

Supplementary Information Available

Rationalization of the inhibition activity of structurally related organometallic compounds against the drug target cathepsin B by DFT

Angela Casini,^a Fabio Edefe,^a Mikael Erlandsson,^b Luca Gonsalvi,^{b,*} Alessandro Marrone,^c
Antonella Ciancetta,^c Nazzareno Re,^{c,*} Andrea Ienco,^b Luigi Messori,^d Maurizio Peruzzini^b and
Paul J. Dyson^{a,*}

^a *Institut des Sciences et Ingénierie Chimiques, Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland.*

^b *Istituto di Chimica dei Composti Organometallici, Consiglio Nazionale delle Ricerche (ICCOM - CNR), Via Madonna del Piano 10, 50019 Sesto Fiorentino (Firenze), Italy.*

^c *Dipartimento di Scienze del Farmaco, Università G.d'Annunzio, Via dei Vestini 31, 66100 Chieti, Italy.*

^d *Dipartimento di Chimica, Università di Firenze, Via della Lastruccia 3, 50019 Sesto Fiorentino (Firenze), Italy.*

Table S1. Crystal data and structure refinement for **3**.

Empirical formula	C ₅₆ H ₉₃ Cl ₆ F ₉ Ir ₃ N ₁₀ O ₉ P ₃ S ₃
Formula weight	2199.79
Temperature (K)	298(2)
Wavelength (Å)	0.71069
Crystal system	Triclinic
Space group	P ₁
Unit cell dimensions	
<i>a</i> (Å)	13.8621(3)
<i>b</i> (Å)	15.8188(4)
<i>c</i> (Å)	18.3948(4)
α (deg)	102.0414(18)
β (deg)	92.5974(18)
γ (deg)	90.3916(19)
Volume (Å ³)	3940.29(16)
<i>Z</i>	2
Calcd density (g/cm ³)	1.854
Absorption coefficient (mm ⁻¹)	5.474
F(000)	2156
Crystal size (mm ³)	0.20 x 0.16 x 0.10
Theta range for data collection (deg)	3.77 to 32.7
Index ranges	-20 ≤ <i>h</i> ≤ 20, -23 ≤ <i>k</i> ≤ 16, -26 ≤ <i>l</i> ≤ 26
Reflections collected	56975
Independent reflections	25286 [<i>R</i> _(int) = 0.0379]
Completeness to theta = 25.00°	99.2 %
Absorption correction	Semi-empirical from equivalents
Max. and min. Transmission	1 and 0.37693
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	25286 / 22 / 892
Goodness-of-fit on F ²	0.934
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0395, <i>wR</i> ₂ = 0.0879
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0955, <i>wR</i> ₂ = 0.1131
Largest diff. peak and hole (e ⁻ ·Å ⁻³)	2.192 and -1.721

Cartesian coordinates of optimized geometries of all considered complexes

[Ru(η^6 -C₁₀H₁₄)(PTA)Cl₂]

C	-13.90430	71.51300	-53.62580
C	-15.17760	72.01940	-53.33480
C	-15.97780	71.45770	-52.28090
C	-15.55930	70.31840	-51.55650
C	-14.23740	69.81930	-51.82220
C	-13.42230	70.42900	-52.79960
H	-15.53810	72.91080	-53.83370
H	-16.92430	71.92890	-52.03630
H	-13.84770	68.98730	-51.24270
H	-12.39920	70.08970	-52.92520
Ru	-14.01630	72.00180	-51.32010
Cl	-14.89940	74.19630	-50.66330
Cl	-11.72940	72.89150	-51.40050
P	-13.60540	71.85160	-49.02650
C	-12.61830	73.19650	-48.15940
H	-13.12540	74.15190	-48.31920
H	-11.63260	73.26270	-48.62590
C	-15.06000	71.80320	-47.83560
H	-15.64760	72.71640	-47.97720
H	-15.70900	70.95100	-48.06610
C	-12.67000	70.37210	-48.33810
H	-13.19360	69.44260	-48.59600
H	-11.67880	70.33290	-48.80470
C	-11.77180	71.65570	-46.47200
H	-10.81420	71.67290	-47.00220
H	-11.57360	71.58110	-45.39680
C	-13.83490	70.47620	-46.19990
H	-13.65840	70.39070	-45.12180
H	-14.42190	69.60850	-46.52230
C	-13.79120	72.86280	-46.04680
H	-13.61600	72.80320	-44.96650
H	-14.34480	73.78250	-46.26020
C	-12.98310	72.08970	-54.68540
H	-11.98610	72.12870	-54.22680
C	-13.34320	73.51660	-55.11760
N	-12.52570	70.45210	-46.87520
N	-12.48690	72.91480	-46.72200
N	-14.61430	71.70230	-46.43640
C	-16.46990	69.63230	-50.57160
H	-17.04340	68.84650	-51.08190
H	-15.90790	69.15190	-49.76400
H	-17.18490	70.33360	-50.13140
C	-12.92310	71.13350	-55.89700
H	-12.19270	71.49850	-56.62850
H	-12.62610	70.11910	-55.60460
H	-13.89840	71.06860	-56.39610

H	-12.57460	73.89670	-55.79970
H	-14.30060	73.55500	-55.65370
H	-13.39270	74.19090	-54.25650

[Os(η^6 -C₁₀H₁₄)(PTA)Cl₂]

C	-13.89450	71.52380	-53.62110
C	-15.17930	72.00180	-53.31210
C	-15.95750	71.42080	-52.24480
C	-15.50470	70.27580	-51.53280
C	-14.17530	69.80070	-51.82260
C	-13.37500	70.44520	-52.80340
H	-15.55250	72.90130	-53.78640
H	-16.90630	71.87570	-51.98000
H	-13.75680	68.98030	-51.24720
H	-12.34400	70.13360	-52.93580
Os	-14.01720	71.96000	-51.33510
Cl	-14.89390	74.17290	-50.68860
Cl	-11.76840	72.96320	-51.43940
P	-13.60110	71.82550	-49.02420
C	-12.54890	73.14040	-48.18930
H	-13.00090	74.11740	-48.38240
H	-11.55630	73.14270	-48.64590
C	-15.06180	71.88600	-47.84380
H	-15.60180	72.82240	-48.01870
H	-15.75010	71.06060	-48.05790
C	-12.74860	70.32130	-48.28750
H	-13.31810	69.41320	-48.52300
H	-11.75730	70.21520	-48.74410
C	-11.79590	71.61050	-46.45170
H	-10.83480	71.56320	-46.97400
H	-11.60860	71.55650	-45.37340
C	-13.91860	70.54750	-46.16140
H	-13.75210	70.48470	-45.08030
H	-14.54780	69.70220	-46.46250
C	-13.75280	72.93260	-46.07780
H	-13.58840	72.89790	-44.99480
H	-14.25660	73.87250	-46.32390
C	-12.99490	72.14060	-54.67770
H	-11.99500	72.19580	-54.22760
C	-13.39020	73.56540	-55.08570
N	-12.60850	70.43630	-46.82690
N	-12.44260	72.89700	-46.74300
N	-14.63150	71.80440	-46.43960
C	-16.38500	69.57480	-50.53200
H	-16.94570	68.77280	-51.03100
H	-15.80080	69.11380	-49.72860
H	-17.11000	70.26280	-50.08680
C	-12.92300	71.20510	-55.90420
H	-12.20620	71.59760	-56.63510
H	-12.60170	70.19320	-55.62960

H	-13.90000	71.12640	-56.39790
H	-12.63480	73.97260	-55.76710
H	-14.35150	73.58970	-55.61560
H	-13.44900	74.22650	-54.21510

[Rh(η^5 -C₅Me₅)(PTA)Cl₂]

Rh	-13.95280	68.19050	-51.42310
Cl	-15.05450	70.24490	-50.67750
Cl	-11.69420	69.13100	-51.58780
P	-13.41730	67.94540	-49.19370
C	-12.70210	69.42320	-48.27750
H	-13.41770	70.24720	-48.33740
H	-11.78820	69.73740	-48.78870
C	-14.75200	67.49740	-47.94960
H	-15.53320	68.26470	-47.98800
H	-15.21280	66.53830	-48.21500
C	-12.13330	66.67730	-48.67290
H	-12.44560	65.67180	-48.97980
H	-11.19400	66.90640	-49.18800
C	-11.42860	68.00790	-46.75630
H	-10.53400	68.27490	-47.32770
H	-11.15200	67.91060	-45.70040
C	-13.15930	66.37800	-46.48150
H	-12.90190	66.26460	-45.42250
H	-13.55830	65.42360	-46.84320
C	-13.63540	68.69900	-46.14620
H	-13.38490	68.61020	-45.08300
H	-14.39070	69.48290	-46.26150
N	-11.92280	66.69520	-47.21600
N	-12.41940	69.08670	-46.87480
N	-14.20510	67.41000	-46.58510
C	-15.75980	67.14690	-52.17270
C	-14.74320	66.15380	-51.94250
C	-13.61990	66.47200	-52.78280
C	-14.00710	67.59050	-53.64260
C	-15.31000	67.99910	-53.27290
C	-17.13160	67.20070	-51.56950
H	-17.42440	68.23470	-51.36290
H	-17.87490	66.76640	-52.25350
H	-17.18290	66.64480	-50.62870
C	-16.12510	69.10960	-53.86030
H	-15.56080	69.67600	-54.60480
H	-17.02350	68.70650	-54.34790
H	-16.44390	69.80970	-53.08040
C	-13.13160	68.17290	-54.70860
H	-13.57700	69.06490	-55.15520
H	-12.15720	68.45670	-54.29590
H	-12.96420	67.43900	-55.50870
C	-12.34360	65.69850	-52.92890
H	-11.48900	66.37620	-53.01370

H	-12.16560	65.04250	-52.07180
H	-12.37080	65.06980	-53.83050
C	-14.87170	64.94890	-51.05750
H	-13.90520	64.62490	-50.66130
H	-15.54730	65.12840	-50.21630
H	-15.28560	64.10810	-51.63220

[Ir(η^5 -C₅Me₅)(PTA)Cl₂]

Ir	-13.95880	68.17190	-51.41960
Cl	-15.00910	70.28360	-50.72880
Cl	-11.75650	69.24720	-51.62180
P	-13.40940	67.92930	-49.19520
C	-12.71580	69.40320	-48.26170
H	-13.44380	70.21770	-48.30560
H	-11.80990	69.74250	-48.77110
C	-14.72860	67.44010	-47.95340
H	-15.52630	68.19120	-47.97760
H	-15.17160	66.47650	-48.23270
C	-12.10510	66.67560	-48.69880
H	-12.40600	65.67070	-49.01920
H	-11.17170	66.92290	-49.21670
C	-11.41160	67.98750	-46.76650
H	-10.52430	68.27740	-47.33810
H	-11.12780	67.87940	-45.71360
C	-13.11350	66.32530	-46.50840
H	-12.85000	66.20010	-45.45230
H	-13.49830	65.36990	-46.88270
C	-13.62620	68.63270	-46.13670
H	-13.36930	68.53180	-45.07610
H	-14.39510	69.40540	-46.23640
N	-11.88580	66.67370	-47.24340
N	-12.42030	69.05200	-46.86440
N	-14.17670	67.34130	-46.59230
C	-15.76140	67.15500	-52.16850
C	-14.73610	66.16820	-51.90600
C	-13.60250	66.46100	-52.75640
C	-13.99070	67.56230	-53.64080
C	-15.29780	67.98290	-53.28430
C	-17.14910	67.19780	-51.60020
H	-17.47140	68.23040	-51.43690
H	-17.86510	66.72020	-52.28450
H	-17.20720	66.67710	-50.63990
C	-16.10500	69.08390	-53.90110
H	-15.52130	69.65560	-54.62620
H	-16.98020	68.66790	-54.41880
H	-16.45850	69.78170	-53.13480
C	-13.11190	68.12050	-54.71770
H	-13.54440	69.01600	-55.17010
H	-12.13010	68.39170	-54.31560
H	-12.96540	67.37450	-55.51060
C	-12.34680	65.65420	-52.90590

H	-11.48190	66.30700	-53.05610
H	-12.15170	65.04380	-52.01910
H	-12.41800	64.97690	-53.76910
C	-14.88250	64.96470	-51.02170
H	-13.92420	64.63940	-50.60700
H	-15.57240	65.14830	-50.19350
H	-15.28790	64.12640	-51.60580

[Ir(η^5 -C₅Me₅)(MePTA)Cl₂]⁺

Ir	-13.96430	68.13100	-51.40910
Cl	-15.02210	70.21210	-50.61230
Cl	-11.74100	69.19860	-51.51370
P	-13.44530	67.81370	-49.20560
C	-12.76660	69.35820	-48.39020
H	-13.51250	70.15260	-48.47520
H	-11.87090	69.67220	-48.93240
C	-14.73250	67.40630	-47.90840
H	-15.54200	68.14110	-47.97040
H	-15.16600	66.41860	-48.09420
C	-12.10300	66.63710	-48.64070
H	-12.37660	65.60250	-48.87040
H	-11.18130	66.86600	-49.18570
C	-11.35850	68.02460	-46.78780
H	-10.50300	68.32340	-47.39870
H	-11.07900	68.01150	-45.73030
C	-13.07140	66.41850	-46.39740
H	-12.79280	66.36480	-45.34000
H	-13.44390	65.44030	-46.70820
C	-13.68340	68.70440	-46.14060
H	-13.38480	68.68570	-45.08840
H	-14.44150	69.47500	-46.30190
N	-11.87690	66.75740	-47.18630
N	-12.41760	69.16160	-46.92940
N	-14.13870	67.41860	-46.55640
C	-15.76540	67.17290	-52.24750
C	-14.75450	66.15930	-52.03200
C	-13.59860	66.49220	-52.83800
C	-13.94910	67.66390	-53.64180
C	-15.26340	68.07800	-53.28260
C	-17.16710	67.18530	-51.71550
H	-17.49630	68.20560	-51.49990
H	-17.85870	66.75500	-52.45290
H	-17.25850	66.60080	-50.79550
C	-16.04370	69.21920	-53.85740
H	-15.41080	69.89280	-54.43880
H	-16.82810	68.83180	-54.52160
H	-16.52330	69.80750	-53.06990
C	-13.05510	68.27850	-54.67360
H	-13.41040	69.26280	-54.98540
H	-12.03550	68.39550	-54.29530
H	-13.01920	67.63270	-55.56140

C	-12.35670	65.67310	-53.02530
H	-11.47850	66.31330	-53.14640
H	-12.17470	65.00950	-52.17500
H	-12.44450	65.04590	-53.92310
C	-14.92430	64.91010	-51.21850
H	-13.97120	64.54050	-50.82900
H	-15.61500	65.05490	-50.38300
H	-15.34390	64.11720	-51.85270
C	-11.88680	70.43850	-46.36150
H	-11.63580	70.29320	-45.30790
H	-10.99540	70.73290	-46.92020
H	-12.64880	71.21510	-46.45960

[*trans*-RuCl₄(dmsO-S)(Im)]⁻

C	-7.25540	-3.44710	-0.60050
C	-7.31340	-2.11710	-0.92090
N	-6.80000	-1.94290	-2.19440
C	-6.41510	-3.13270	-2.62340
N	-6.66140	-4.07370	-1.68240
Ru	-6.62100	-0.11010	-3.23020
S	-6.25980	2.00770	-4.32220
C	-4.62460	2.65020	-3.84180
Cl	-5.15590	0.57480	-1.35920
Cl	-4.65560	-1.01650	-4.40960
O	-7.23300	3.15710	-4.23600
C	-5.93250	1.75080	-6.09970
Cl	-8.51990	0.76840	-1.93050
H	-5.95790	-3.33110	-3.57870
H	-7.66970	-1.27300	-0.35290
H	-6.70640	-5.06080	-1.89780
H	-7.55870	-3.98810	0.28310
H	-5.17050	0.97850	-6.21430
H	-5.62400	2.71370	-6.51560
H	-6.87120	1.42120	-6.54650
H	-3.88110	1.86240	-3.98510
H	-4.68800	2.90490	-2.78360
H	-4.42970	3.53280	-4.45870
Cl	-8.13790	-0.69180	-5.09780

[Ru(η⁶-C₁₀H₁₄)(PTA)ClH₂O]⁺

C	-13.83280	71.50290	-53.61780
C	-15.15050	71.91400	-53.37680
C	-15.93480	71.32900	-52.32240
C	-15.46420	70.24260	-51.54950
C	-14.09010	69.87410	-51.74010
C	-13.28630	70.52340	-52.70750
H	-15.58270	72.71800	-53.96240
H	-16.94100	71.70120	-52.14890
H	-13.64850	69.10100	-51.11930
H	-12.23640	70.25970	-52.78560
Ru	-14.04140	72.05250	-51.30130

O	-14.76780	74.05030	-50.59510
Cl	-12.03260	73.40880	-51.43370
P	-13.55300	71.77910	-48.99480
C	-12.42320	73.00950	-48.11500
H	-12.83000	74.01950	-48.23050
H	-11.43900	72.99590	-48.59090
C	-14.99750	71.84520	-47.78220
H	-15.50120	72.81300	-47.88330
H	-15.72590	71.06390	-48.02650
C	-12.74800	70.19590	-48.35910
H	-13.36350	69.32820	-48.62520
H	-11.77000	70.07160	-48.83880
C	-11.70710	71.35150	-46.48280
H	-10.75750	71.29010	-47.02340
H	-11.50410	71.23290	-45.41410
C	-13.87520	70.36500	-46.20490
H	-13.69210	70.23760	-45.13370
H	-14.54580	69.56480	-46.53550
C	-13.60090	72.73660	-45.99650
H	-13.41590	72.63280	-44.92290
H	-14.06680	73.71110	-46.17340
C	-12.95050	72.06350	-54.71620
H	-11.95830	72.20890	-54.26920
C	-13.41420	73.41460	-55.27430
N	-12.58410	70.24260	-46.90540
N	-12.30720	72.67790	-46.69430
N	-14.53250	71.66830	-46.40440
C	-16.35870	69.49800	-50.59480
H	-16.83040	68.65680	-51.11980
H	-15.80110	69.08070	-49.75100
H	-17.15870	70.13590	-50.20770
C	-12.81980	71.00720	-55.83980
H	-12.11810	71.36510	-56.60050
H	-12.44420	70.04850	-55.46430
H	-13.78520	70.82740	-56.32760
H	-12.67640	73.78320	-55.99400
H	-14.37050	73.33600	-55.80660
H	-13.50650	74.16710	-54.48350
H	-15.49130	74.44860	-51.10750
H	-13.95710	74.57290	-50.79370

[Os(η^6 -C₁₀H₁₄)(PTA)ClH₂O]⁺

C	-13.81080	71.51210	-53.61560
C	-15.13850	71.89220	-53.36300
C	-15.89950	71.29000	-52.29350
C	-15.40390	70.19150	-51.53870
C	-14.02240	69.85310	-51.74570
C	-13.23140	70.54210	-52.70910
H	-15.58700	72.70040	-53.93040
H	-16.90870	71.64450	-52.10200
H	-13.55590	69.09140	-51.12920

H	-12.17600	70.30390	-52.79210
OS	-14.04040	72.01070	-51.31030
O	-14.86060	73.99000	-50.60780
Cl	-12.13130	73.51570	-51.45250
P	-13.55520	71.77130	-48.99700
C	-12.32960	72.93380	-48.15700
H	-12.65660	73.96960	-48.29560
H	-11.35170	72.83690	-48.63750
C	-14.97900	71.97330	-47.77640
H	-15.41530	72.97060	-47.89920
H	-15.76130	71.23850	-47.99920
C	-12.86630	70.15040	-48.32640
H	-13.54720	69.32510	-48.56680
H	-11.90440	69.94120	-48.80950
C	-11.72460	71.26950	-46.48740
H	-10.78650	71.12360	-47.03200
H	-11.52220	71.16240	-45.41740
C	-13.95720	70.45500	-46.16920
H	-13.77380	70.34190	-45.09650
H	-14.68860	69.69890	-46.47370
C	-13.50530	72.80400	-46.02470
H	-13.31990	72.71480	-44.94990
H	-13.89900	73.80570	-46.22410
C	-12.94360	72.11940	-54.70230
H	-11.96060	72.29920	-54.24770
C	-13.45560	73.45660	-55.25210
N	-12.68550	70.21910	-46.87610
N	-12.22510	72.63130	-46.72880
N	-14.51710	71.79790	-46.39870
C	-16.27750	69.42920	-50.57900
H	-16.74510	68.58680	-51.10550
H	-15.70540	69.01350	-49.74440
H	-17.07940	70.05600	-50.17790
C	-12.76520	71.08020	-55.83450
H	-12.07430	71.47270	-56.58800
H	-12.35410	70.13370	-55.46550
H	-13.72000	70.86700	-56.32950
H	-12.72840	73.85930	-55.96430
H	-14.40480	73.34490	-55.79110
H	-13.58190	74.19930	-54.45680
H	-15.61340	74.33120	-51.12030
H	-14.09170	74.57610	-50.80020

[Rh(η^5 -C₅Me₅)(PTA)ClOH]

Rh	-14.11790	68.20270	-51.37210
Cl	-15.22050	70.28840	-50.72540
O	-12.28280	69.16640	-51.38580
P	-13.42480	67.94810	-49.18990
C	-12.95990	69.48750	-48.22260
H	-13.83520	70.13860	-48.14610
H	-12.19210	70.02320	-48.78750

C	-14.48460	67.13390	-47.86570
H	-15.42070	67.69520	-47.76070
H	-14.74610	66.11220	-48.16630
C	-11.85130	66.97320	-48.89050
H	-11.97430	65.94270	-49.24550
H	-11.05120	67.43590	-49.47780
C	-11.24710	68.31180	-46.94690
H	-10.50120	68.80760	-47.57610
H	-10.84220	68.21960	-45.93260
C	-12.53650	66.31990	-46.64580
H	-12.14800	66.20550	-45.62760
H	-12.75310	65.32280	-47.04580
C	-13.47190	68.44740	-46.07990
H	-13.09420	68.35570	-45.05530
H	-14.38930	69.04490	-46.05940
N	-11.48720	66.95140	-47.46360
N	-12.45730	69.14580	-46.88260
N	-13.78920	67.09140	-46.56710
C	-15.88920	67.22600	-52.36410
C	-15.00300	66.20500	-51.91440
C	-13.72300	66.40280	-52.57280
C	-13.88230	67.48640	-53.52560
C	-15.19180	68.01280	-53.38160
C	-17.32920	67.41890	-51.98970
H	-17.54840	68.47720	-51.81670
H	-17.99080	67.06170	-52.79200
H	-17.58800	66.87250	-51.07800
C	-15.81260	69.15200	-54.13250
H	-15.08340	69.66010	-54.76840
H	-16.62840	68.79220	-54.77420
H	-16.22670	69.89480	-53.44190
C	-12.77670	68.00130	-54.39520
H	-13.13340	68.75620	-55.10100
H	-12.00050	68.46080	-53.76670
H	-12.32060	67.18690	-54.97210
C	-12.52020	65.50680	-52.50010
H	-11.59530	66.08770	-52.56850
H	-12.49100	64.93830	-51.56540
H	-12.52060	64.77980	-53.32580
C	-15.35130	65.05960	-51.00800
H	-14.48510	64.71280	-50.43610
H	-16.14280	65.32370	-50.30080
H	-15.71030	64.20570	-51.60040
H	-12.51710	70.11090	-51.39100

[Ir(η^5 -C₅Me₅)(PTA)ClOH]

Ir	-14.08090	68.14830	-51.39310
Cl	-15.28100	70.14720	-50.59330
O	-12.40550	69.36690	-51.55750
P	-13.37250	67.89360	-49.22550
C	-12.47510	69.33050	-48.42530

H	-13.12430	70.21090	-48.46240
H	-11.58140	69.55220	-49.01540
C	-14.62690	67.57690	-47.86830
H	-15.36100	68.38990	-47.88090
H	-15.16560	66.64250	-48.06850
C	-12.14770	66.54930	-48.75450
H	-12.55970	65.56200	-48.99730
H	-11.23360	66.67940	-49.34580
C	-11.19680	67.87880	-46.94720
H	-10.33010	68.05880	-47.59170
H	-10.84810	67.79350	-45.91170
C	-13.01280	66.39350	-46.48130
H	-12.68020	66.29490	-45.44200
H	-13.50650	65.46030	-46.77520
C	-13.29340	68.75280	-46.20200
H	-12.96940	68.68380	-45.15740
H	-13.99780	69.58560	-46.29350
N	-11.81770	66.59310	-47.32030
N	-12.10970	69.02700	-47.03170
N	-13.98560	67.49580	-46.54510
C	-15.81670	67.11120	-52.32560
C	-14.84500	66.13700	-51.92840
C	-13.60300	66.42010	-52.64580
C	-13.87700	67.50880	-53.57330
C	-15.21140	67.95530	-53.36170
C	-17.25430	67.19230	-51.90250
H	-17.55400	68.23110	-51.73420
H	-17.91080	66.76850	-52.67590
H	-17.43320	66.64220	-50.97410
C	-15.92940	69.06690	-54.06900
H	-15.24670	69.66200	-54.68110
H	-16.71100	68.66350	-54.72760
H	-16.40570	69.74400	-53.35190
C	-12.84700	68.11960	-54.47370
H	-13.29780	68.80230	-55.19910
H	-12.12900	68.68980	-53.86630
H	-12.30390	67.34530	-55.02840
C	-12.36050	65.57610	-52.66270
H	-11.46890	66.19320	-52.80860
H	-12.23350	65.02460	-51.72610
H	-12.39710	64.83850	-53.47810
C	-15.09290	64.94710	-51.04600
H	-14.18580	64.63100	-50.52220
H	-15.86500	65.14910	-50.29790
H	-15.43250	64.09430	-51.65090
H	-12.73420	70.27580	-51.44630

[*trans*-RuCl₂(dmsO-S)(Im)H₂OOH]

C	-0.03960	-3.37560	3.67080
C	0.52480	-2.22190	3.19790
N	-0.20830	-1.78020	2.11340

C	-1.19540	-2.64150	1.92150
N	-1.12630	-3.62480	2.85080
Ru	0.22490	-0.06380	0.96560
S	0.61100	1.92530	-0.22180
C	2.33190	2.50930	-0.15030
O	1.34170	0.48410	2.53900
Cl	1.96230	-1.16130	-0.19770
O	-0.27880	3.05010	0.28210
C	0.40870	1.77760	-2.01660
O	-1.22550	1.10740	2.15700
H	-1.93680	-2.57270	1.14010
H	1.38230	-1.66350	3.53860
H	-1.76240	-4.40660	2.92030
H	0.22550	-4.02610	4.49000
H	1.09990	1.01000	-2.37430
H	0.60700	2.75590	-2.46240
H	-0.62050	1.45880	-2.18570
H	2.98680	1.69860	-0.47990
H	2.53860	2.77870	0.88780
H	2.42520	3.39470	-0.78450
H	-0.61070	1.27440	2.90170
H	-1.27970	1.96190	1.66860
Cl	-1.57910	-0.55910	-0.57820
H	2.11950	1.01290	2.30240

[Ru(η^6 -C₁₀H₁₄)(PTA)Cl]⁺

C	-2.80850	-2.35170	-29.76270
C	-2.71810	-3.14820	-28.60800
C	-1.44350	-3.57210	-28.11450
C	-0.23360	-3.37180	-28.85390
C	-0.31870	-2.55680	-30.00980
C	-1.56370	-1.98440	-30.39560
H	-3.60110	-3.34980	-28.01260
H	-1.39730	-4.09770	-27.16480
H	0.58140	-2.29650	-30.55750
H	-1.58560	-1.28460	-31.22630
Ru	-1.24190	-1.39110	-28.30840
Cl	-2.52780	0.04760	-27.00610
P	0.58440	0.01130	-27.72960
C	0.45000	1.84100	-28.21690
H	-0.48250	2.23970	-27.80550
H	0.40380	1.91930	-29.30860
C	0.94670	0.27140	-25.88580
H	0.03060	0.62030	-25.39930
H	1.22800	-0.68690	-25.43560
C	2.35940	-0.27800	-28.30440
H	2.70750	-1.25560	-27.95150
H	2.39830	-0.28440	-29.40030
C	2.86950	2.10710	-28.27450
H	2.80500	2.09580	-29.36730
H	3.65770	2.80760	-27.98280

C	3.28690	0.78850	-26.31700
H	4.07910	1.47770	-26.00940
H	3.53500	-0.21050	-25.94410
C	1.67780	2.56770	-26.24200
H	2.45540	3.27280	-25.93360
H	0.72340	2.89430	-25.81850
C	-4.11200	-1.81410	-30.32260
H	-3.90970	-0.78600	-30.65410
C	-5.26530	-1.76790	-29.31170
N	3.24800	0.76690	-27.79080
N	1.59540	2.58780	-27.71340
N	2.02340	1.23820	-25.70870
C	1.05970	-3.98920	-28.39600
H	1.10730	-5.02900	-28.74560
H	1.92880	-3.46510	-28.80270
H	1.13440	-4.00740	-27.30420
C	-4.49080	-2.64410	-31.57360
H	-5.38980	-2.22160	-32.03460
H	-3.69560	-2.64470	-32.32790
H	-4.70640	-3.68460	-31.30390
H	-6.12910	-1.27590	-29.77000
H	-5.58960	-2.77320	-29.01570
H	-4.99520	-1.20420	-28.41280

[Os(η^6 -C₁₀H₁₄)(PTA)Cl]⁺

C	-2.86550	-2.35990	-29.68520
C	-2.72230	-3.14590	-28.52890
C	-1.41700	-3.53510	-28.06490
C	-0.23590	-3.33970	-28.85870
C	-0.37090	-2.52330	-30.01050
C	-1.64080	-1.95350	-30.34380
H	-3.58020	-3.35270	-27.89970
H	-1.33170	-4.05910	-27.11760
H	0.50680	-2.24480	-30.58460
H	-1.69860	-1.25380	-31.17210
Os	-1.25790	-1.37470	-28.28420
Cl	-2.57740	0.06740	-27.02270
P	0.56710	-0.00670	-27.68090
C	0.45890	1.82630	-28.16230
H	-0.47890	2.23320	-27.77110
H	0.43830	1.90900	-29.25440
C	0.88430	0.24360	-25.82720
H	-0.03970	0.60030	-25.36150
H	1.14440	-0.71920	-25.37410
C	2.34770	-0.31390	-28.21390
H	2.67620	-1.29600	-27.85560
H	2.41230	-0.31800	-29.30860
C	2.88080	2.06690	-28.16240
H	2.84170	2.06040	-29.25640
H	3.66930	2.75800	-27.84960
C	3.23850	0.73730	-26.20050

H	4.03030	1.41700	-25.87190
H	3.46720	-0.26540	-25.82530
C	1.64670	2.53330	-26.15650
H	2.42410	3.22900	-25.82730
H	0.68640	2.86890	-25.75410
C	-4.19650	-1.84750	-30.20500
H	-4.03050	-0.80810	-30.52130
C	-5.32710	-1.85290	-29.16750
N	3.23340	0.72110	-27.67500
N	1.59890	2.55950	-27.62930
N	1.96560	1.19840	-25.62020
C	1.07830	-3.94540	-28.44630
H	1.11840	-4.98650	-28.79220
H	1.92780	-3.41780	-28.88840
H	1.19360	-3.95640	-27.35790
C	-4.58280	-2.66540	-31.46070
H	-5.50280	-2.25980	-31.89450
H	-3.80540	-2.63260	-32.23250
H	-4.76480	-3.71570	-31.20430
H	-6.21700	-1.38360	-29.59890
H	-5.61130	-2.87250	-28.87920
H	-5.05660	-1.29280	-28.26650

[Rh(η^5 -C₅Me₅)(PTA)Cl]⁺

C	-2.41670	-3.21720	-28.43090
C	-0.97640	-3.40220	-28.66160
C	-0.60730	-2.69200	-29.85730
C	-1.77330	-1.97060	-30.29190
C	-2.90400	-2.34170	-29.42760
C	-3.19960	-3.86310	-27.33190
H	-4.10620	-3.30130	-27.09690
H	-3.49830	-4.87670	-27.63390
H	-2.61240	-3.95190	-26.41380
C	-4.31120	-1.86630	-29.60530
H	-4.34860	-0.83420	-29.96600
H	-4.82530	-2.49500	-30.34640
H	-4.87580	-1.91640	-28.67180
C	-1.88430	-1.11350	-31.51130
H	-2.57510	-0.27940	-31.35990
H	-0.91640	-0.71120	-31.81990
H	-2.27530	-1.71330	-32.34630
C	0.70370	-2.78500	-30.57950
H	0.92580	-1.87780	-31.14710
H	1.53670	-2.97370	-29.89750
H	0.67180	-3.61840	-31.29480
C	-0.10040	-4.31330	-27.86410
H	0.95910	-4.07600	-27.98690
H	-0.34310	-4.27940	-26.79820
H	-0.24900	-5.35020	-28.19970
Rh	-1.27270	-1.26810	-28.28110
Cl	-2.35880	-0.02000	-26.63220

P	0.56830	0.17730	-27.94220
C	0.24730	2.02840	-28.18400
H	-0.60920	2.31180	-27.56470
H	-0.01260	2.21620	-29.23170
C	1.26470	0.26740	-26.18320
H	0.44110	0.49410	-25.49930
H	1.67760	-0.70940	-25.90760
C	2.21240	0.07690	-28.86700
H	2.67280	-0.90430	-28.70340
H	2.04140	0.18850	-29.94400
C	2.59260	2.47770	-28.65600
H	2.32060	2.57440	-29.71200
H	3.38510	3.19950	-28.43660
C	3.44740	0.99820	-26.97530
H	4.24640	1.70880	-26.74320
H	3.81540	-0.01280	-26.77290
C	1.79050	2.63610	-26.39980
H	2.57350	3.36150	-26.15960
H	0.91860	2.84450	-25.77300
N	3.12710	1.12580	-28.40900
N	1.42700	2.80450	-27.81830
N	2.30310	1.28810	-26.09550

[Ir(η^5 -C₅Me₅)(PTA)Cl]⁺

C	-1.64810	-3.27420	-28.19990
C	-0.56710	-3.13380	-29.14700
C	-1.08030	-2.37180	-30.26070
C	-2.52290	-2.16160	-30.05740
C	-2.87010	-2.71410	-28.79870
C	-1.60230	-4.02910	-26.90910
H	-2.26770	-3.59160	-26.15990
H	-1.93060	-5.06470	-27.07840
H	-0.59220	-4.06540	-26.49370
C	-4.22900	-2.74570	-28.17090
H	-4.87090	-1.95030	-28.55570
H	-4.71490	-3.70690	-28.38750
H	-4.17590	-2.63850	-27.08410
C	-3.43960	-1.48770	-31.03020
H	-4.31070	-1.05650	-30.53220
H	-2.93280	-0.68610	-31.57410
H	-3.79800	-2.21720	-31.76940
C	-0.33680	-2.01650	-31.50950
H	-0.67470	-1.06340	-31.92530
H	0.74060	-1.95460	-31.33780
H	-0.50920	-2.78940	-32.27210
C	0.78250	-3.78120	-29.05850
H	1.54430	-3.21760	-29.60280
H	1.11570	-3.89750	-28.02410
H	0.73700	-4.78450	-29.50330
Ir	-1.26900	-1.13910	-28.46840
Cl	-2.45080	0.80220	-27.93440

P	0.61380	-0.12380	-27.52880
C	1.14420	1.53190	-28.27770
H	0.28320	2.20770	-28.26790
H	1.44300	1.37630	-29.32020
C	0.46960	0.44510	-25.72950
H	-0.41270	1.08660	-25.63930
H	0.32190	-0.42900	-25.08590
C	2.31410	-0.92530	-27.42200
H	2.25240	-1.85560	-26.84570
H	2.67010	-1.17970	-28.42700
C	3.44440	1.23400	-27.54240
H	3.70330	0.99660	-28.57930
H	4.27720	1.78660	-27.09720
C	2.87730	0.32000	-25.40030
H	3.70550	0.86490	-24.93750
H	2.71150	-0.60180	-24.83350
C	1.88970	2.38510	-26.12160
H	2.70760	2.94970	-25.66440
H	0.98590	3.00100	-26.09810
N	3.26880	-0.01670	-26.78160
N	2.25350	2.09990	-27.52120
N	1.67250	1.16360	-25.32610

[*trans*-RuCl₂(dmsO-S)(Im)OH]

C	-0.97110	-3.58780	3.20190
C	-1.15300	-2.30120	2.77270
N	-0.10470	-1.95910	1.93950
C	0.70340	-3.00540	1.86370
N	0.20770	-4.01670	2.61560
Ru	0.19030	-0.07360	1.05060
S	0.33090	2.08160	0.09270
C	1.95610	2.87080	0.26630
Cl	1.79180	0.45130	2.64220
Cl	1.62180	-0.99440	-0.67010
O	-0.73250	3.03350	0.59220
C	0.20040	2.01950	-1.72090
O	-1.56240	0.39150	1.72260
H	1.61320	-3.04920	1.28460
H	-1.93690	-1.59060	2.98460
H	0.63800	-4.92360	2.73160
H	-1.55450	-4.22110	3.85210
H	0.98680	1.37120	-2.11330
H	0.27330	3.04250	-2.10000
H	-0.78280	1.60190	-1.95010
H	2.71250	2.20450	-0.15640
H	2.12990	3.00370	1.33480
H	1.91990	3.83340	-0.25040
H	-1.74360	1.34750	1.61210

[Ru(η^6 -C₁₀H₁₄)(PTA)ClCys]

C	-2.75360	-2.48840	-29.63640
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C	-2.81450	-3.13990	-28.39720
C	-1.61400	-3.48650	-27.69270
C	-0.33330	-3.29840	-28.26020
C	-0.27750	-2.61630	-29.52400
C	-1.45060	-2.19050	-30.17420
H	-3.76680	-3.30760	-27.90930
H	-1.69660	-3.92060	-26.70070
H	0.68670	-2.40550	-29.97550
H	-1.37510	-1.62110	-31.09500
Ru	-1.40450	-1.26890	-28.04880
Cl	-2.51350	0.80690	-28.79760
P	0.46140	0.03880	-27.52090
C	0.40150	1.92370	-27.52150
H	-0.29820	2.27650	-26.75980
H	0.03630	2.26070	-28.49620
C	1.40980	-0.20150	-25.90930
H	0.75070	0.01060	-25.06350
H	1.71780	-1.25050	-25.82320
C	1.95250	-0.13780	-28.67180
H	2.28410	-1.18270	-28.69230
H	1.64800	0.13270	-29.69060
C	2.71440	2.13410	-28.27320
H	2.32550	2.39660	-29.26320
H	3.62580	2.71550	-28.09260
C	3.55580	0.35660	-26.91140
H	4.47250	0.92560	-26.72040
H	3.80090	-0.71160	-26.88070
C	2.23500	2.09770	-25.92860
H	3.13940	2.68080	-25.72050
H	1.48040	2.33710	-25.17550
C	-3.98120	-2.05550	-30.41960
H	-3.79360	-1.01770	-30.72610
C	-5.28160	-2.07100	-29.60710
N	3.08470	0.70440	-28.26510
N	1.72910	2.49200	-27.25210
N	2.59590	0.66540	-25.84360
C	0.90270	-3.84430	-27.59230
H	1.08530	-4.87520	-27.92580
H	1.79480	-3.26040	-27.83920
H	0.78910	-3.86050	-26.50410
C	-4.11890	-2.91870	-31.69400
H	-4.95650	-2.55810	-32.30250
H	-3.21600	-2.88460	-32.31440
H	-4.31360	-3.96810	-31.43900
H	-6.09380	-1.64400	-30.20610
H	-5.58110	-3.09070	-29.33230
H	-5.18880	-1.47770	-28.69230
C	-1.84010	4.52010	-22.96170
C	-1.78390	3.49040	-24.07900
O	-0.77250	3.36310	-24.78200
N	-2.89760	2.74150	-24.25320

C	-3.03510	1.68190	-25.25160
C	-4.54070	1.37840	-25.32140
O	-5.24870	1.48930	-24.31130
C	-2.19480	0.45520	-24.81240
S	-2.29700	-1.10670	-25.77130
N	-5.01460	1.02340	-26.52990
C	-6.39920	0.62680	-26.71950
H	-2.79530	4.53310	-22.42710
H	-1.03430	4.31440	-22.24900
H	-1.65610	5.51170	-23.38830
H	-3.68880	2.82300	-23.62150
H	-2.67410	2.04500	-26.21700
H	-1.16230	0.79810	-24.71520
H	-2.53350	0.16030	-23.81150
H	-4.34560	0.88240	-27.28530
H	-6.63070	0.65780	-27.78740
H	-6.58660	-0.38550	-26.33730
H	-7.05680	1.31870	-26.18630

[Os(η^6 -C₁₀H₁₄)(PTA)ClCys]

C	-2.76750	-2.48620	-29.60670
C	-2.79200	-3.15840	-28.37400
C	-1.56550	-3.49160	-27.68990
C	-0.29460	-3.28820	-28.29090
C	-0.27440	-2.58040	-29.54620
C	-1.47700	-2.14140	-30.15910
H	-3.73020	-3.32630	-27.86040
H	-1.62140	-3.93060	-26.69880
H	0.67580	-2.33810	-30.01050
H	-1.42830	-1.54170	-31.06180
Os	-1.39770	-1.32090	-28.06030
Cl	-2.50820	0.78490	-28.79880
P	0.46710	0.00890	-27.52220
C	0.39950	1.89290	-27.53710
H	-0.31430	2.24800	-26.78940
H	0.04930	2.22280	-28.51980
C	1.39010	-0.21630	-25.89530
H	0.71770	-0.00030	-25.06070
H	1.69940	-1.26390	-25.79840
C	1.97380	-0.16640	-28.64940
H	2.30950	-1.20980	-28.66430
H	1.68110	0.10050	-29.67280
C	2.72230	2.10920	-28.25390
H	2.34810	2.36430	-29.25160
H	3.62850	2.69530	-28.06300
C	3.54880	0.34240	-26.86900
H	4.46080	0.91490	-26.66710
H	3.79630	-0.72490	-26.82850
C	2.20690	2.08520	-25.91700
H	3.10580	2.67300	-25.69900
H	1.44020	2.32650	-25.17700

C	-4.01820	-2.05020	-30.35030
H	-3.85210	-1.00300	-30.63620
C	-5.30100	-2.10590	-29.51200
N	3.09720	0.68120	-28.23130
N	1.71980	2.46910	-27.25050
N	2.57140	0.65470	-25.81810
C	0.95840	-3.83430	-27.65690
H	1.13740	-4.85790	-28.01390
H	1.84220	-3.24190	-27.91150
H	0.86660	-3.87050	-26.56720
C	-4.16810	-2.88490	-31.64180
H	-5.02230	-2.52220	-32.22530
H	-3.27760	-2.82210	-32.27780
H	-4.34290	-3.94300	-31.40910
H	-6.13110	-1.67410	-30.08250
H	-5.58080	-3.13710	-29.26040
H	-5.19840	-1.53810	-28.58220
C	-1.84900	4.49430	-22.97930
C	-1.80490	3.46750	-24.09960
O	-0.79510	3.32930	-24.80270
N	-2.92800	2.73330	-24.27680
C	-3.07890	1.68310	-25.28260
C	-4.58890	1.39940	-25.35210
O	-5.29930	1.53060	-24.34640
C	-2.24700	0.44450	-24.85660
S	-2.37850	-1.11720	-25.81650
N	-5.06300	1.04020	-26.56040
C	-6.45150	0.65910	-26.75460
H	-2.80260	4.51370	-22.44210
H	-1.04290	4.27990	-22.26970
H	-1.65820	5.48550	-23.40380
H	-3.72020	2.82390	-23.64750
H	-2.71670	2.05070	-26.24580
H	-1.20990	0.77560	-24.77330
H	-2.57700	0.15250	-23.85250
H	-4.39130	0.87700	-27.30770
H	-6.68140	0.69910	-27.82260
H	-6.65080	-0.35350	-26.37920
H	-7.10150	1.35520	-26.21810

[Rh(η^5 -C₅Me₅)(PTA)ClCys]

C	-2.39720	-3.27960	-28.23430
C	-0.94480	-3.34360	-28.28520
C	-0.52370	-2.73860	-29.53360
C	-1.66690	-2.15140	-30.14310
C	-2.83210	-2.49750	-29.33140
C	-3.24050	-3.94670	-27.19460
H	-4.30330	-3.89450	-27.44450
H	-2.96500	-5.00510	-27.10300
H	-3.10780	-3.47940	-26.20850
C	-4.24010	-2.13880	-29.69340

H	-4.32040	-1.07070	-29.92060
H	-4.56400	-2.69920	-30.58170
H	-4.93490	-2.36310	-28.88020
C	-1.73980	-1.43750	-31.45920
H	-2.33760	-0.52400	-31.37420
H	-0.74690	-1.15600	-31.82170
H	-2.20530	-2.07530	-32.22450
C	0.83600	-2.88670	-30.14860
H	1.08010	-2.06610	-30.82780
H	1.62450	-2.95930	-29.39460
H	0.86750	-3.81670	-30.73450
C	-0.10360	-4.17280	-27.36040
H	0.95360	-3.89670	-27.41730
H	-0.42460	-4.04650	-26.32180
H	-0.18130	-5.24090	-27.61150
Rh	-1.38520	-1.16510	-28.08800
Cl	-2.64720	0.87880	-28.68020
P	0.49160	0.15360	-27.69130
C	0.29940	2.01980	-27.49630
H	-0.34250	2.24860	-26.64200
H	-0.18720	2.41310	-28.39350
C	1.61410	-0.16350	-26.21340
H	1.03030	-0.08420	-25.29230
H	2.00030	-1.18910	-26.26230
C	1.85450	0.19940	-28.99860
H	2.25430	-0.80690	-29.15280
H	1.42590	0.53700	-29.95000
C	2.49700	2.48020	-28.44690
H	1.98710	2.80340	-29.36100
H	3.38120	3.11130	-28.30110
C	3.59680	0.65400	-27.36270
H	4.48750	1.27280	-27.20700
H	3.91580	-0.38980	-27.46480
C	2.27260	2.18640	-26.08210
H	3.15140	2.81630	-25.90390
H	1.58710	2.29400	-25.23760
N	2.96030	1.08950	-28.61920
N	1.60450	2.66330	-27.30160
N	2.73720	0.78490	-26.17780
C	-1.86670	4.28810	-22.72440
C	-1.78220	3.29730	-23.87440
O	-0.81170	3.28730	-24.64250
N	-2.82870	2.44680	-24.00420
C	-2.92240	1.40950	-25.03000
C	-4.38490	0.93590	-25.00900
O	-5.01640	0.90530	-23.94410
C	-1.92280	0.27340	-24.69670
S	-1.92100	-1.24650	-25.72110
N	-4.91060	0.58820	-26.19710
C	-6.25440	0.04640	-26.30550
H	-2.77230	4.17920	-22.11910

H	-0.98890	4.16210	-22.08190
H	-1.83150	5.30360	-23.13310
H	-3.57520	2.42430	-23.31610
H	-2.67350	1.84030	-26.00310
H	-0.92810	0.72340	-24.65140
H	-2.15760	-0.09800	-23.69120
H	-4.30770	0.60180	-27.01830
H	-6.51930	-0.01760	-27.36380
H	-6.32130	-0.95130	-25.85300
H	-6.96840	0.69870	-25.79340

[Ir(η^5 -C₅Me₅)(PTA)ClCys]

C	-2.01150	-3.39340	-28.15220
C	-0.63980	-3.25060	-28.59050
C	-0.65730	-2.51550	-29.85480
C	-2.00630	-2.13300	-30.11470
C	-2.85290	-2.65680	-29.05150
C	-2.47890	-4.22200	-26.99550
H	-3.36760	-3.79480	-26.52440
H	-2.73170	-5.23100	-27.35080
H	-1.71110	-4.31530	-26.22370
C	-4.34890	-2.56180	-29.00220
H	-4.69700	-1.62980	-29.45720
H	-4.81530	-3.39620	-29.54600
H	-4.71360	-2.58560	-27.97120
C	-2.51180	-1.39720	-31.31780
H	-3.16140	-0.56700	-31.02470
H	-1.69410	-0.98450	-31.91450
H	-3.08970	-2.07770	-31.95850
C	0.48770	-2.38700	-30.81840
H	0.47180	-1.43490	-31.35620
H	1.45560	-2.47770	-30.32120
H	0.43310	-3.18960	-31.56850
C	0.52890	-4.00710	-28.02560
H	1.47910	-3.51770	-28.25820
H	0.45800	-4.09650	-26.93810
H	0.57270	-5.02330	-28.44370
Ir	-1.37820	-1.20960	-28.10190
Cl	-2.56170	0.88660	-28.68430
P	0.52200	0.00270	-27.54310
C	0.50040	1.88390	-27.54610
H	-0.22850	2.24980	-26.81780
H	0.18400	2.23130	-28.53500
C	1.38970	-0.26180	-25.89300
H	0.70080	-0.04270	-25.07390
H	1.67100	-1.31820	-25.80260
C	2.05490	-0.22130	-28.61770
H	2.35840	-1.27480	-28.60570
H	1.81130	0.04140	-29.65350
C	2.84810	2.03730	-28.19500
H	2.50860	2.30340	-29.20220

H	3.76390	2.59890	-27.97830
C	3.59030	0.24870	-26.79180
H	4.50870	0.80050	-26.56190
H	3.81220	-0.82390	-26.74660
C	2.26310	2.01980	-25.87410
H	3.16860	2.58390	-25.62350
H	1.47930	2.27490	-25.15630
N	3.18570	0.60000	-28.16500
N	1.82730	2.42510	-27.21950
N	2.58870	0.58050	-25.77070
C	-1.95890	4.40190	-22.97990
C	-1.90310	3.36770	-24.09270
O	-0.92150	3.28500	-24.84270
N	-2.98570	2.56230	-24.21040
C	-3.11420	1.50920	-25.21470
C	-4.59880	1.11390	-25.22300
O	-5.27550	1.17950	-24.18770
C	-2.18280	0.32860	-24.83460
S	-2.21860	-1.22190	-25.81530
N	-5.09030	0.71590	-26.41190
C	-6.44520	0.20960	-26.54820
H	-2.87610	4.35340	-22.38420
H	-1.09550	4.26210	-22.32100
H	-1.87510	5.39960	-23.42400
H	-3.75180	2.60740	-23.54540
H	-2.81600	1.90350	-26.18840
H	-1.17200	0.73640	-24.77380
H	-2.45960	-0.00770	-23.82740
H	-4.44390	0.63760	-27.19410
H	-6.68440	0.13190	-27.61190
H	-6.55550	-0.77700	-26.07930
H	-7.15120	0.89360	-26.06840

[*trans*-RuCl₂(dmsO-S)(Im)OHCys]⁻

C	-0.56860	-3.50170	3.43400
C	-0.68160	-2.18360	3.08140
N	-0.04700	-1.99600	1.86770
C	0.45860	-3.15970	1.50180
N	0.17920	-4.10170	2.43520
Ru	0.08330	-0.15370	0.87280
S	0.27510	2.00530	-0.05260
C	1.87090	2.76210	0.37960
Cl	1.25740	0.69310	2.92130
Cl	2.27970	-0.77850	-0.13750
O	-0.81190	3.01190	0.27180
C	0.46930	1.98470	-1.86370
O	-1.66400	0.28980	1.79600
H	1.02540	-3.33210	0.60020
H	-1.15080	-1.34970	3.57920
H	0.21770	-5.09450	2.25050
H	-0.93270	-4.05390	4.28700

H	1.28970	1.30630	-2.11170
H	0.65990	3.00970	-2.19490
H	-0.46660	1.60890	-2.28100
H	2.66440	2.07160	0.08300
H	1.87210	2.87580	1.46410
H	1.93240	3.72630	-0.13410
C	-3.63930	-6.63980	-0.23780
C	-2.81320	-5.40490	0.11060
O	-1.70100	-5.52470	0.64250
N	-3.38540	-4.22270	-0.19980
C	-2.83570	-2.88540	0.03600
C	-4.05420	-1.93940	-0.02990
O	-5.07120	-2.28730	-0.66310
C	-1.75540	-2.56280	-1.03120
S	-1.06800	-0.85920	-1.09860
N	-3.94880	-0.77920	0.62590
C	-4.99940	0.21910	0.52890
H	-4.60250	-6.40660	-0.70390
H	-3.05800	-7.27350	-0.91640
H	-3.81700	-7.21410	0.67810
H	-4.30820	-4.18830	-0.62770
H	-2.38530	-2.84870	1.02980
H	-0.95160	-3.29500	-0.91470
H	-2.20340	-2.72130	-2.01980
H	-3.04450	-0.46930	1.04260
H	-4.72270	1.06570	1.16220
H	-5.12530	0.56960	-0.50360
H	-5.95780	-0.19180	0.86630
H	-1.76280	1.25670	1.75400