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A novel platinum-based anticancer drug: a complete vibrational study

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Novel Platinum-based Anticancer Drug: a Complete Vibrational Study

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Supplementary material

Cartesian coordinates for the solid phase conformer of Pt₂Spm

Symbol	X	Y	Z
Pt	-4.0763460	0.2599500	-0.0711900
N	-4.7042880	-1.2505510	1.1952630
H	-4.0093990	-1.4348830	1.9180640
H	-5.5090750	-0.8305460	1.6703750
N	-2.7753210	-0.9997980	-1.1000870
H	-2.6311460	-0.4583050	-1.9576880
Cl	-3.4313100	1.9034930	-1.5997620
Cl	-5.5777470	1.6029530	1.1057380
C	-3.4288040	-2.2757080	-1.4706430
C	-5.0813830	-2.5005400	0.5058540
C	-3.9225200	-3.0978560	-0.2828850
H	-4.2696920	-2.0217360	-2.1215660
H	-2.7201180	-2.8800590	-2.0517570
H	-5.4389310	-3.2317580	1.2402950
H	-5.9122090	-2.2550230	-0.1599160
H	-4.2600960	-4.0612370	-0.6796620
H	-3.0925760	-3.3361670	0.3934570
C	-1.4451770	-1.1904430	-0.4706190
C	-0.6797340	0.1152420	-0.3269660
H	-0.8714360	-1.9045040	-1.0775940
H	-1.5954660	-1.6450900	0.5119810
H	-0.5526630	0.5724940	-1.3155330
H	-1.2823070	0.8198300	0.2551660
C	0.6797340	-0.1152420	0.3269660
C	1.4451770	1.1904430	0.4706190
H	0.5526630	-0.5724940	1.3155330
H	1.2823070	-0.8198300	-0.2551660
N	2.7753210	0.9997980	1.1000870
H	0.8714360	1.9045040	1.0775940
H	1.5954660	1.6450900	-0.5119810
Pt	4.0763460	-0.2599500	0.0711900
H	2.6311460	0.4583050	1.9576880
C	3.4288040	2.2757080	1.4706430
N	4.7042880	1.2505510	-1.1952630
Cl	3.4313100	-1.9034930	1.5997620
Cl	5.5777470	-1.6029530	-1.1057380
C	3.9225200	3.0978560	0.2828850
H	4.2696920	2.0217360	2.1215660
H	2.7201180	2.8800590	2.0517570
H	4.0093990	1.4348830	-1.9180640
H	5.5090750	0.8305460	-1.6703750
C	5.0813830	2.5005400	-0.5058540
H	4.2600960	4.0612370	0.6796620
H	3.0925760	3.3361670	-0.3934570
H	5.4389310	3.2317580	-1.2402950
H	5.9122090	2.2550230	0.1599160

Cartesian coordinates for the most stable conformer of Pt₂Spm

Symbol	X	Y	Z
Pt	2.0794570	-0.1879770	-0.3867160
N	1.3683240	1.5014850	-1.3613840
H	1.8850180	1.4881060	-2.2403040
H	0.3855230	1.3430200	-1.6259360
N	2.6970670	0.7642130	1.3881900
H	3.6983290	0.5928940	1.2828990
Cl	2.9606830	-2.1816900	0.4893960
Cl	1.5216840	-1.2696900	-2.3928160
C	2.5206920	2.2333740	1.4790990
C	1.4616570	2.8370200	-0.7413440
C	2.6768810	2.9764920	0.1618530
H	1.5204990	2.4242980	1.8725050
H	3.2389480	2.6102710	2.2179260
H	1.4826190	3.5915390	-1.5336910
H	0.5424800	2.9947500	-0.1707350
H	2.8037260	4.0382000	0.3994500
H	3.5884870	2.6625780	-0.3617040
C	2.3424520	0.1117510	2.6898760
C	0.8664660	0.1155120	3.0651970
H	2.9103640	0.6364570	3.4696270
H	2.7125110	-0.9111970	2.6229820
H	0.4708510	1.1378540	3.0873510
H	0.8231910	-0.2357440	4.1041780
C	-0.0318940	-0.7528930	2.1885100
C	-1.4896040	-0.6029220	2.5924340
H	0.0695830	-0.4322930	1.1445630
H	0.3072570	-1.7927530	2.2290500
N	-2.4755470	-0.9159090	1.5159440
H	-1.6904020	0.4397780	2.8468300
H	-1.7328550	-1.2217190	3.4668340
Pt	-2.1988460	0.2508730	-0.1964850
H	-3.3535600	-0.5179690	1.8524070
C	-2.7152600	-2.3630950	1.2989690
N	-1.6082640	-1.2882240	-1.4404970
Cl	-2.8933290	2.0476650	1.1480420
Cl	-1.8737460	1.6046340	-2.0884010
C	-1.7835140	-3.0437000	0.3037220
H	-3.7463370	-2.4612560	0.9446590
H	-2.6519590	-2.8671370	2.2708860
H	-0.5814100	-1.2721540	-1.5269020
H	-1.9386770	-1.0082420	-2.3651700
C	-2.0429490	-2.6637050	-1.1448160
H	-1.9453220	-4.1228690	0.4000730
H	-0.7316760	-2.8699020	0.5510950
H	-1.5048350	-3.3478900	-1.8091950
H	-3.1106080	-2.7380530	-1.3725350