-0.738755000000	0.053138000000
C	-1.756028000000	-12.949811000000	-0.081399000000	C	-8.128115000000	-10.232283000000	-0.051214000000
C	-0.547673000000	-13.048907000000	-0.068380000000	C	-7.126620000000	-10.915095000000	-0.043155000000
C	6.558585000000	-10.961894000000	-3.390994000000	C	0.039511000000	-12.732670000000	-3.390787000000
C	7.592770000000	-10.279357000000	-2.762318000000	C	1.278917000000	-12.671271000000	-2.765988000000
C	5.454650000000	-11.551222000000	-2.786948000000	C	-1.208232000000	-12.673672000000	-2.782480000000
C	8.640871000000	-9.570102000000	-3.444472000000	C	2.540709000000	-12.604093000000	-3.452746000000
N	7.733032000000	-10.119168000000	-1.420001000000	N	1.485184000000	-12.597716000000	-1.424535000000
C	4.343411000000	-12.127363000000	-3.493962000000	C	-2.460883000000	-12.608613000000	-3.485911000000
N	5.223461000000	-11.610568000000	-1.449012000000	N	-1.432466000000	-12.600961000000	-1.443892000000
C	9.385266000000	-8.960218000000	-2.490549000000	C	3.494816000000	-12.457072000000	-2.502562000000
H	8.773960000000	-9.535532000000	-4.516809000000	H	2.669755000000	-12.652851000000	-4.524943000000
C	8.805673000000	-9.319685000000	-1.222497000000	C	2.815695000000	-12.461504000000	-1.232056000000
Zn	6.471610000000	-10.881482000000	-0.001216000000	Zn	0.016890000000	-12.617329000000	-0.000033000000
C	3.435706000000	-12.499138000000	-2.558992000000	C	-3.427787000000	-12.463727000000	-2.548361000000
H	4.268658000000	-12.218290000000	-4.568663000000	H	-2.575549000000	-12.657363000000	-4.559746000000
C	4.005638000000	-12.172911000000	-1.277770000000	C	-2.765658000000	-12.467416000000	-1.268972000000
H	10.251346000000	-8.328785000000	-2.619235000000	H	4.562044000000	-12.365443000000	-2.636394000000
C	9.287113000000	-8.894864000000	0.032956000000	C	3.447791000000	-12.340554000000	0.022644000000
N	5.199662000000	-11.626067000000	1.417585000000	N	-1.451449000000	-12.601727000000	1.424469000000
N	7.709706000000	-10.135436000000	1.446593000000	N	1.466198000000	-12.597331000000	1.443828000000
H	2.470394000000	-12.958623000000	-2.708548000000	H	-4.493359000000	-12.374512000000	-2.696241000000
C	3.380440000000	-12.404106000000	-0.035099000000	C	-3.414722000000	-12.349517000000	-0.022677000000
C	8.785848000000	-9.334628000000	1.275506000000	C	2.799038000000	-12.460293000000	1.268922000000
C	10.287817000000	-7.886261000000	0.046523000000	C	4.822535000000	-11.983467000000	0.031260000000
C	3.984456000000	-12.185591000000	1.220238000000	C	-2.782312000000	-12.468969000000	1.232006000000
C	5.408222000000	-11.580827000000	2.759828000000	C	-1.244990000000	-12.674902000000	2.765913000000
C	7.547763000000	-10.311343000000	2.784454000000	C	1.242156000000	-12.670786000000	2.782408000000
C	2.016192000000	-12.800996000000	-0.048330000000	C	-4.790388000000	-11.995994000000	-0.031253000000
C	9.345628000000	-8.991312000000	2.556739000000	C	3.461156000000	-12.455030000000	2.548312000000
C	11.025657000000	-6.924332000000	0.056486000000	C	5.952775000000	-11.544750000000	0.037856000000
C	3.392328000000	-12.523952000000	2.488302000000	C	-3.461442000000	-12.466462000000	2.502513000000
C	4.284498000000	-12.162799000000	3.442059000000	C	-2.506955000000	-12.611104000000	3.452679000000
C	6.502600000000	-10.999605000000	3.388432000000	C	-0.005429000000	-12.733125000000	3.390707000000
C	8.585557000000	-9.611590000000	3.491549000000	C	2.494635000000	-12.602545000000	3.485846000000
C	0.818606000000	-12.989421000000	-0.058020000000	C	-5.921760000000	-11.560206000000	-0.037776000000
H	10.210873000000	-8.363403000000	2.706419000000	H	4.526492000000	-12.363059000000	2.696201000000
H	2.423685000000	-12.982759000000	2.617099000000	H	-4.528906000000	-12.377637000000	2.636354000000
H	4.191122000000	-12.264219000000	4.514350000000	H	-2.635873000000	-12.660324000000	4.524871000000
H	8.701768000000	-9.590442000000	4.566206000000	H	2.609429000000	-12.651125000000	4.559674000000
C	11.579001000000	6.051545000000	-0.067034000000	C	13.041761000000	-0.704062000000	-0.053056000000
C	10.844207000000	7.204952000000	-0.056551000000	C	12.994402000000	0.655842000000	-0.042591000000
C	12.097415000000	4.955553000000	-0.080132000000	C	12.950987000000	-1.915706000000	-0.065643000000
C	10.082003000000	8.147698000000	-0.046763000000	C	12.811599000000	1.857136000000	-0.032953000000
C	12.559452000000	3.613726000000	-0.072398000000	C	12.672230000000	-3.298726000000	-0.062194000000
C	9.055739000000	9.130289000000	-0.033503000000	C	12.433536000000	3.218609000000	-0.020797000000
C	12.683453000000	2.987596000000	-1.279259000000	C	12.474367000000	-3.903891000000	-1.287755000000
C	12.800375000000	3.040753000000	1.240244000000	C	12.589659000000	-3.931665000000	1.228468000000
C	8.543106000000	9.556370000000	-1.276175000000	C	12.216087000000	3.847069000000	-1.268394000000
C	8.563774000000	9.543251000000	1.221832000000	C	12.220601000000	3.825566000000	1.238059000000
C	12.590308000000	3.588434000000	-2.586407000000	C	12.740927000000	-3.350541000000	-2.577606000000
O	12.945711000000	1.672743000000	-1.427346000000	O	12.010416000000	-5.155550000000	-1.434417000000
C	12.938236000000	3.688731000000	2.436194000000	C	13.025070000000	-3.444801000000	2.440086000000
O	12.909679000000	1.713862000000	1.419361000000	O	12.050816000000	-5.150604000000	1.389926000000
N	7.446726000000	10.329189000000	-1.447465000000	N	11.661032000000	5.065575000000	-1.438381000000
C	9.111303000000	9.226899000000	-2.557339000000	C	12.552743000000	3.279237000000	-2.546984000000
N	7.470952000000	10.314972000000	1.419132000000	N	11.668185000000	5.041976000000	1.430756000000
C	9.152644000000	9.199470000000	2.489956000000	C	12.561663000000	3.235636000000	2.505530000000

C	12.829725000000	2.618626000000	-3.484092000000	C	12.450405000000	-4.311770000000	-3.482607000000
H	12.386679000000	4.633411000000	-2.760613000000	H	13.125505000000	-2.357590000000	-2.750368000000
C	13.016260000000	1.387225000000	-2.759987000000	C	11.952317000000	-5.440183000000	-2.762494000000
C	13.139804000000	2.681428000000	3.404148000000	C	12.728698000000	-4.433623000000	3.385586000000
H	12.895025000000	4.756127000000	2.583689000000	H	13.503613000000	-2.491531000000	2.599701000000
C	13.105025000000	1.488046000000	2.735093000000	C	12.117522000000	-5.460993000000	2.700286000000
C	7.280081000000	10.500195000000	-2.785384000000	C	11.616650000000	5.302180000000	-2.776696000000
Zn	6.190061000000	11.043811000000	0.000197000000	Zn	10.943382000000	6.323261000000	0.008596000000
C	8.335394000000	9.826980000000	-3.492319000000	C	12.194235000000	4.192231000000	-3.482624000000
H	9.992355000000	8.621333000000	-2.706861000000	H	13.014017000000	2.314991000000	-2.697468000000
C	7.326827000000	10.472166000000	2.761396000000	C	11.630907000000	5.256486000000	2.773002000000
C	8.392959000000	9.790473000000	3.443709000000	C	12.209323000000	4.133670000000	3.457730000000
H	10.034717000000	8.590614000000	2.618801000000	H	13.021018000000	2.267826000000	2.638054000000
H	12.854860000000	2.699770000000	-4.561362000000	H	12.540606000000	-4.262022000000	-4.558267000000
C	13.149760000000	0.160948000000	-3.295661000000	C	11.419062000000	-6.565135000000	-3.301297000000
O	12.951860000000	-1.382040000000	-1.417120000000	O	10.461402000000	-7.778934000000	-1.424778000000
O	12.982195000000	-1.340068000000	1.429643000000	O	10.541626000000	-7.793934000000	1.394437000000
H	13.276825000000	2.804703000000	4.468180000000	H	12.917795000000	-4.410813000000	4.448530000000
C	13.144192000000	0.176440000000	3.298257000000	C	11.534864000000	-6.626503000000	3.255234000000
C	6.217467000000	11.161055000000	-3.389512000000	C	11.040007000000	6.412915000000	-3.380964000000
N	4.899152000000	11.754740000000	-1.418744000000	N	10.188412000000	7.587317000000	-1.413678000000
N	4.923780000000	11.741235000000	1.447860000000	N	10.199151000000	7.565925000000	1.455363000000
H	8.451920000000	9.808271000000	-4.566987000000	H	12.299187000000	4.122543000000	-4.556271000000
C	6.275508000000	11.128144000000	3.389918000000	C	11.060828000000	6.358883000000	3.398366000000
H	8.527081000000	9.759884000000	4.516039000000	H	12.318859000000	4.045685000000	4.529565000000
C	13.143492000000	-1.151244000000	-2.732533000000	C	10.713542000000	-7.652515000000	-2.744455000000
C	12.876490000000	-2.711310000000	-1.238153000000	C	9.669210000000	-8.847271000000	-1.258460000000
C	13.043194000000	-1.052856000000	2.762390000000	C	10.802805000000	-7.629923000000	2.718777000000
C	12.754059000000	-2.661220000000	1.281147000000	C	9.677875000000	-8.816551000000	1.253476000000
C	5.108594000000	11.714229000000	-2.760999000000	C	10.360338000000	7.450927000000	-2.755967000000
C	3.670004000000	12.282961000000	-1.221457000000	C	9.402404000000	8.667324000000	-1.221401000000
C	3.691876000000	12.272002000000	1.276556000000	C	9.413095000000	8.649575000000	1.285146000000
C	5.156636000000	11.688512000000	2.785785000000	C	10.380124000000	7.408492000000	2.794126000000
C	13.210141000000	-2.343321000000	-3.401500000000	C	10.086286000000	-8.673138000000	-3.430602000000
C	13.032979000000	-3.355502000000	-2.433854000000	C	9.406484000000	-9.435654000000	-2.478011000000
C	12.648204000000	-3.290313000000	0.074085000000	C	9.213667000000	-9.266038000000	0.039955000000
C	12.887190000000	-2.288659000000	3.486214000000	C	10.090499000000	-8.640761000000	3.442728000000
C	12.674222000000	-3.264276000000	2.588161000000	C	9.370998000000	-9.348285000000	2.547813000000
C	3.970172000000	12.266780000000	-3.443324000000	C	9.670419000000	8.508967000000	-3.440798000000
C	3.069170000000	12.605356000000	-2.489588000000	C	9.060623000000	9.256912000000	-2.489068000000
C	3.060770000000	12.486502000000	0.033876000000	C	8.976839000000	9.150376000000	0.037210000000
C	3.113940000000	12.584072000000	2.557718000000	C	9.081768000000	9.220485000000	2.564034000000
C	4.031051000000	12.236205000000	3.492714000000	C	9.697146000000	8.457218000000	3.499930000000
H	13.352070000000	-2.463008000000	-4.465298000000	H	10.116177000000	-8.823045000000	-4.499752000000
H	13.017530000000	-4.423657000000	-2.581388000000	H	8.799905000000	-10.313522000000	-2.633741000000
C	12.220821000000	-4.643576000000	0.081170000000	C	8.155573000000	-10.210947000000	0.051324000000
H	12.912625000000	-2.369148000000	4.563526000000	H	10.127366000000	-8.765614000000	4.515410000000
H	12.497203000000	-4.314138000000	2.762068000000	H	8.703251000000	-10.177118000000	2.724370000000
H	3.874056000000	12.365251000000	-4.515648000000	H	9.650874000000	8.649302000000	-4.512486000000
H	2.089041000000	13.039062000000	-2.618447000000	H	8.445982000000	10.134287000000	-2.621878000000
C	1.686800000000	12.848310000000	0.047090000000	C	7.979192000000	10.151197000000	0.047960000000
H	2.137159000000	13.018660000000	2.707223000000	H	8.469771000000	10.096865000000	2.714460000000
H	3.954158000000	12.325711000000	4.567384000000	H	9.685681000000	8.581217000000	4.573752000000
C	11.730645000000	-5.752478000000	0.067551000000	C	7.155926000000	-10.896460000000	0.043283000000
C	0.484803000000	13.006165000000	0.056817000000	C	7.026574000000	10.905441000000	0.055030000000
C	-0.882547000000	13.030851000000	0.067343000000	C	5.868160000000	11.620024000000	0.060583000000
C	-2.087989000000	12.901057000000	0.080536000000	C	4.772478000000	12.144723000000	0.067598000000
C	-3.473645000000	12.594579000000	0.072987000000	C	3.433904000000	12.592226000000	0.056265000000
C	-4.071974000000	12.372410000000	1.279871000000	C	2.807527000000	12.748473000000	1.277550000000
C	-4.088541000000	12.502081000000	-1.239530000000	C	2.844392000000	12.813849000000	-1.237084000000
C	-3.510311000000	12.605366000000	2.587005000000	C	3.417676000000	12.729709000000	2.569277000000
O	-5.330297000000	11.909573000000	1.428057000000	O	1.492159000000	12.977244000000	1.415858000000
O	-5.277539000000	11.903045000000	-1.418741000000	O	1.521656000000	12.958425000000	-1.401049000000
C	-3.608071000000	12.958706000000	-2.435283000000	C	3.486166000000	12.922358000000	-2.452765000000
C	-4.462072000000	12.302415000000	3.484810000000	C	2.438594000000	12.980776000000	3.466741000000
H	-2.512639000000	12.977010000000	2.761141000000	H	4.469317000000	12.568144000000	2.747306000000
C	-5.610066000000	11.819415000000	2.760731000000	C	1.213820000000	13.100628000000	2.741465000000
C	-5.572503000000	11.952852000000	-2.734344000000	C	1.286616000000	13.148462000000	-2.716275000000
C	-4.572841000000	12.605771000000	-3.403208000000	C	2.485095000000	13.146519000000	-3.400929000000
H	-2.675016000000	13.478940000000	-2.582664000000	H	4.550840000000	12.852484000000	-2.609719000000
H	-4.405516000000	12.365151000000	4.562118000000	H	2.524852000000	13.057914000000	4.541146000000
C	-6.725470000000	11.292656000000	3.296377000000	C	-0.027390000000	13.218934000000	3.274398000000
O	-7.939338000000	10.320675000000	1.417360000000	O	-1.556156000000	12.954194000000	1.401295000000
O	-7.920488000000	10.371186000000	-1.429422000000	O	-1.526715000000	12.973288000000	-1.415611000000

C	-6.712015000000	11.302330000000	-3.297659000000	C	-0.007819000000	13.219195000000	-3.274133000000
H	-4.539502000000	12.787793000000	-4.467111000000	H	2.600716000000	13.279329000000	-4.466503000000
C	-7.841746000000	10.603026000000	2.733056000000	C	-1.321628000000	13.144771000000	2.716533000000
C	-9.033966000000	9.562826000000	1.238116000000	C	-2.878502000000	12.806098000000	1.237317000000
C	-8.928533000000	9.487178000000	-1.281335000000	C	-2.841463000000	12.740974000000	-1.277320000000
C	-7.707809000000	10.574281000000	-2.762065000000	C	-1.248707000000	13.097511000000	-2.741210000000
C	-8.892977000000	10.036901000000	3.401949000000	C	-2.520099000000	13.139588000000	3.401184000000
C	-9.664453000000	9.358669000000	2.433935000000	C	-3.520565000000	12.912814000000	2.453003000000
C	-9.409441000000	9.067426000000	-0.074483000000	C	-3.467419000000	12.582976000000	-0.056045000000
C	-9.401921000000	9.105696000000	-2.588516000000	C	-3.451558000000	12.720651000000	-2.569050000000
C	-8.681000000000	9.797131000000	-3.486223000000	C	-2.473154000000	12.974415000000	-3.466495000000
H	-9.068538000000	10.094232000000	4.465916000000	H	-2.636075000000	13.272016000000	4.466768000000
H	-10.567427000000	8.787811000000	2.581303000000	H	-4.585048000000	12.840086000000	2.609951000000
C	-10.340892000000	7.996736000000	-0.082222000000	C	-4.804789000000	12.131889000000	-0.067391000000
H	-10.205335000000	8.407155000000	-2.762743000000	H	-4.502761000000	12.556270000000	-2.747092000000
H	-8.763361000000	9.777834000000	-4.563520000000	H	-2.559620000000	13.051397000000	-4.540894000000
C	-11.031157000000	7.000001000000	-0.069054000000	C	-5.899055000000	11.604243000000	-0.060369000000
C	-11.662976000000	5.787127000000	-0.058388000000	C	-7.055390000000	10.886540000000	-0.054845000000
C	-12.098622000000	4.655788000000	-0.048332000000	C	-8.006147000000	10.129762000000	-0.047850000000
C	-12.436922000000	3.275844000000	-0.034516000000	C	-9.001170000000	9.126327000000	-0.037233000000
C	-12.548602000000	2.643827000000	1.221073000000	C	-9.425654000000	8.642218000000	1.221338000000
C	-12.550120000000	2.618432000000	-1.276928000000	C	-9.435931000000	8.624327000000	-1.285208000000
C	-12.544802000000	3.326168000000	2.488941000000	C	-9.085618000000	9.232765000000	2.489027000000
N	-12.671090000000	1.311686000000	1.418894000000	N	-10.208842000000	7.560154000000	1.413548000000
N	-12.671838000000	1.282518000000	-1.447685000000	N	-10.219107000000	7.538604000000	-1.455490000000
C	-12.548832000000	3.274745000000	-2.558345000000	C	-9.105922000000	9.196050000000	-2.564075000000
C	-12.677092000000	2.373182000000	3.443072000000	C	-9.693590000000	8.483264000000	3.440701000000
H	-12.458046000000	4.394504000000	2.617366000000	H	-8.473315000000	10.111766000000	2.621889000000
C	-12.735071000000	1.108806000000	2.761245000000	C	-10.380612000000	7.423375000000	2.625817000000
Zn	-12.662879000000	-0.162560000000	0.000521000000	Zn	-10.960255000000	6.294038000000	-0.008778000000
C	-12.736989000000	1.052209000000	-2.785507000000	C	-10.399474000000	7.380636000000	-2.794272000000
C	-12.681194000000	2.302450000000	-3.492928000000	C	-9.719160000000	8.431128000000	-3.500024000000
H	-12.464488000000	4.340447000000	-2.708288000000	H	-8.496209000000	10.074028000000	-2.714452000000
H	-12.717450000000	2.505053000000	4.515358000000	H	-9.674580000000	8.623704000000	4.512385000000
C	-12.777999000000	-0.129393000000	3.390241000000	C	-11.057628000000	6.383598000000	3.380761000000
N	-12.634191000000	-1.607383000000	1.448718000000	N	-11.674802000000	5.034531000000	1.438150000000
N	-12.634056000000	-1.636540000000	-1.417864000000	N	-11.681480000000	5.010791000000	-1.430986000000
C	-12.778722000000	-0.198681000000	-3.389150000000	C	-11.077313000000	6.329207000000	-3.398567000000
H	-12.723422000000	2.412329000000	-4.567629000000	H	-9.707866000000	8.555109000000	-4.573850000000
C	-12.704557000000	-1.378814000000	2.786568000000	C	-11.631243000000	5.271320000000	2.776461000000
C	-12.478455000000	-2.939755000000	1.277894000000	C	-12.226638000000	3.814569000000	1.268139000000
C	-12.477442000000	-2.965110000000	-1.220105000000	C	-12.230734000000	3.792944000000	-1.238313000000
C	-12.703817000000	-1.435378000000	-2.760183000000	C	-11.644572000000	5.225338000000	-2.773236000000
C	-12.616450000000	-2.627212000000	3.493962000000	C	-12.206016000000	4.159885000000	3.482356000000
C	-12.459755000000	-3.595812000000	2.559304000000	C	-12.561995000000	3.245914000000	2.546704000000
C	-12.349069000000	-3.594061000000	0.035440000000	C	-12.442264000000	3.185491000000	0.020538000000
C	-12.456765000000	-3.647139000000	-2.487977000000	C	-12.570066000000	3.202066000000	-2.505809000000
C	-12.613804000000	-2.697854000000	-3.442047000000	C	-12.219939000000	4.100977000000	-3.457998000000
H	-12.655317000000	-2.738125000000	4.568684000000	H	-12.310947000000	4.089972000000	4.555990000000
H	-12.348109000000	-4.659009000000	2.709194000000	H	-13.020765000000	2.280470000000	2.697164000000
C	-11.975494000000	-4.964875000000	0.049096000000	C	-12.816774000000	1.823039000000	0.032694000000
H	-12.342762000000	-4.712905000000	-2.616450000000	H	-13.026864000000	2.233051000000	-2.638356000000
H	-12.651257000000	-2.830719000000	-4.514315000000	H	-12.329088000000	4.012658000000	-4.529846000000
C	-11.510921000000	-6.084647000000	0.058981000000	C	-12.996398000000	0.621268000000	0.042478000000
H	6.588623000000	-10.991314000000	-4.474127000000	H	0.046755000000	-12.781588000000	-4.473498000000
H	13.209383000000	0.156167000000	-4.377976000000	H	11.484413000000	-6.607707000000	-4.382398000000
H	6.228336000000	11.202336000000	-4.472620000000	H	11.083212000000	6.448666000000	-4.463443000000
H	-6.737167000000	11.355802000000	-4.380013000000	H	-0.001751000000	13.323073000000	-4.353056000000
H	-12.820108000000	-0.210307000000	-4.472246000000	H	-11.126937000000	6.347268000000	-4.481209000000
H	-6.466813000000	-11.508392000000	-4.379322000000	H	-11.621813000000	-6.714655000000	-4.332309000000
H	-6.760173000000	11.339919000000	4.378757000000	H	-0.033737000000	13.322711000000	4.353330000000
H	6.304987000000	11.155892000000	4.473029000000	H	11.110564000000	6.377121000000	4.481000000000
H	13.201921000000	0.182731000000	4.380667000000	H	11.639945000000	-6.684003000000	4.332358000000
H	6.514702000000	-11.041111000000	4.471518000000	H	-0.012547000000	-12.782187000000	4.473412000000
H	-6.443529000000	-11.525811000000	4.379445000000	H	-11.467008000000	-6.638286000000	4.382463000000
H	-12.819154000000	-0.118817000000	4.473357000000	H	-11.101091000000	6.419289000000	4.463233000000
c-P3Iso3⁴⁺				c-P3Iso3⁶⁺			
C	12.397932000000	-4.579453000000	1.262756000000	C	-5.034004000000	12.372224000000	1.249126000000
C	12.357754000000	-5.203056000000	2.530543000000	C	-4.568121000000	12.812563000000	2.497803000000
C	12.786325000000	-4.273449000000	3.431647000000	C	-5.566495000000	12.545052000000	3.398921000000
C	13.036701000000	-3.081652000000	2.713738000000	C	-6.595854000000	11.904165000000	2.684997000000
O	12.809963000000	-3.314978000000	1.397042000000	O	-6.253474000000	11.835743000000	1.382834000000
H	12.067317000000	-6.226830000000	2.708070000000	H	-3.617984000000	13.293292000000	2.675517000000
H	12.903809000000	-4.389459000000	4.499810000000	H	-5.578865000000	12.757512000000	4.458832000000

C	13.343432000000	-1.857560000000	3.248657000000	C	-7.726469000000	11.320220000000	3.226039000000
C	13.405809000000	-0.577812000000	2.702678000000	C	-8.682454000000	10.480370000000	2.685001000000
C	13.539439000000	0.620102000000	3.403828000000	C	-9.654504000000	9.755495000000	3.398941000000
O	13.222287000000	-0.304288000000	1.391579000000	O	-8.743664000000	10.136692000000	1.382819000000
C	13.396264000000	1.640326000000	2.483054000000	C	-10.267673000000	8.923449000000	2.497811000000
H	13.707945000000	0.707054000000	4.467632000000	H	-9.847751000000	9.844410000000	4.458872000000
C	13.208402000000	1.024872000000	1.247072000000	C	-9.687857000000	9.196791000000	1.249106000000
H	13.438094000000	2.704944000000	2.652021000000	H	-11.061715000000	8.213970000000	2.675522000000
C	13.051903000000	1.654176000000	-0.020822000000	C	-10.043358000000	8.643917000000	-0.000089000000
C	13.179310000000	1.015354000000	-1.261772000000	C	-9.687787000000	9.196676000000	-1.249314000000
C	13.311923000000	1.626052000000	-2.529524000000	C	-10.267544000000	8.923244000000	-2.498026000000
O	13.229442000000	-0.313623000000	-1.395961000000	O	-8.743564000000	10.136544000000	-1.383055000000
C	13.469941000000	0.614563000000	-3.430518000000	C	-9.654307000000	9.755195000000	-3.399193000000
H	13.312976000000	2.690217000000	-2.707115000000	H	-11.061600000000	8.213776000000	-2.675723000000
C	13.384141000000	-0.600185000000	-2.712574000000	C	-8.682276000000	10.480108000000	-2.685264000000
H	13.615125000000	0.693911000000	-4.498627000000	H	-9.847502000000	9.844021000000	-4.459141000000
C	13.344167000000	-1.861536000000	-3.247435000000	C	-7.726235000000	11.319882000000	-3.226316000000
C	13.053518000000	-3.109397000000	-2.701498000000	C	-6.595650000000	11.903865000000	-2.685248000000
C	12.854298000000	-4.298173000000	-3.402663000000	C	-5.566222000000	12.544646000000	-3.399168000000
O	12.801597000000	-3.322149000000	-1.390481000000	O	-6.253376000000	11.835597000000	-1.383050000000
C	12.436895000000	-5.240145000000	-2.482008000000	C	-4.567914000000	12.812246000000	-2.498001000000
H	12.992974000000	-4.428001000000	-4.466406000000	H	-5.578507000000	12.756970000000	-4.459107000000
C	12.424261000000	-4.596703000000	-1.246053000000	C	-5.033908000000	12.372073000000	-1.249308000000
H	12.185692000000	-6.275541000000	-2.651009000000	H	-3.617746000000	13.292926000000	-2.675693000000
C	12.101009000000	-5.159060000000	0.021740000000	C	-4.389542000000	12.501598000000	-0.000072000000
C	11.430589000000	-6.392806000000	0.026134000000	C	-3.016916000000	12.796821000000	-0.000035000000
C	10.711573000000	-7.375725000000	0.022423000000	C	-1.799807000000	12.861092000000	0.000012000000
C	12.744759000000	3.024278000000	-0.025395000000	C	-10.818760000000	7.473417000000	-0.000055000000
C	12.322138000000	4.166441000000	-0.021852000000	C	-11.322317000000	6.363509000000	-0.000026000000
C	7.754693000000	9.964612000000	-3.388782000000	C	-12.423728000000	-0.937037000000	-3.387509000000
C	6.733518000000	10.677080000000	-2.771626000000	C	-12.265436000000	-2.174090000000	-2.774367000000
C	8.700188000000	9.148569000000	-2.779617000000	C	-12.452979000000	0.309777000000	-2.774372000000
C	5.710762000000	11.409853000000	-3.464318000000	C	-12.134046000000	-3.423643000000	-3.473087000000
N	6.512841000000	10.738883000000	-1.430464000000	N	-12.157432000000	-2.384240000000	-1.434189000000
C	9.659292000000	8.341027000000	-3.480254000000	C	-12.510678000000	1.564883000000	-3.473106000000
N	8.820463000000	8.943727000000	-1.439832000000	N	-12.377739000000	0.533764000000	-1.434206000000
C	4.862809000000	11.882982000000	-2.518273000000	C	-11.918401000000	-4.373795000000	-2.531917000000
H	5.651438000000	11.537386000000	-4.536089000000	H	-12.197982000000	-3.549315000000	-4.544806000000
C	5.387280000000	11.457487000000	-1.247934000000	C	-11.944852000000	-3.702729000000	-1.257626000000
Zn	7.683019000000	9.855047000000	-0.000358000000	Zn	-12.293649000000	-0.927196000000	0.000015000000
C	10.330501000000	7.631057000000	-2.540429000000	C	-12.440117000000	2.536653000000	-2.531945000000
H	9.792897000000	8.320051000000	-4.552724000000	H	-12.592756000000	1.679520000000	-4.544826000000
C	9.794289000000	8.028452000000	-1.265883000000	C	-12.365504000000	1.869235000000	-1.257651000000
H	3.974359000000	12.479626000000	-2.658928000000	H	-11.777120000000	-5.433760000000	-2.678868000000
C	4.808503000000	11.754123000000	0.010736000000	C	-11.781712000000	-4.334648000000	0.000029000000
N	8.826356000000	8.936705000000	1.429748000000	N	-12.377687000000	0.533785000000	1.434217000000
N	6.521191000000	10.735008000000	1.439121000000	N	-12.157365000000	-2.384217000000	1.434233000000
H	11.126786000000	6.917397000000	-2.687831000000	H	-12.459573000000	3.605813000000	-2.678911000000
C	10.227585000000	7.532425000000	-0.011429000000	C	-12.299035000000	2.518486000000	-0.000011000000
C	5.395446000000	11.455358000000	1.265149000000	C	-11.944806000000	-3.702711000000	1.257679000000
C	3.521042000000	12.322754000000	0.015203000000	C	-11.360726000000	-5.678316000000	0.000035000000
C	9.798432000000	8.021170000000	1.247257000000	C	-12.365437000000	1.869253000000	1.257641000000
C	8.712479000000	9.135669000000	2.770956000000	C	-12.452842000000	0.309818000000	2.774390000000
C	6.749234000000	10.668574000000	2.778851000000	C	-12.265323000000	-2.174050000000	2.774412000000
C	11.093766000000	6.423196000000	-0.015870000000	C	-12.084339000000	3.910113000000	-0.000026000000
C	4.879003000000	11.878083000000	2.539678000000	C	-11.918322000000	-4.373762000000	2.531977000000
C	2.361268000000	12.694365000000	0.018628000000	C	-10.895483000000	-6.805094000000	0.000051000000
C	10.339392000000	7.616793000000	2.517607000000	C	-12.439956000000	2.536690000000	2.531932000000
C	9.673265000000	8.323290000000	3.463635000000	C	-12.510473000000	1.564934000000	3.473111000000
C	7.771888000000	9.951469000000	3.388060000000	C	-12.423576000000	-0.936988000000	3.387545000000
C	5.731635000000	11.400968000000	3.479507000000	C	-12.133924000000	-3.423596000000	3.473143000000
C	11.737695000000	5.389453000000	-0.019132000000	C	-11.793321000000	5.093910000000	-0.000028000000
H	3.992222000000	12.475574000000	2.687093000000	H	-11.777048000000	-5.433726000000	2.678936000000
H	11.135286000000	6.901333000000	2.658254000000	H	-12.459382000000	3.605852000000	2.678884000000
H	9.811518000000	8.297061000000	4.535398000000	H	-12.592483000000	1.679587000000	4.544834000000
H	5.678622000000	11.525387000000	4.551976000000	H	-12.197825000000	-3.549254000000	4.544865000000
C	-9.769539000000	8.586602000000	-0.022101000000	C	0.149770000000	-12.985464000000	-0.000065000000
C	-10.536825000000	7.469169000000	-0.019243000000	C	1.484760000000	-12.758470000000	-0.000073000000
C	-8.991372000000	9.523393000000	-0.025715000000	C	-1.063196000000	-13.104525000000	-0.000054000000
C	-11.110542000000	6.394885000000	-0.015872000000	C	2.655471000000	-12.418618000000	-0.000076000000
C	-7.958151000000	10.474202000000	-0.021200000000	C	-2.464593000000	-13.018509000000	0.000005000000
C	-11.638394000000	5.090244000000	-0.011313000000	C	3.968033000000	-11.908817000000	-0.000067000000
C	-7.468490000000	10.903587000000	-1.262071000000	C	-3.121166000000	-12.987211000000	-1.249183000000
C	-7.491343000000	10.924351000000	1.246830000000	C	-3.121062000000	-12.987077000000	1.249246000000

C	-11.851515000000	4.466939000000	-1.265700000000	C	4.563546000000	-11.641808000000	-1.257713000000
C	-11.847183000000	4.474385000000	1.247433000000	C	4.563551000000	-11.641832000000	1.257584000000
C	-8.063540000000	10.712722000000	-2.529956000000	C	-2.594463000000	-13.352563000000	-2.497889000000
O	-6.342613000000	11.611479000000	-1.396354000000	O	-4.407322000000	-12.639758000000	-1.382889000000
C	-8.118300000000	10.779606000000	2.482686000000	C	-2.594240000000	-13.352264000000	2.497951000000
O	-6.346933000000	11.600569000000	1.391310000000	O	-4.407216000000	-12.639648000000	1.383021000000
N	-12.157545000000	3.165967000000	-1.439537000000	N	5.726332000000	-10.984878000000	-1.434278000000
C	-11.775389000000	5.129872000000	-2.540285000000	C	4.022743000000	-12.039900000000	-2.532004000000
N	-12.154302000000	3.174830000000	1.430062000000	N	5.726350000000	-10.984925000000	1.434157000000
C	-11.767300000000	5.145145000000	2.517701000000	C	4.022747000000	-12.040028000000	2.531872000000
C	-7.266577000000	11.355097000000	-3.430969000000	C	-3.621643000000	-13.237792000000	-3.399015000000
H	-8.985623000000	10.181468000000	-2.707492000000	H	-1.582943000000	-13.685257000000	-2.675615000000
C	-6.171639000000	11.888400000000	-2.713049000000	C	-4.735530000000	-12.758650000000	-2.685076000000
C	-7.306024000000	11.413460000000	3.403533000000	C	-3.621349000000	-13.237420000000	3.399151000000
H	-9.061382000000	10.283889000000	2.651705000000	H	-1.582690000000	-13.684896000000	2.675625000000
C	-6.201755000000	11.896255000000	2.702379000000	C	-4.735311000000	-12.758398000000	2.685248000000
C	-12.274882000000	2.959318000000	-2.779271000000	C	5.957908000000	-10.938056000000	-2.774447000000
Zn	-12.378211000000	1.725436000000	0.000082000000	Zn	6.949706000000	-10.181874000000	-0.000055000000
C	-12.054876000000	4.193567000000	-3.480028000000	C	4.899655000000	-11.615347000000	-3.473175000000
H	-11.555261000000	6.176243000000	-2.687796000000	H	3.106443000000	-12.591241000000	-2.678965000000
C	-12.269666000000	2.976899000000	2.771261000000	C	5.957932000000	-10.938131000000	2.774325000000
C	-12.046262000000	4.215145000000	3.463827000000	C	4.899670000000	-11.615417000000	3.473046000000
H	-11.545407000000	6.192101000000	2.658258000000	H	3.106438000000	-12.591264000000	2.678827000000
H	-7.407789000000	11.440913000000	-4.499111000000	H	-3.601969000000	-13.449597000000	-4.458948000000
C	-5.059385000000	12.484317000000	-3.247982000000	C	-5.940934000000	-12.350906000000	-3.226109000000
O	-3.523065000000	12.744979000000	-1.391087000000	O	-7.124157000000	-11.333448000000	-1.382843000000
O	-3.533351000000	12.748786000000	1.396547000000	O	-7.124062000000	-11.333348000000	1.383084000000
H	-7.465533000000	11.515960000000	4.467336000000	H	-3.601583000000	-13.449088000000	4.459109000000
C	-5.061947000000	12.481878000000	3.248327000000	C	-5.940681000000	-12.350630000000	3.226342000000
C	-12.509072000000	1.732409000000	-3.388343000000	C	7.023174000000	-10.289521000000	-3.387592000000
N	-12.558769000000	0.269988000000	-1.429894000000	N	8.143596000000	-9.335618000000	-1.434261000000
N	-12.559521000000	0.279414000000	1.439700000000	N	8.143614000000	-9.335665000000	1.434165000000
H	-12.103509000000	4.319677000000	-4.552507000000	H	4.841367000000	-11.743708000000	-4.544897000000
C	-12.506073000000	1.754472000000	3.388506000000	C	7.023215000000	-10.289628000000	3.387479000000
H	-12.092605000000	4.348096000000	4.535580000000	H	4.841386000000	-11.743796000000	4.544766000000
C	-3.833293000000	12.856757000000	-2.702081000000	C	-7.012120000000	-11.664030000000	-2.685029000000
C	-2.230640000000	13.055738000000	-1.246676000000	C	-8.198699000000	-10.545878000000	-1.249087000000
C	-3.848637000000	12.828152000000	2.713335000000	C	-7.011925000000	-11.663826000000	2.685289000000
C	-2.232230000000	13.024014000000	1.262149000000	C	-8.198621000000	-10.545796000000	1.249348000000
C	-12.615657000000	0.491920000000	-2.771110000000	C	8.015530000000	-9.534156000000	-2.774445000000
C	-12.618454000000	-1.064018000000	-1.247274000000	C	9.179291000000	-8.492446000000	-1.257697000000
C	-12.620628000000	-1.055657000000	1.265875000000	C	9.179315000000	-8.492497000000	1.257614000000
C	-12.615982000000	0.510277000000	2.779446000000	C	8.015574000000	-9.534257000000	2.774343000000
C	-2.704369000000	13.278806000000	-3.403241000000	C	-8.081964000000	-11.093245000000	-3.398922000000
C	-1.679842000000	13.388565000000	-2.482521000000	C	-8.813026000000	-10.362647000000	-2.497753000000
C	-1.581983000000	13.056976000000	0.021233000000	C	-8.633100000000	-10.052599000000	0.000129000000
C	-2.691044000000	13.206909000000	3.431211000000	C	-8.081730000000	-11.093007000000	3.399213000000
C	-1.671860000000	13.300563000000	2.530090000000	C	-8.812864000000	-10.362484000000	2.498044000000
C	-12.739061000000	-0.760261000000	-3.463674000000	C	9.032091000000	-8.795745000000	-3.473164000000
C	-12.724857000000	-1.731087000000	-2.517548000000	C	9.747259000000	-8.134066000000	-2.531991000000
C	-12.585933000000	-1.713495000000	0.011484000000	C	9.645088000000	-8.035324000000	-0.000038000000
C	-12.728561000000	-1.714162000000	2.540466000000	C	9.747315000000	-8.134176000000	2.531912000000
C	-12.741590000000	-0.737124000000	3.480203000000	C	9.032159000000	-8.795887000000	3.473071000000
H	-2.661311000000	13.463816000000	-4.466983000000	H	-8.259719000000	-11.210148000000	-4.458847000000
H	-0.657640000000	13.688964000000	-2.651551000000	H	-9.704556000000	-9.780365000000	-2.675424000000
C	-0.178256000000	13.093409000000	0.025550000000	C	-9.575223000000	-9.011610000000	0.000124000000
H	-2.649189000000	13.366396000000	4.499408000000	H	-8.259421000000	-11.209837000000	4.459157000000
H	-0.639952000000	13.560681000000	2.707543000000	H	-9.704398000000	-9.780215000000	2.675739000000
H	-12.819935000000	-0.875494000000	-4.535429000000	H	9.172859000000	-8.788251000000	-4.544887000000
H	-12.797476000000	-2.798834000000	-2.658107000000	H	10.594673000000	-7.481860000000	-2.678951000000
C	-12.434716000000	-3.112702000000	0.016087000000	C	10.598347000000	-6.999005000000	-0.000028000000
H	-12.802731000000	-2.780862000000	2.687980000000	H	10.594741000000	-7.481988000000	2.678883000000
H	-12.822850000000	-0.845143000000	4.552682000000	H	9.172948000000	-8.788439000000	4.544792000000
C	1.032491000000	12.962483000000	0.021721000000	C	-10.239440000000	-7.989698000000	0.000093000000
C	-12.176653000000	-4.302940000000	0.019541000000	C	11.341588000000	-6.032733000000	-0.000022000000
C	-11.744267000000	-5.587611000000	0.022448000000	C	12.039482000000	-4.872292000000	-0.000030000000
C	-11.252132000000	-6.701589000000	0.026127000000	C	12.592420000000	-3.786130000000	-0.000036000000
C	-10.518604000000	-7.898857000000	0.021607000000	C	13.023024000000	-2.449778000000	-0.000042000000
C	-10.164789000000	-8.445650000000	1.262522000000	C	13.233119000000	-1.826967000000	1.249176000000
C	-10.193261000000	-8.459911000000	-1.246360000000	C	13.233023000000	-1.826951000000	-1.249266000000
C	-10.684544000000	-8.099037000000	2.530450000000	C	13.381582000000	-2.450612000000	2.497839000000
O	-9.275575000000	-9.434601000000	1.396713000000	O	13.378053000000	-0.502613000000	1.382920000000
O	-9.277699000000	-9.423585000000	-1.390905000000	O	13.377974000000	-0.502599000000	-1.383009000000
C	-10.757134000000	-8.149457000000	-2.482117000000	C	13.381364000000	-2.450585000000	-2.497948000000

C	-10.093533000000	-8.934862000000	3.431457000000	C	13.648915000000	-1.452220000000	3.398991000000
H	-11.426003000000	-7.335708000000	2.708072000000	H	13.323009000000	-3.513835000000	2.675522000000
C	-9.186574000000	-9.747540000000	2.713421000000	C	13.608391000000	-0.240313000000	2.685100000000
C	-9.219489000000	-9.748107000000	-2.701902000000	C	13.608197000000	-0.240288000000	-2.685207000000
C	-10.149733000000	-8.981698000000	-3.402933000000	C	13.648631000000	-1.452187000000	-3.399116000000
H	-11.528608000000	-7.414612000000	-2.651051000000	H	13.322741000000	-3.513806000000	-2.675632000000
H	-10.252553000000	-8.978586000000	4.499649000000	C	13.839076000000	-1.547735000000	4.458906000000
C	-8.279678000000	-10.625034000000	3.248248000000	H	13.667729000000	1.030800000000	3.226175000000
O	-6.873949000000	-11.296526000000	1.391045000000	O	13.151212000000	2.503381000000	1.382931000000
O	-6.885801000000	-11.297982000000	-1.396521000000	O	13.151139000000	2.503400000000	-1.382997000000
C	-8.283718000000	-10.623470000000	-3.247958000000	C	13.667510000000	1.030828000000	-3.226283000000
H	-10.331632000000	-9.036962000000	-4.466646000000	H	13.838682000000	-1.547685000000	-4.459052000000
C	-7.202504000000	-11.318845000000	2.702158000000	C	13.418233000000	2.278591000000	2.685122000000
C	-5.715907000000	-11.949044000000	1.246415000000	C	12.809155000000	3.790981000000	1.249193000000
C	-5.709619000000	-11.918738000000	-1.262392000000	C	12.809080000000	3.790996000000	-1.249230000000
C	-7.211271000000	-11.288439000000	-2.713181000000	C	13.418065000000	2.278619000000	-2.685210000000
C	-6.231863000000	-12.033518000000	3.403175000000	C	13.276319000000	3.482841000000	3.399042000000
C	-5.276759000000	-12.419564000000	2.482268000000	C	12.862229000000	4.429815000000	2.497892000000
C	-5.092756000000	-12.128022000000	-0.021613000000	C	12.508055000000	4.375250000000	-0.000060000000
C	-5.246819000000	-12.338479000000	-2.530354000000	C	12.862057000000	4.429835000000	-2.497931000000
C	-6.201820000000	-11.969743000000	-3.431235000000	C	13.276096000000	3.482871000000	-3.399113000000
H	-6.240731000000	-12.223007000000	4.466964000000	H	13.449911000000	3.605777000000	4.458975000000
H	-4.375671000000	-12.988099000000	2.651135000000	H	12.644681000000	5.472189000000	2.675584000000
C	-3.752551000000	-12.547104000000	-0.026257000000	C	11.881826000000	5.631898000000	0.000017000000
H	-4.325564000000	-12.871132000000	-2.707997000000	H	12.644499000000	5.472209000000	-2.675608000000
H	-6.205619000000	-12.134925000000	-4.499380000000	H	13.449614000000	3.605821000000	-4.459056000000
C	-2.552151000000	-12.752262000000	-0.022731000000	C	11.172175000000	6.622785000000	0.000040000000
C	-1.200704000000	-12.857725000000	-0.019909000000	C	10.308044000000	7.665383000000	0.000095000000
C	0.016473000000	-12.817093000000	-0.016551000000	C	9.428278000000	8.509229000000	0.000132000000
C	1.410302000000	-12.621794000000	-0.011901000000	C	8.330368000000	9.390887000000	0.000121000000
C	2.047928000000	-12.494607000000	1.246859000000	C	7.801298000000	9.773022000000	1.257761000000
C	2.056695000000	-12.494648000000	-1.266221000000	C	7.801330000000	9.773030000000	-1.257532000000
C	1.427006000000	-12.760746000000	2.517105000000	C	8.416550000000	9.503843000000	2.532064000000
N	3.326940000000	-12.110784000000	1.429583000000	N	6.650891000000	10.451402000000	1.434314000000
N	3.336410000000	-12.109175000000	-1.440001000000	N	6.650916000000	10.451390000000	-1.434110000000
C	1.444590000000	-12.760158000000	-2.540853000000	C	8.416624000000	9.503874000000	-2.531819000000
C	2.371815000000	-12.537277000000	3.463288000000	C	7.610258000000	10.050845000000	3.473224000000
H	0.409360000000	-13.092056000000	2.657604000000	H	9.352165000000	8.986060000000	2.679042000000
C	3.555927000000	-12.111669000000	2.770782000000	C	6.494501000000	10.628509000000	2.774481000000
Zn	4.694198000000	-11.580031000000	-0.000311000000	Zn	5.343646000000	11.109120000000	0.000088000000
C	3.574103000000	-12.107452000000	-2.779705000000	C	6.494561000000	10.628507000000	-2.774281000000
C	2.395240000000	-12.534019000000	-3.480540000000	C	7.610349000000	10.050870000000	-3.472996000000
H	0.428352000000	-13.092710000000	-2.688423000000	H	9.352255000000	8.986112000000	-2.678775000000
H	2.279770000000	-12.643827000000	4.535039000000	H	7.750548000000	10.064552000000	4.544948000000
C	4.732752000000	-11.705181000000	3.388115000000	C	5.400097000000	11.226576000000	3.387619000000
N	6.037080000000	-11.014066000000	1.439376000000	N	4.013674000000	11.719627000000	1.434289000000
N	6.045056000000	-11.008762000000	-1.430204000000	N	4.013704000000	11.719624000000	-1.434143000000
C	4.753783000000	-11.696837000000	-3.388729000000	C	5.400162000000	11.226557000000	-3.387444000000
H	2.310398000000	-12.639161000000	-4.553027000000	H	7.750670000000	10.064590000000	-4.544716000000
C	5.865249000000	-11.178322000000	2.779122000000	C	4.249643000000	11.708038000000	2.774472000000
C	7.223924000000	-10.399603000000	1.265611000000	C	2.765538000000	12.194765000000	1.257715000000
C	7.230244000000	-10.393598000000	-1.247511000000	C	2.765555000000	12.194742000000	-1.257595000000
C	5.881338000000	-11.168952000000	-2.771436000000	C	4.249689000000	11.708007000000	-2.774322000000
C	7.008346000000	-10.663476000000	3.479947000000	C	3.101775000000	12.218974000000	3.473186000000
C	7.848098000000	-10.163824000000	2.540258000000	C	2.171118000000	12.507334000000	2.532005000000
C	7.776432000000	-10.040791000000	0.011261000000	C	2.136724000000	12.369443000000	0.000055000000
C	7.861235000000	-10.152256000000	-2.517768000000	C	2.171147000000	12.507269000000	-2.531900000000
C	7.027566000000	-10.649839000000	-3.463938000000	C	3.101821000000	12.218906000000	-3.473062000000
H	7.142436000000	-10.679820000000	4.552436000000	H	3.024874000000	12.337121000000	4.544909000000
H	8.809013000000	-9.694807000000	2.687818000000	H	1.182509000000	12.914933000000	2.678957000000
C	8.912791000000	-9.210480000000	0.015916000000	C	0.762570000000	12.676628000000	0.000043000000
H	8.822303000000	-9.681383000000	-2.658262000000	H	1.182533000000	12.914847000000	-2.678875000000
H	7.167845000000	-10.662273000000	-4.535686000000	H	3.024932000000	12.337026000000	-4.544789000000
C	9.814834000000	-8.392215000000	0.019413000000	C	-0.445885000000	12.837005000000	0.000030000000
H	7.791793000000	10.018014000000	-4.470790000000	H	-12.495782000000	-0.942478000000	-4.468999000000
H	-5.114633000000	12.627220000000	-4.321339000000	H	-6.025551000000	-12.526842000000	-4.292673000000
H	-12.573897000000	1.737774000000	-4.470350000000	H	7.063860000000	-10.349152000000	-4.469086000000
H	-8.379968000000	-10.742782000000	-4.321302000000	H	13.862081000000	1.045513000000	-4.292865000000
H	4.781605000000	-11.755669000000	-4.470734000000	H	5.431468000000	11.291623000000	-4.468936000000
H	13.495755000000	-1.885227000000	-4.320760000000	H	-7.836229000000	11.481098000000	-4.292892000000
H	-8.371617000000	-10.747175000000	4.321653000000	H	13.862390000000	1.045489000000	4.292741000000
H	-12.569920000000	1.767043000000	4.470511000000	H	7.063914000000	-10.349292000000	4.468970000000
H	-5.121546000000	12.622552000000	4.321746000000	H	-6.025200000000	-12.526463000000	4.292930000000
H	7.814608000000	10.000579000000	4.470064000000	H	-12.495578000000	-0.942414000000	4.469038000000

H	13.495284000000	-1.876234000000	4.322045000000	H	-7.836553000000	11.481545000000	4.292589000000
H	4.753708000000	-11.766740000000	4.470123000000	H	5.431384000000	11.291651000000	4.469112000000