

## Synthesis of an unusual Quinazoline alkaloid: Theoretical and Experimental Investigations of its Structural, Electronic, Molecular and Biological properties

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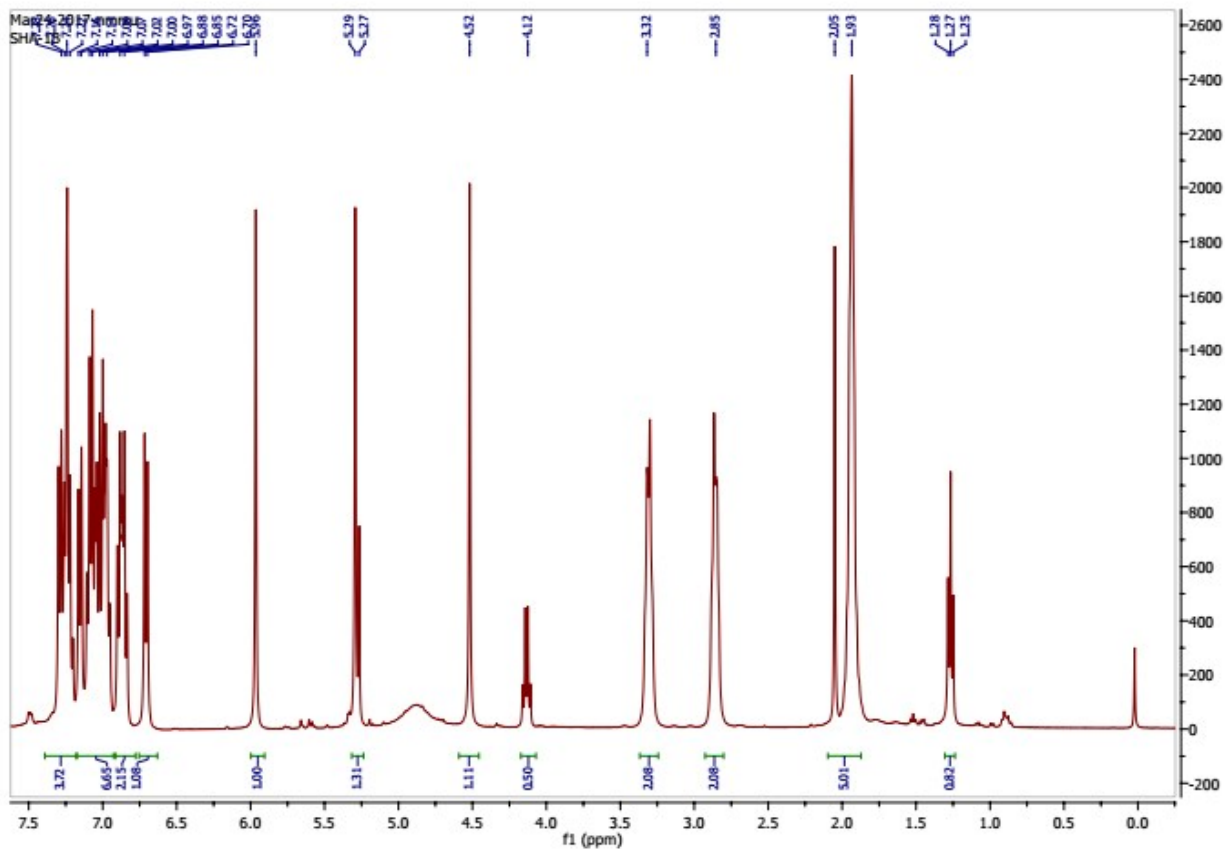
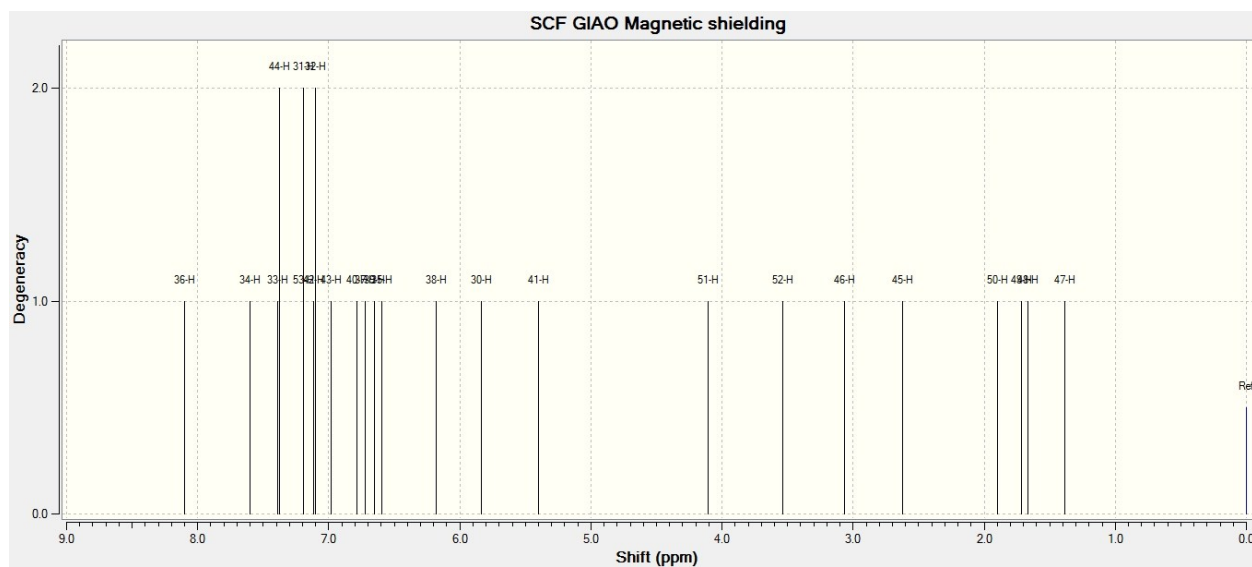
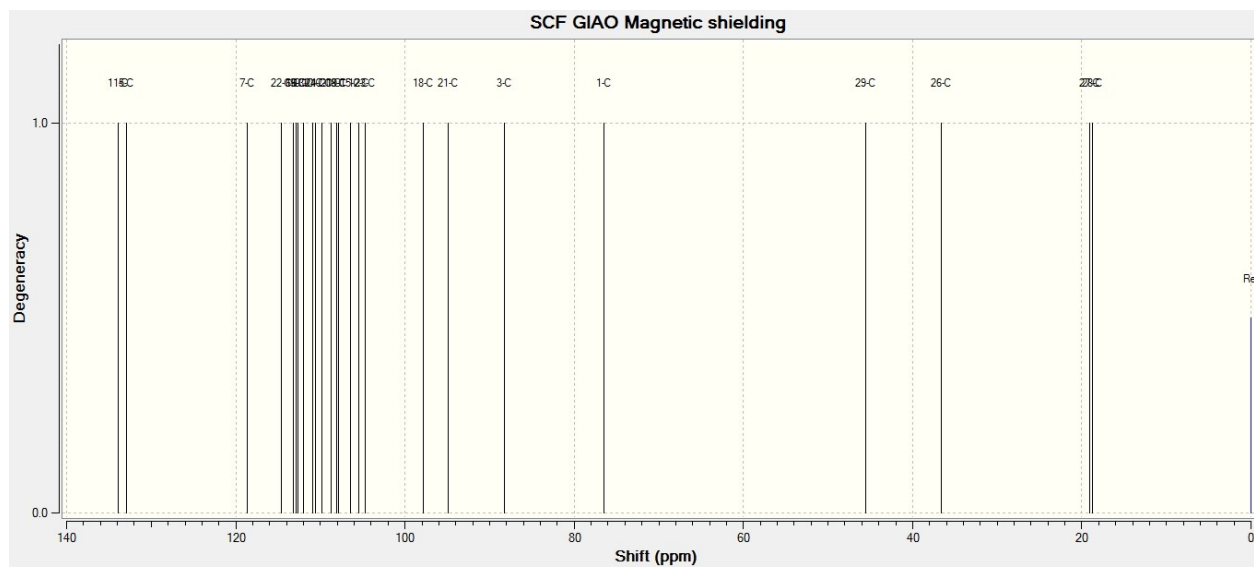
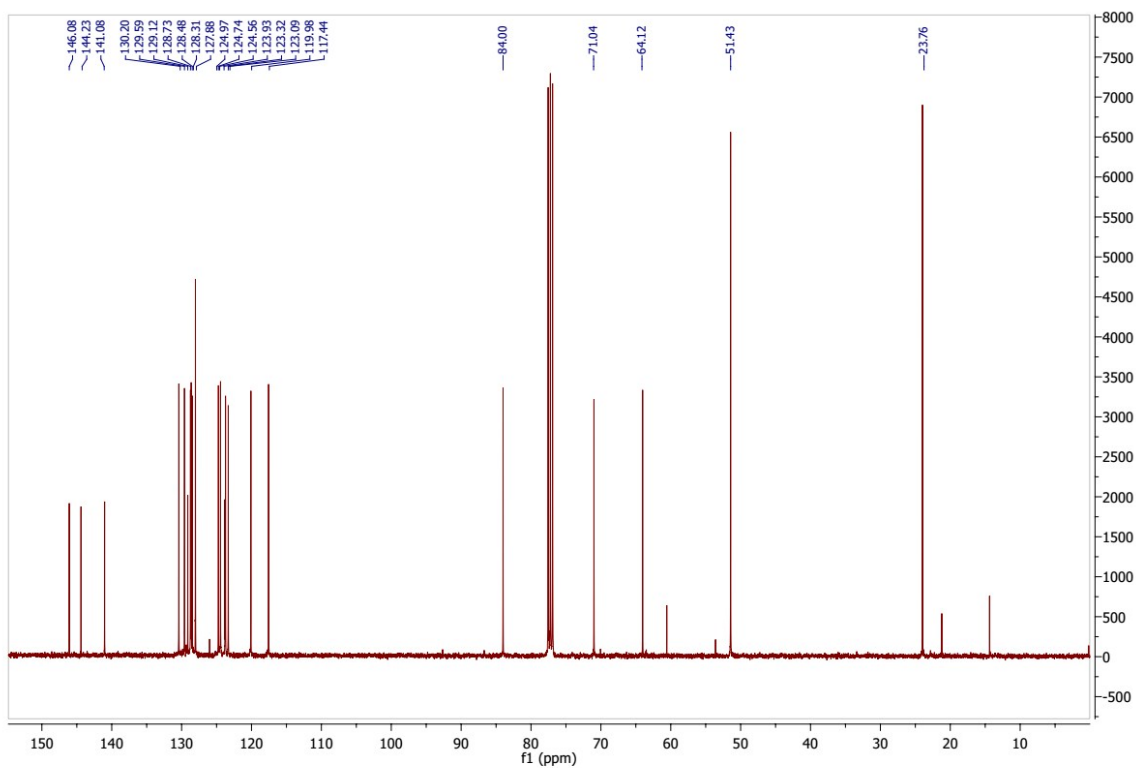


Fig. S1 Experimental  $^1\text{H}$  NMR of Compound 1

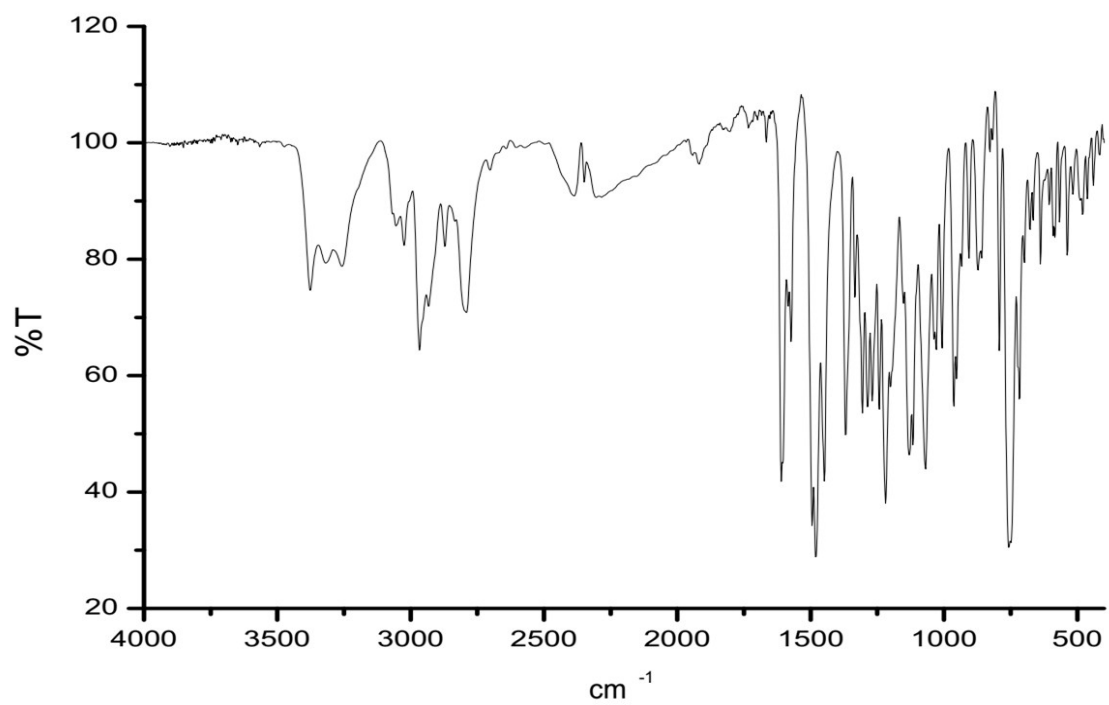


**Fig. S2** Theoretical  $^1\text{H}$  NMR of Compound **1**

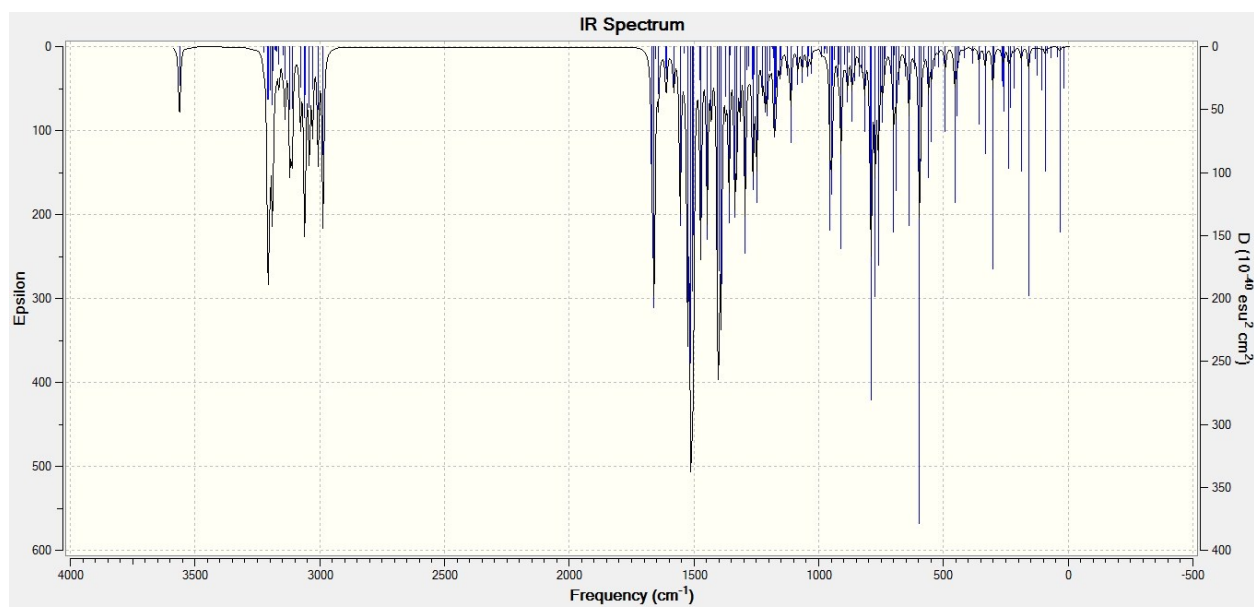


**Fig. S3** Experimental  $^{13}\text{C}$  NMR of Compound **1**

**Fig. S4** Theoretical  $^{13}\text{C}$  NMR of Compound **1**



**Fig. S5** Experimental FT-IR of Compound **1**



**Fig. S6** Theoretical FT-IR of Compound **1****Table S1.** Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **1**.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.

	x	y	z	$U(\text{eq})$
N(1A)	1272(2)	3353(2)	1652(1)	26(1)
N(2A)	1165(2)	2427(2)	767(1)	24(1)
N(3A)	2462(2)	3255(2)	261(1)	23(1)
N(4A)	2645(2)	2038(2)	-454(1)	26(1)
C(1A)	960(3)	4174(3)	1973(2)	32(1)
C(2A)	1018(3)	3866(3)	2605(2)	41(1)
C(3A)	1150(4)	2810(3)	2577(2)	49(1)
C(4A)	864(3)	2496(3)	1935(2)	36(1)
C(5A)	862(2)	3320(2)	1028(1)	25(1)
C(6A)	509(2)	2154(2)	217(1)	25(1)
C(7A)	-508(3)	1713(2)	218(2)	32(1)
C(8A)	-1159(3)	1430(3)	-304(2)	39(1)
C(9A)	-796(3)	1568(3)	-828(2)	39(1)
C(10A)	213(3)	1995(2)	-828(2)	32(1)
C(11A)	878(2)	2304(2)	-304(1)	25(1)
C(12A)	1990(2)	2773(2)	-314(1)	24(1)
C(13A)	2005(2)	4141(2)	357(1)	23(1)
C(14A)	2339(3)	4940(2)	60(2)	28(1)
C(15A)	1911(3)	5808(2)	118(2)	33(1)
C(16A)	1136(3)	5878(2)	464(2)	35(1)
C(17A)	812(3)	5085(2)	758(2)	31(1)
C(18A)	1248(2)	4206(2)	721(1)	25(1)
C(19A)	2284(2)	2562(2)	706(1)	22(1)
C(20A)	2723(2)	1630(2)	557(1)	23(1)
C(21A)	2981(2)	984(2)	993(1)	26(1)
C(22A)	3510(3)	186(2)	893(2)	28(1)
C(23A)	3798(2)	42(2)	349(2)	27(1)

C(24A)	3517(2)	650(2)	-97(1)	26(1)
C(25A)	2967(2)	1450(2)	0(1)	22(1)
N(1B)	8192(2)	6459(2)	2034(1)	25(1)
N(2B)	6775(2)	5210(2)	1961(1)	26(1)
N(3B)	5805(2)	5343(2)	986(1)	33(1)
N(4B)	4849(3)	3799(2)	805(2)	56(1)
C(1B)	8594(3)	7474(2)	2208(2)	29(1)
C(2B)	9785(3)	7454(3)	2426(2)	35(1)
C(3B)	9957(3)	6385(3)	2480(2)	43(1)
C(4B)	8850(3)	5888(2)	2452(2)	33(1)
C(5B)	7070(2)	6263(2)	2064(1)	24(1)
C(6B)	5795(2)	4922(2)	2152(2)	31(1)
C(7B)	5778(3)	4893(2)	2745(2)	38(1)
C(8B)	4839(4)	4605(3)	2939(2)	53(1)
C(9B)	3925(3)	4343(3)	2541(3)	62(2)
C(10B)	3943(3)	4378(3)	1951(3)	52(1)
C(11B)	4867(3)	4671(2)	1743(2)	38(1)
C(12B)	4857(3)	4735(2)	1092(2)	40(1)
C(13B)	5730(3)	6333(2)	1136(2)	28(1)
C(14B)	4982(3)	6812(2)	772(2)	34(1)
C(15B)	4829(3)	7757(2)	901(2)	33(1)
C(16B)	5448(3)	8248(2)	1388(2)	30(1)
C(17B)	6191(3)	7777(2)	1749(2)	27(1)
C(18B)	6350(2)	6817(2)	1630(1)	25(1)
C(19B)	6719(2)	4963(2)	1338(2)	27(1)
C(20B)	6687(3)	3883(2)	1219(2)	28(1)
C(21B)	7596(2)	3420(2)	1371(1)	26(1)
C(22B)	7616(3)	2449(2)	1233(2)	29(1)
C(23B)	6704(3)	1933(2)	926(2)	30(1)
C(24B)	5782(3)	2372(2)	778(2)	33(1)
C(25B)	5760(3)	3351(2)	929(2)	33(1)
N(1C)	5824(2)	1195(2)	2790(1)	26(1)
N(2C)	7216(2)	223(2)	2693(1)	26(1)
N(3C)	8408(2)	602(2)	3614(1)	26(1)
N(4C)	9422(2)	-763(2)	3663(1)	34(1)
C(1C)	5358(3)	2125(2)	2729(2)	34(1)

C(2C)	4168(3)	1857(3)	2696(2)	38(1)
C(3C)	4017(3)	760(2)	2606(2)	32(1)
C(4C)	5042(3)	517(2)	2417(2)	30(1)
C(5C)	6874(3)	1211(2)	2637(1)	27(1)
C(6C)	7439(2)	26(2)	3318(1)	25(1)
C(7C)	7528(2)	-1027(2)	3437(1)	27(1)
C(8C)	6612(3)	-1656(2)	3388(2)	31(1)
C(9C)	6649(3)	-2607(3)	3551(2)	36(1)
C(10C)	7624(3)	-2926(3)	3777(2)	38(1)
C(11C)	8539(3)	-2322(3)	3821(2)	35(1)
C(12C)	8504(3)	-1371(2)	3644(1)	30(1)
C(13C)	8398(3)	1599(2)	3477(1)	29(1)
C(14C)	9172(3)	2253(3)	3814(2)	34(1)
C(15C)	9212(3)	3220(3)	3704(2)	40(1)
C(16C)	8509(3)	3552(3)	3260(2)	42(1)
C(17C)	7745(3)	2909(2)	2915(2)	35(1)
C(18C)	7680(3)	1923(2)	3026(2)	29(1)
C(19C)	9310(2)	165(2)	3416(2)	30(1)
C(20C)	9130(3)	88(2)	2751(2)	30(1)
C(21C)	9981(3)	1(2)	2457(2)	34(1)
C(22C)	9840(3)	-43(2)	1856(2)	36(1)
C(23C)	8831(3)	-28(2)	1528(2)	35(1)
C(24C)	7979(3)	51(2)	1810(2)	30(1)
C(25C)	8121(3)	117(2)	2421(1)	27(1)
N(1D)	7203(2)	2495(2)	6968(1)	32(1)
N(2D)	6866(2)	1596(2)	6060(1)	32(1)
N(3D)	8465(2)	2038(3)	5669(1)	38(1)
N(4D)	8483(2)	797(3)	4964(1)	40(1)
C(1D)	7149(3)	3380(3)	7312(2)	42(1)
C(2D)	7273(4)	3039(3)	7945(2)	50(1)
C(3D)	6924(4)	1930(4)	7871(2)	50(1)
C(4D)	6563(3)	1774(3)	7231(2)	41(1)
C(5D)	6848(3)	2559(3)	6342(2)	33(1)
C(6D)	7968(3)	1398(3)	6061(2)	34(1)
C(7D)	8029(3)	352(3)	5890(2)	35(1)
C(8D)	7803(3)	-370(3)	6265(2)	37(1)

C(9D)	7871(3)	-1332(3)	6130(2)	41(1)
C(10D)	8177(3)	-1590(3)	5602(2)	44(1)
C(11D)	8393(3)	-892(3)	5218(2)	41(1)
C(12D)	8302(3)	80(3)	5352(2)	38(1)
C(13D)	8295(3)	3021(3)	5757(2)	41(1)
C(14D)	8880(4)	3720(4)	5486(2)	55(1)
C(15D)	8714(5)	4682(4)	5530(2)	66(2)
C(16D)	7962(5)	4974(4)	5844(2)	65(1)
C(17D)	7376(4)	4291(3)	6115(2)	51(1)
C(18D)	7539(3)	3314(3)	6079(2)	40(1)
C(19D)	8007(3)	1669(3)	5064(2)	36(1)
C(20D)	6798(3)	1509(3)	4994(2)	33(1)
C(21D)	6195(3)	1361(3)	4436(2)	39(1)
C(22D)	5105(3)	1180(3)	4362(2)	47(1)
C(23D)	4602(3)	1168(3)	4841(2)	45(1)
C(24D)	5179(3)	1340(3)	5395(2)	38(1)
C(25D)	6282(3)	1497(3)	5477(2)	33(1)
C(1S)	5934(4)	4206(3)	4537(3)	98(4)
Cl(1S)	6886(2)	3858(2)	4107(1)	82(1)
Cl(2S)	5797(2)	5442(2)	4442(1)	86(1)
Cl(3S)	4718(2)	3507(2)	4280(1)	88(1)
C(1T)	5109(6)	3377(8)	4750(3)	98(4)
Cl(1T)	4927(5)	3942(5)	5410(2)	82(1)
Cl(2T)	6239(5)	3921(5)	4504(3)	86(1)
Cl(3T)	3963(5)	3432(5)	4213(3)	88(1)

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**Table S2.** Bond lengths [Å] and angles [°] for compound 1.

N(1A)-C(5A)	1.458(4)	C(10A)-H(10A)	0.9500
N(1A)-C(1A)	1.469(4)	C(11A)-C(12A)	1.525(4)
N(1A)-C(4A)	1.477(4)	C(12A)-H(12A)	1.0000
N(2A)-C(6A)	1.432(4)	C(13A)-C(14A)	1.397(5)
N(2A)-C(19A)	1.469(4)	C(13A)-C(18A)	1.401(4)
N(2A)-C(5A)	1.480(4)	C(14A)-C(15A)	1.387(4)
N(3A)-C(13A)	1.441(3)	C(14A)-H(14A)	0.9500
N(3A)-C(19A)	1.465(4)	C(15A)-C(16A)	1.390(5)
N(3A)-C(12A)	1.488(4)	C(15A)-H(15A)	0.9500
N(4A)-C(25A)	1.383(4)	C(16A)-C(17A)	1.384(5)
N(4A)-C(12A)	1.448(4)	C(16A)-H(16A)	0.9500
N(4A)-H(4A)	0.80(5)	C(17A)-C(18A)	1.399(4)
C(1A)-C(2A)	1.530(5)	C(17A)-H(17A)	0.9500
C(1A)-H(1AA)	0.9900	C(19A)-C(20A)	1.517(4)
C(1A)-H(1AB)	0.9900	C(19A)-H(19A)	1.0000
C(2A)-C(3A)	1.496(6)	C(20A)-C(21A)	1.392(4)
C(2A)-H(2AA)	0.9900	C(20A)-C(25A)	1.404(4)
C(2A)-H(2AB)	0.9900	C(21A)-C(22A)	1.388(4)
C(3A)-C(4A)	1.518(6)	C(21A)-H(21A)	0.9500
C(3A)-H(3AA)	0.9900	C(22A)-C(23A)	1.391(5)
C(3A)-H(3AB)	0.9900	C(22A)-H(22A)	0.9500
C(4A)-H(4AA)	0.9900	C(23A)-C(24A)	1.378(5)
C(4A)-H(4AB)	0.9900	C(23A)-H(23A)	0.9500
C(5A)-C(18A)	1.528(4)	C(24A)-C(25A)	1.406(4)
C(5A)-H(5AA)	1.0000	C(24A)-H(24A)	0.9500
C(6A)-C(11A)	1.385(5)	N(1B)-C(5B)	1.462(4)
C(6A)-C(7A)	1.399(4)	N(1B)-C(4B)	1.478(4)
C(7A)-C(8A)	1.380(5)	N(1B)-C(1B)	1.482(4)
C(7A)-H(7AA)	0.9500	N(2B)-C(6B)	1.436(4)
C(8A)-C(9A)	1.388(6)	N(2B)-C(19B)	1.467(4)
C(8A)-H(8AA)	0.9500	N(2B)-C(5B)	1.484(4)
C(9A)-C(10A)	1.381(5)	N(3B)-C(13B)	1.429(4)
C(9A)-H(9AA)	0.9500	N(3B)-C(19B)	1.467(4)
C(10A)-C(11A)	1.400(4)	N(3B)-C(12B)	1.483(5)

N(4B)-C(25B)	1.372(4)	C(17B)-C(18B)	1.398(4)
N(4B)-C(12B)	1.445(4)	C(17B)-H(17B)	0.9500
N(4B)-H(4B)	0.88(5)	C(19B)-C(20B)	1.517(4)
C(1B)-C(2B)	1.538(4)	C(19B)-H(19B)	1.0000
C(1B)-H(1BA)	0.9900	C(20B)-C(21B)	1.387(4)
C(1B)-H(1BB)	0.9900	C(20B)-C(25B)	1.406(4)
C(2B)-C(3B)	1.531(5)	C(21B)-C(22B)	1.385(4)
C(2B)-H(2BA)	0.9900	C(21B)-H(21B)	0.9500
C(2B)-H(2BB)	0.9900	C(22B)-C(23B)	1.397(5)
C(3B)-C(4B)	1.520(5)	C(22B)-H(22B)	0.9500
C(3B)-H(3BA)	0.9900	C(23B)-C(24B)	1.382(5)
C(3B)-H(3BB)	0.9900	C(23B)-H(23B)	0.9500
C(4B)-H(4BA)	0.9900	C(24B)-C(25B)	1.404(4)
C(4B)-H(4BB)	0.9900	C(24B)-H(24B)	0.9500
C(5B)-C(18B)	1.527(4)	N(1C)-C(5C)	1.454(4)
C(5B)-H(5BA)	1.0000	N(1C)-C(4C)	1.467(4)
C(6B)-C(7B)	1.383(6)	N(1C)-C(1C)	1.477(4)
C(6B)-C(11B)	1.408(5)	N(2C)-C(25C)	1.433(4)
C(7B)-C(8B)	1.390(5)	N(2C)-C(6C)	1.469(4)
C(7B)-H(7BA)	0.9500	N(2C)-C(5C)	1.485(4)
C(8B)-C(9B)	1.386(8)	N(3C)-C(13C)	1.434(4)
C(8B)-H(8BA)	0.9500	N(3C)-C(6C)	1.477(4)
C(9B)-C(10B)	1.376(8)	N(3C)-C(19C)	1.491(4)
C(9B)-H(9BA)	0.9500	N(4C)-C(12C)	1.386(5)
C(10B)-C(11B)	1.392(6)	N(4C)-C(19C)	1.438(5)
C(10B)-H(10B)	0.9500	N(4C)-H(4C)	0.86(5)
C(11B)-C(12B)	1.514(6)	C(1C)-C(2C)	1.536(5)
C(12B)-H(12B)	1.0000	C(1C)-H(1CA)	0.9900
C(13B)-C(14B)	1.401(5)	C(1C)-H(1CB)	0.9900
C(13B)-C(18B)	1.403(4)	C(2C)-C(3C)	1.527(5)
C(14B)-C(15B)	1.380(5)	C(2C)-H(2CA)	0.9900
C(14B)-H(14B)	0.9500	C(2C)-H(2CB)	0.9900
C(15B)-C(16B)	1.393(5)	C(3C)-C(4C)	1.523(5)
C(15B)-H(15B)	0.9500	C(3C)-H(3CA)	0.9900
C(16B)-C(17B)	1.388(5)	C(3C)-H(3CB)	0.9900
C(16B)-H(16B)	0.9500	C(4C)-H(4CA)	0.9900

C(4C)-H(4CB)	0.9900	C(24C)-H(24C)	0.9500
C(5C)-C(18C)	1.528(4)	N(1D)-C(4D)	1.455(5)
C(5C)-H(5CA)	1.0000	N(1D)-C(5D)	1.456(4)
C(6C)-C(7C)	1.511(4)	N(1D)-C(1D)	1.464(4)
C(6C)-H(6CA)	1.0000	N(2D)-C(25D)	1.433(4)
C(7C)-C(8C)	1.393(5)	N(2D)-C(6D)	1.472(4)
C(7C)-C(12C)	1.401(5)	N(2D)-C(5D)	1.481(4)
C(8C)-C(9C)	1.390(5)	N(3D)-C(13D)	1.421(6)
C(8C)-H(8CA)	0.9500	N(3D)-C(6D)	1.473(5)
C(9C)-C(10C)	1.396(5)	N(3D)-C(19D)	1.491(4)
C(9C)-H(9CA)	0.9500	N(4D)-C(12D)	1.392(5)
C(10C)-C(11C)	1.374(6)	N(4D)-C(19D)	1.439(5)
C(10C)-H(10C)	0.9500	N(4D)-H(4D)	0.96(6)
C(11C)-C(12C)	1.399(5)	C(1D)-C(2D)	1.544(6)
C(11C)-H(11A)	0.9500	C(1D)-H(1DA)	0.9900
C(13C)-C(18C)	1.391(5)	C(1D)-H(1DB)	0.9900
C(13C)-C(14C)	1.407(5)	C(2D)-C(3D)	1.566(7)
C(14C)-C(15C)	1.376(5)	C(2D)-H(2DA)	0.9900
C(14C)-H(14C)	0.9500	C(2D)-H(2DB)	0.9900
C(15C)-C(16C)	1.373(6)	C(3D)-C(4D)	1.485(5)
C(15C)-H(15C)	0.9500	C(3D)-H(3DA)	0.9900
C(16C)-C(17C)	1.399(5)	C(3D)-H(3DB)	0.9900
C(16C)-H(16C)	0.9500	C(4D)-H(4DA)	0.9900
C(17C)-C(18C)	1.403(5)	C(4D)-H(4DB)	0.9900
C(17C)-H(17C)	0.9500	C(5D)-C(18D)	1.524(5)
C(19C)-C(20C)	1.524(5)	C(5D)-H(5DA)	1.0000
C(19C)-H(19C)	1.0000	C(6D)-C(7D)	1.512(5)
C(20C)-C(21C)	1.397(5)	C(6D)-H(6DA)	1.0000
C(20C)-C(25C)	1.400(5)	C(7D)-C(8D)	1.391(6)
C(21C)-C(22C)	1.377(5)	C(7D)-C(12D)	1.406(5)
C(21C)-H(21C)	0.9500	C(8D)-C(9D)	1.382(6)
C(22C)-C(23C)	1.397(6)	C(8D)-H(8DA)	0.9500
C(22C)-H(22C)	0.9500	C(9D)-C(10D)	1.398(6)
C(23C)-C(24C)	1.381(5)	C(9D)-H(9DA)	0.9500
C(23C)-H(23C)	0.9500	C(10D)-C(11D)	1.378(6)
C(24C)-C(25C)	1.398(5)	C(10D)-H(10D)	0.9500

C(11D)-C(12D)	1.399(6)	C(6A)-N(2A)-C(19A)	111.1(2)
C(11D)-H(11B)	0.9500	C(6A)-N(2A)-C(5A)	111.7(2)
C(13D)-C(14D)	1.404(6)	C(19A)-N(2A)-C(5A)	109.4(2)
C(13D)-C(18D)	1.404(6)	C(13A)-N(3A)-C(19A)	111.4(2)
C(14D)-C(15D)	1.380(8)	C(13A)-N(3A)-C(12A)	111.7(2)
C(14D)-H(14D)	0.9500	C(19A)-N(3A)-C(12A)	106.6(2)
C(15D)-C(16D)	1.389(8)	C(25A)-N(4A)-C(12A)	115.0(3)
C(15D)-H(15D)	0.9500	C(25A)-N(4A)-H(4A)	117(3)
C(16D)-C(17D)	1.391(7)	C(12A)-N(4A)-H(4A)	117(3)
C(16D)-H(16D)	0.9500	N(1A)-C(1A)-C(2A)	105.5(3)
C(17D)-C(18D)	1.398(6)	N(1A)-C(1A)-H(1AA)	110.6
C(17D)-H(17D)	0.9500	C(2A)-C(1A)-H(1AA)	110.6
C(19D)-C(20D)	1.536(5)	N(1A)-C(1A)-H(1AB)	110.6
C(19D)-H(19D)	1.0000	C(2A)-C(1A)-H(1AB)	110.6
C(20D)-C(25D)	1.396(5)	H(1AA)-C(1A)-H(1AB)	108.8
C(20D)-C(21D)	1.396(5)	C(3A)-C(2A)-C(1A)	104.8(3)
C(21D)-C(22D)	1.386(6)	C(3A)-C(2A)-H(2AA)	110.8
C(21D)-H(21D)	0.9500	C(1A)-C(2A)-H(2AA)	110.8
C(22D)-C(23D)	1.378(6)	C(3A)-C(2A)-H(2AB)	110.8
C(22D)-H(22D)	0.9500	C(1A)-C(2A)-H(2AB)	110.8
C(23D)-C(24D)	1.378(5)	H(2AA)-C(2A)-H(2AB)	108.9
C(23D)-H(23D)	0.9500	C(2A)-C(3A)-C(4A)	105.6(3)
C(24D)-C(25D)	1.401(5)	C(2A)-C(3A)-H(3AA)	110.6
C(24D)-H(24D)	0.9500	C(4A)-C(3A)-H(3AA)	110.6
C(1S)-Cl(2S)	1.763(5)	C(2A)-C(3A)-H(3AB)	110.6
C(1S)-Cl(3S)	1.774(5)	C(4A)-C(3A)-H(3AB)	110.6
C(1S)-Cl(1S)	1.796(5)	H(3AA)-C(3A)-H(3AB)	108.7
C(1S)-H(1SA)	1.0000	N(1A)-C(4A)-C(3A)	101.7(3)
C(1T)-Cl(1T)	1.765(5)	N(1A)-C(4A)-H(4AA)	111.4
C(1T)-Cl(2T)	1.769(6)	C(3A)-C(4A)-H(4AA)	111.4
C(1T)-Cl(3T)	1.776(5)	N(1A)-C(4A)-H(4AB)	111.4
C(1T)-H(1TA)	1.0000	C(3A)-C(4A)-H(4AB)	111.4
		H(4AA)-C(4A)-H(4AB)	109.3
C(5A)-N(1A)-C(1A)	113.5(3)	N(1A)-C(5A)-N(2A)	107.9(2)
C(5A)-N(1A)-C(4A)	111.7(2)	N(1A)-C(5A)-C(18A)	113.3(2)
C(1A)-N(1A)-C(4A)	104.4(3)	N(2A)-C(5A)-C(18A)	110.8(2)

N(1A)-C(5A)-H(5AA)	108.3	C(17A)-C(16A)-C(15A)	119.8(3)
N(2A)-C(5A)-H(5AA)	108.3	C(17A)-C(16A)-H(16A)	120.1
C(18A)-C(5A)-H(5AA)	108.3	C(15A)-C(16A)-H(16A)	120.1
C(11A)-C(6A)-C(7A)	120.7(3)	C(16A)-C(17A)-C(18A)	121.8(3)
C(11A)-C(6A)-N(2A)	121.0(3)	C(16A)-C(17A)-H(17A)	119.1
C(7A)-C(6A)-N(2A)	118.3(3)	C(18A)-C(17A)-H(17A)	119.1
C(8A)-C(7A)-C(6A)	119.9(3)	C(17A)-C(18A)-C(13A)	117.6(3)
C(8A)-C(7A)-H(7AA)	120.0	C(17A)-C(18A)-C(5A)	121.7(3)
C(6A)-C(7A)-H(7AA)	120.0	C(13A)-C(18A)-C(5A)	120.5(3)
C(7A)-C(8A)-C(9A)	119.9(3)	N(3A)-C(19A)-N(2A)	111.6(2)
C(7A)-C(8A)-H(8AA)	120.1	N(3A)-C(19A)-C(20A)	108.5(2)
C(9A)-C(8A)-H(8AA)	120.1	N(2A)-C(19A)-C(20A)	113.1(2)
C(10A)-C(9A)-C(8A)	120.0(3)	N(3A)-C(19A)-H(19A)	107.8
C(10A)-C(9A)-H(9AA)	120.0	N(2A)-C(19A)-H(19A)	107.8
C(8A)-C(9A)-H(9AA)	120.0	C(20A)-C(19A)-H(19A)	107.8
C(9A)-C(10A)-C(11A)	120.9(3)	C(21A)-C(20A)-C(25A)	119.3(3)
C(9A)-C(10A)-H(10A)	119.5	C(21A)-C(20A)-C(19A)	119.5(3)
C(11A)-C(10A)-H(10A)	119.5	C(25A)-C(20A)-C(19A)	120.9(3)
C(6A)-C(11A)-C(10A)	118.5(3)	C(22A)-C(21A)-C(20A)	121.2(3)
C(6A)-C(11A)-C(12A)	121.5(3)	C(22A)-C(21A)-H(21A)	119.4
C(10A)-C(11A)-C(12A)	120.0(3)	C(20A)-C(21A)-H(21A)	119.4
N(4A)-C(12A)-N(3A)	109.3(2)	C(21A)-C(22A)-C(23A)	119.1(3)
N(4A)-C(12A)-C(11A)	108.9(2)	C(21A)-C(22A)-H(22A)	120.5
N(3A)-C(12A)-C(11A)	111.1(2)	C(23A)-C(22A)-H(22A)	120.5
N(4A)-C(12A)-H(12A)	109.2	C(24A)-C(23A)-C(22A)	120.8(3)
N(3A)-C(12A)-H(12A)	109.2	C(24A)-C(23A)-H(23A)	119.6
C(11A)-C(12A)-H(12A)	109.2	C(22A)-C(23A)-H(23A)	119.6
C(14A)-C(13A)-C(18A)	120.9(3)	C(23A)-C(24A)-C(25A)	120.2(3)
C(14A)-C(13A)-N(3A)	116.9(3)	C(23A)-C(24A)-H(24A)	119.9
C(18A)-C(13A)-N(3A)	122.2(3)	C(25A)-C(24A)-H(24A)	119.9
C(15A)-C(14A)-C(13A)	120.1(3)	N(4A)-C(25A)-C(20A)	120.3(3)
C(15A)-C(14A)-H(14A)	120.0	N(4A)-C(25A)-C(24A)	120.4(3)
C(13A)-C(14A)-H(14A)	120.0	C(20A)-C(25A)-C(24A)	119.2(3)
C(14A)-C(15A)-C(16A)	119.8(3)	C(5B)-N(1B)-C(4B)	111.5(3)
C(14A)-C(15A)-H(15A)	120.1	C(5B)-N(1B)-C(1B)	112.2(2)
C(16A)-C(15A)-H(15A)	120.1	C(4B)-N(1B)-C(1B)	104.1(2)

C(6B)-N(2B)-C(19B)	111.3(3)	N(1B)-C(5B)-H(5BA)	108.2
C(6B)-N(2B)-C(5B)	111.4(2)	N(2B)-C(5B)-H(5BA)	108.2
C(19B)-N(2B)-C(5B)	108.8(2)	C(18B)-C(5B)-H(5BA)	108.2
C(13B)-N(3B)-C(19B)	112.2(2)	C(7B)-C(6B)-C(11B)	120.6(3)
C(13B)-N(3B)-C(12B)	110.6(3)	C(7B)-C(6B)-N(2B)	118.8(3)
C(19B)-N(3B)-C(12B)	106.6(3)	C(11B)-C(6B)-N(2B)	120.7(3)
C(25B)-N(4B)-C(12B)	116.2(3)	C(6B)-C(7B)-C(8B)	119.7(4)
C(25B)-N(4B)-H(4B)	122(3)	C(6B)-C(7B)-H(7BA)	120.2
C(12B)-N(4B)-H(4B)	122(3)	C(8B)-C(7B)-H(7BA)	120.2
N(1B)-C(1B)-C(2B)	105.3(3)	C(9B)-C(8B)-C(7B)	120.3(5)
N(1B)-C(1B)-H(1BA)	110.7	C(9B)-C(8B)-H(8BA)	119.9
C(2B)-C(1B)-H(1BA)	110.7	C(7B)-C(8B)-H(8BA)	119.9
N(1B)-C(1B)-H(1BB)	110.7	C(10B)-C(9B)-C(8B)	119.9(4)
C(2B)-C(1B)-H(1BB)	110.7	C(10B)-C(9B)-H(9BA)	120.1
H(1BA)-C(1B)-H(1BB)	108.8	C(8B)-C(9B)-H(9BA)	120.1
C(3B)-C(2B)-C(1B)	105.3(3)	C(9B)-C(10B)-C(11B)	121.2(4)
C(3B)-C(2B)-H(2BA)	110.7	C(9B)-C(10B)-H(10B)	119.4
C(1B)-C(2B)-H(2BA)	110.7	C(11B)-C(10B)-H(10B)	119.4
C(3B)-C(2B)-H(2BB)	110.7	C(10B)-C(11B)-C(6B)	118.3(4)
C(1B)-C(2B)-H(2BB)	110.7	C(10B)-C(11B)-C(12B)	120.1(4)
H(2BA)-C(2B)-H(2BB)	108.8	C(6B)-C(11B)-C(12B)	121.5(3)
C(4B)-C(3B)-C(2B)	103.9(3)	N(4B)-C(12B)-N(3B)	108.1(3)
C(4B)-C(3B)-H(3BA)	111.0	N(4B)-C(12B)-C(11B)	112.4(3)
C(2B)-C(3B)-H(3BA)	111.0	N(3B)-C(12B)-C(11B)	109.9(3)
C(4B)-C(3B)-H(3BB)	111.0	N(4B)-C(12B)-H(12B)	108.8
C(2B)-C(3B)-H(3BB)	111.0	N(3B)-C(12B)-H(12B)	108.8
H(3BA)-C(3B)-H(3BB)	109.0	C(11B)-C(12B)-H(12B)	108.8
N(1B)-C(4B)-C(3B)	103.3(3)	C(14B)-C(13B)-C(18B)	120.2(3)
N(1B)-C(4B)-H(4BA)	111.1	C(14B)-C(13B)-N(3B)	117.2(3)
C(3B)-C(4B)-H(4BA)	111.1	C(18B)-C(13B)-N(3B)	122.6(3)
N(1B)-C(4B)-H(4BB)	111.1	C(15B)-C(14B)-C(13B)	120.6(3)
C(3B)-C(4B)-H(4BB)	111.1	C(15B)-C(14B)-H(14B)	119.7
H(4BA)-C(4B)-H(4BB)	109.1	C(13B)-C(14B)-H(14B)	119.7
N(1B)-C(5B)-N(2B)	108.3(2)	C(14B)-C(15B)-C(16B)	119.6(3)
N(1B)-C(5B)-C(18B)	113.8(3)	C(14B)-C(15B)-H(15B)	120.2
N(2B)-C(5B)-C(18B)	109.9(2)	C(16B)-C(15B)-H(15B)	120.2

C(17B)-C(16B)-C(15B)	119.9(3)	C(25C)-N(2C)-C(6C)	111.2(2)
C(17B)-C(16B)-H(16B)	120.0	C(25C)-N(2C)-C(5C)	111.6(2)
C(15B)-C(16B)-H(16B)	120.0	C(6C)-N(2C)-C(5C)	108.2(2)
C(16B)-C(17B)-C(18B)	121.4(3)	C(13C)-N(3C)-C(6C)	111.4(2)
C(16B)-C(17B)-H(17B)	119.3	C(13C)-N(3C)-C(19C)	111.6(3)
C(18B)-C(17B)-H(17B)	119.3	C(6C)-N(3C)-C(19C)	106.3(2)
C(17B)-C(18B)-C(13B)	118.2(3)	C(12C)-N(4C)-C(19C)	116.8(3)
C(17B)-C(18B)-C(5B)	121.3(3)	C(12C)-N(4C)-H(4C)	117(3)
C(13B)-C(18B)-C(5B)	120.0(3)	C(19C)-N(4C)-H(4C)	120(3)
N(2B)-C(19B)-N(3B)	111.0(3)	N(1C)-C(1C)-C(2C)	104.5(3)
N(2B)-C(19B)-C(20B)	112.1(3)	N(1C)-C(1C)-H(1CA)	110.9
N(3B)-C(19B)-C(20B)	110.1(2)	C(2C)-C(1C)-H(1CA)	110.9
N(2B)-C(19B)-H(19B)	107.8	N(1C)-C(1C)-H(1CB)	110.9
N(3B)-C(19B)-H(19B)	107.8	C(2C)-C(1C)-H(1CB)	110.9
C(20B)-C(19B)-H(19B)	107.8	H(1CA)-C(1C)-H(1CB)	108.9
C(21B)-C(20B)-C(25B)	119.4(3)	C(3C)-C(2C)-C(1C)	105.0(3)
C(21B)-C(20B)-C(19B)	119.7(3)	C(3C)-C(2C)-H(2CA)	110.8
C(25B)-C(20B)-C(19B)	120.8(3)	C(1C)-C(2C)-H(2CA)	110.8
C(22B)-C(21B)-C(20B)	121.4(3)	C(3C)-C(2C)-H(2CB)	110.8
C(22B)-C(21B)-H(21B)	119.3	C(1C)-C(2C)-H(2CB)	110.8
C(20B)-C(21B)-H(21B)	119.3	H(2CA)-C(2C)-H(2CB)	108.8
C(21B)-C(22B)-C(23B)	118.9(3)	C(4C)-C(3C)-C(2C)	103.4(3)
C(21B)-C(22B)-H(22B)	120.5	C(4C)-C(3C)-H(3CA)	111.1
C(23B)-C(22B)-H(22B)	120.5	C(2C)-C(3C)-H(3CA)	111.1
C(24B)-C(23B)-C(22B)	120.8(3)	C(4C)-C(3C)-H(3CB)	111.1
C(24B)-C(23B)-H(23B)	119.6	C(2C)-C(3C)-H(3CB)	111.1
C(22B)-C(23B)-H(23B)	119.6	H(3CA)-C(3C)-H(3CB)	109.0
C(23B)-C(24B)-C(25B)	120.0(3)	N(1C)-C(4C)-C(3C)	101.7(3)
C(23B)-C(24B)-H(24B)	120.0	N(1C)-C(4C)-H(4CA)	111.4
C(25B)-C(24B)-H(24B)	120.0	C(3C)-C(4C)-H(4CA)	111.4
N(4B)-C(25B)-C(24B)	121.4(3)	N(1C)-C(4C)-H(4CB)	111.4
N(4B)-C(25B)-C(20B)	119.2(3)	C(3C)-C(4C)-H(4CB)	111.4
C(24B)-C(25B)-C(20B)	119.4(3)	H(4CA)-C(4C)-H(4CB)	109.3
C(5C)-N(1C)-C(4C)	113.1(2)	N(1C)-C(5C)-N(2C)	108.0(2)
C(5C)-N(1C)-C(1C)	114.2(3)	N(1C)-C(5C)-C(18C)	112.6(2)
C(4C)-N(1C)-C(1C)	103.7(2)	N(2C)-C(5C)-C(18C)	109.5(3)

N(1C)-C(5C)-H(5CA)	108.9	C(15C)-C(16C)-C(17C)	120.3(3)
N(2C)-C(5C)-H(5CA)	108.9	C(15C)-C(16C)-H(16C)	119.9
C(18C)-C(5C)-H(5CA)	108.9	C(17C)-C(16C)-H(16C)	119.9
N(2C)-C(6C)-N(3C)	111.2(3)	C(16C)-C(17C)-C(18C)	120.1(4)
N(2C)-C(6C)-C(7C)	113.8(2)	C(16C)-C(17C)-H(17C)	119.9
N(3C)-C(6C)-C(7C)	109.2(2)	C(18C)-C(17C)-H(17C)	119.9
N(2C)-C(6C)-H(6CA)	107.4	C(13C)-C(18C)-C(17C)	118.9(3)
N(3C)-C(6C)-H(6CA)	107.4	C(13C)-C(18C)-C(5C)	120.6(3)
C(7C)-C(6C)-H(6CA)	107.4	C(17C)-C(18C)-C(5C)	120.4(3)
C(8C)-C(7C)-C(12C)	119.0(3)	N(4C)-C(19C)-N(3C)	109.8(3)
C(8C)-C(7C)-C(6C)	119.3(3)	N(4C)-C(19C)-C(20C)	111.4(3)
C(12C)-C(7C)-C(6C)	121.5(3)	N(3C)-C(19C)-C(20C)	109.5(3)
C(9C)-C(8C)-C(7C)	121.2(3)	N(4C)-C(19C)-H(19C)	108.7
C(9C)-C(8C)-H(8CA)	119.4	N(3C)-C(19C)-H(19C)	108.7
C(7C)-C(8C)-H(8CA)	119.4	C(20C)-C(19C)-H(19C)	108.7
C(8C)-C(9C)-C(10C)	118.9(3)	C(21C)-C(20C)-C(25C)	118.7(3)
C(8C)-C(9C)-H(9CA)	120.5	C(21C)-C(20C)-C(19C)	120.1(3)
C(10C)-C(9C)-H(9CA)	120.5	C(25C)-C(20C)-C(19C)	121.2(3)
C(11C)-C(10C)-C(9C)	120.7(3)	C(22C)-C(21C)-C(20C)	121.0(3)
C(11C)-C(10C)-H(10C)	119.6	C(22C)-C(21C)-H(21C)	119.5
C(9C)-C(10C)-H(10C)	119.6	C(20C)-C(21C)-H(21C)	119.5
C(10C)-C(11C)-C(12C)	120.3(3)	C(21C)-C(22C)-C(23C)	120.2(3)
C(10C)-C(11C)-H(11A)	119.8	C(21C)-C(22C)-H(22C)	119.9
C(12C)-C(11C)-H(11A)	119.8	C(23C)-C(22C)-H(22C)	119.9
N(4C)-C(12C)-C(11C)	121.1(3)	C(24C)-C(23C)-C(22C)	119.6(3)
N(4C)-C(12C)-C(7C)	119.2(3)	C(24C)-C(23C)-H(23C)	120.2
C(11C)-C(12C)-C(7C)	119.7(3)	C(22C)-C(23C)-H(23C)	120.2
C(18C)-C(13C)-C(14C)	120.3(3)	C(23C)-C(24C)-C(25C)	120.5(3)
C(18C)-C(13C)-N(3C)	122.8(3)	C(23C)-C(24C)-H(24C)	119.7
C(14C)-C(13C)-N(3C)	116.9(3)	C(25C)-C(24C)-H(24C)	119.7
C(15C)-C(14C)-C(13C)	119.9(4)	C(24C)-C(25C)-C(20C)	120.0(3)
C(15C)-C(14C)-H(14C)	120.1	C(24C)-C(25C)-N(2C)	118.4(3)
C(13C)-C(14C)-H(14C)	120.1	C(20C)-C(25C)-N(2C)	121.6(3)
C(16C)-C(15C)-C(14C)	120.6(3)	C(4D)-N(1D)-C(5D)	113.0(3)
C(16C)-C(15C)-H(15C)	119.7	C(4D)-N(1D)-C(1D)	103.2(3)
C(14C)-C(15C)-H(15C)	119.7	C(5D)-N(1D)-C(1D)	114.2(3)



C(25D)-N(2D)-C(6D)	110.1(3)	N(1D)-C(5D)-H(5DA)	108.9
C(25D)-N(2D)-C(5D)	113.2(3)	N(2D)-C(5D)-H(5DA)	108.9
C(6D)-N(2D)-C(5D)	109.4(3)	C(18D)-C(5D)-H(5DA)	108.9
C(13D)-N(3D)-C(6D)	112.7(3)	N(2D)-C(6D)-N(3D)	110.9(3)
C(13D)-N(3D)-C(19D)	111.5(3)	N(2D)-C(6D)-C(7D)	110.9(3)
C(6D)-N(3D)-C(19D)	105.9(3)	N(3D)-C(6D)-C(7D)	110.5(3)
C(12D)-N(4D)-C(19D)	114.0(3)	N(2D)-C(6D)-H(6DA)	108.2
C(12D)-N(4D)-H(4D)	111(3)	N(3D)-C(6D)-H(6DA)	108.2
C(19D)-N(4D)-H(4D)	125(3)	C(7D)-C(6D)-H(6DA)	108.2
N(1D)-C(1D)-C(2D)	103.2(3)	C(8D)-C(7D)-C(12D)	118.3(4)
N(1D)-C(1D)-H(1DA)	111.1	C(8D)-C(7D)-C(6D)	120.2(3)
C(2D)-C(1D)-H(1DA)	111.1	C(12D)-C(7D)-C(6D)	121.6(3)
N(1D)-C(1D)-H(1DB)	111.1	C(9D)-C(8D)-C(7D)	122.0(4)
C(2D)-C(1D)-H(1DB)	111.1	C(9D)-C(8D)-H(8DA)	119.0
H(1DA)-C(1D)-H(1DB)	109.1	C(7D)-C(8D)-H(8DA)	119.0
C(1D)-C(2D)-C(3D)	104.0(3)	C(8D)-C(9D)-C(10D)	119.2(4)
C(1D)-C(2D)-H(2DA)	111.0	C(8D)-C(9D)-H(9DA)	120.4
C(3D)-C(2D)-H(2DA)	111.0	C(10D)-C(9D)-H(9DA)	120.4
C(1D)-C(2D)-H(2DB)	111.0	C(11D)-C(10D)-C(9D)	120.2(4)
C(3D)-C(2D)-H(2DB)	110.9	C(11D)-C(10D)-H(10D)	119.9
H(2DA)-C(2D)-H(2DB)	109.0	C(9D)-C(10D)-H(10D)	119.9
C(4D)-C(3D)-C(2D)	103.4(3)	C(10D)-C(11D)-C(12D)	120.4(4)
C(4D)-C(3D)-H(3DA)	111.1	C(10D)-C(11D)-H(11B)	119.8
C(2D)-C(3D)-H(3DA)	111.1	C(12D)-C(11D)-H(11B)	119.8
C(4D)-C(3D)-H(3DB)	111.1	N(4D)-C(12D)-C(11D)	121.7(3)
C(2D)-C(3D)-H(3DB)	111.1	N(4D)-C(12D)-C(7D)	118.4(4)
H(3DA)-C(3D)-H(3DB)	109.1	C(11D)-C(12D)-C(7D)	119.9(4)
N(1D)-C(4D)-C(3D)	105.0(3)	C(14D)-C(13D)-C(18D)	119.2(4)
N(1D)-C(4D)-H(4DA)	110.8	C(14D)-C(13D)-N(3D)	117.9(4)
C(3D)-C(4D)-H(4DA)	110.8	C(18D)-C(13D)-N(3D)	122.8(3)
N(1D)-C(4D)-H(4DB)	110.8	C(15D)-C(14D)-C(13D)	120.8(5)
C(3D)-C(4D)-H(4DB)	110.8	C(15D)-C(14D)-H(14D)	119.6
H(4DA)-C(4D)-H(4DB)	108.8	C(13D)-C(14D)-H(14D)	119.6
N(1D)-C(5D)-N(2D)	108.1(3)	C(14D)-C(15D)-C(16D)	120.3(4)
N(1D)-C(5D)-C(18D)	111.7(3)	C(14D)-C(15D)-H(15D)	119.9
N(2D)-C(5D)-C(18D)	110.4(3)	C(16D)-C(15D)-H(15D)	119.9

C(15D)-C(16D)-C(17D)	119.6(5)	C(22D)-C(23D)-C(24D)	120.1(4)
C(15D)-C(16D)-H(16D)	120.2	C(22D)-C(23D)-H(23D)	119.9
C(17D)-C(16D)-H(16D)	120.2	C(24D)-C(23D)-H(23D)	119.9
C(16D)-C(17D)-C(18D)	120.9(5)	C(23D)-C(24D)-C(25D)	120.3(3)
C(16D)-C(17D)-H(17D)	119.6	C(23D)-C(24D)-H(24D)	119.9
C(18D)-C(17D)-H(17D)	119.6	C(25D)-C(24D)-H(24D)	119.9
C(17D)-C(18D)-C(13D)	119.3(4)	C(20D)-C(25D)-C(24D)	119.9(3)
C(17D)-C(18D)-C(5D)	120.8(4)	C(20D)-C(25D)-N(2D)	121.1(3)
C(13D)-C(18D)-C(5D)	119.8(4)	C(24D)-C(25D)-N(2D)	118.9(3)
N(4D)-C(19D)-N(3D)	106.8(3)	Cl(2S)-C(1S)-Cl(3S)	110.4(3)
N(4D)-C(19D)-C(20D)	112.8(3)	Cl(2S)-C(1S)-Cl(1S)	107.8(3)
N(3D)-C(19D)-C(20D)	110.1(3)	Cl(3S)-C(1S)-Cl(1S)	108.2(3)
N(4D)-C(19D)-H(19D)	109.0	Cl(2S)-C(1S)-H(1SA)	110.1
N(3D)-C(19D)-H(19D)	109.0	Cl(3S)-C(1S)-H(1SA)	110.1
C(20D)-C(19D)-H(19D)	109.0	Cl(1S)-C(1S)-H(1SA)	110.1
C(25D)-C(20D)-C(21D)	118.9(3)	Cl(1T)-C(1T)-Cl(2T)	111.1(4)
C(25D)-C(20D)-C(19D)	121.6(3)	Cl(1T)-C(1T)-Cl(3T)	109.5(4)
C(21D)-C(20D)-C(19D)	119.6(3)	Cl(2T)-C(1T)-Cl(3T)	110.6(4)
C(22D)-C(21D)-C(20D)	120.6(4)	Cl(1T)-C(1T)-H(1TA)	108.5
C(22D)-C(21D)-H(21D)	119.7	Cl(2T)-C(1T)-H(1TA)	108.5
C(20D)-C(21D)-H(21D)	119.7	Cl(3T)-C(1T)-H(1TA)	108.5
C(23D)-C(22D)-C(21D)	120.2(3)		
C(23D)-C(22D)-H(22D)	119.9		
C(21D)-C(22D)-H(22D)	119.9		

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Symmetry transformations used to generate equivalent atoms:

**Table S3.** Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **1**. The anisotropic displacement factor exponent takes the form:  $-2p^2[ h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12} ]$

	U11	U22	U33	U23	U13	U12
N(1A)	23(1)	25(1)	27(1)	-6(1)	3(1)	1(1)
N(2A)	21(1)	20(1)	29(1)	-6(1)	2(1)	1(1)
N(3A)	21(1)	14(1)	32(1)	-4(1)	2(1)	1(1)
N(4A)	26(1)	20(1)	32(1)	-1(1)	7(1)	5(1)
C(1A)	27(2)	34(2)	36(2)	-11(1)	7(1)	2(1)
C(2A)	34(2)	55(2)	35(2)	-8(2)	10(1)	5(2)
C(3A)	58(3)	49(2)	41(2)	4(2)	14(2)	6(2)
C(4A)	33(2)	37(2)	37(2)	2(1)	6(1)	-2(1)
C(5A)	20(1)	24(1)	28(2)	-8(1)	1(1)	3(1)
C(6A)	23(1)	19(1)	31(2)	-7(1)	1(1)	2(1)
C(7A)	24(2)	28(2)	43(2)	-9(1)	5(1)	-2(1)
C(8A)	23(2)	34(2)	55(2)	-20(2)	1(2)	-4(1)
C(9A)	28(2)	38(2)	45(2)	-21(2)	-8(1)	6(1)
C(10A)	29(2)	32(2)	33(2)	-10(1)	-2(1)	11(1)
C(11A)	21(1)	19(1)	32(2)	-5(1)	-1(1)	7(1)
C(12A)	26(1)	17(1)	29(2)	-2(1)	4(1)	5(1)
C(13A)	20(1)	16(1)	31(2)	-6(1)	-2(1)	3(1)
C(14A)	26(1)	22(1)	35(2)	-2(1)	0(1)	2(1)
C(15A)	39(2)	19(2)	39(2)	-1(1)	-1(1)	3(1)
C(16A)	40(2)	20(2)	43(2)	-6(1)	-2(2)	9(1)
C(17A)	29(2)	28(2)	36(2)	-7(1)	0(1)	10(1)
C(18A)	23(1)	21(1)	30(2)	-6(1)	-2(1)	3(1)
C(19A)	18(1)	18(1)	29(1)	-3(1)	1(1)	2(1)
C(20A)	18(1)	16(1)	31(2)	-4(1)	-1(1)	1(1)
C(21A)	24(1)	21(1)	30(2)	-3(1)	-1(1)	2(1)
C(22A)	27(2)	16(1)	38(2)	0(1)	-3(1)	2(1)
C(23A)	21(1)	16(1)	43(2)	-3(1)	1(1)	1(1)
C(24A)	23(1)	17(1)	36(2)	-5(1)	4(1)	1(1)
C(25A)	18(1)	15(1)	32(2)	-3(1)	1(1)	0(1)
N(1B)	21(1)	17(1)	36(1)	-4(1)	2(1)	-1(1)
N(2B)	22(1)	14(1)	39(1)	-4(1)	2(1)	-1(1)

N(3B)	29(1)	21(1)	45(2)	-7(1)	-10(1)	6(1)
N(4B)	32(2)	27(2)	95(3)	-27(2)	-28(2)	9(1)
C(1B)	27(2)	21(1)	37(2)	-5(1)	4(1)	-2(1)
C(2B)	27(2)	29(2)	45(2)	-3(1)	0(1)	-2(1)
C(3B)	25(2)	29(2)	71(3)	-8(2)	-2(2)	1(1)
C(4B)	25(2)	23(2)	47(2)	-4(1)	-4(1)	3(1)
C(5B)	22(1)	14(1)	34(2)	-3(1)	1(1)	-2(1)
C(6B)	22(1)	15(1)	56(2)	0(1)	7(1)	1(1)
C(7B)	35(2)	23(2)	61(2)	6(2)	16(2)	4(1)
C(8B)	52(2)	26(2)	91(3)	7(2)	41(2)	6(2)
C(9B)	35(2)	24(2)	134(5)	-3(2)	41(3)	-3(2)
C(10B)	23(2)	22(2)	111(4)	-13(2)	15(2)	-2(1)
C(11B)	22(2)	14(1)	74(3)	-8(1)	2(2)	-1(1)
C(12B)	23(2)	18(2)	72(3)	-13(2)	-11(2)	2(1)
C(13B)	26(2)	18(1)	38(2)	-2(1)	-1(1)	3(1)
C(14B)	31(2)	28(2)	39(2)	-1(1)	-4(1)	6(1)
C(15B)	29(2)	23(2)	46(2)	7(1)	2(1)	6(1)
C(16B)	30(2)	20(1)	43(2)	2(1)	10(1)	6(1)
C(17B)	27(2)	21(1)	35(2)	-1(1)	7(1)	2(1)
C(18B)	22(1)	18(1)	36(2)	-1(1)	3(1)	-1(1)
C(19B)	24(1)	19(1)	36(2)	-4(1)	-4(1)	2(1)
C(20B)	27(2)	18(1)	37(2)	-5(1)	-1(1)	1(1)
C(21B)	24(1)	20(1)	34(2)	-2(1)	2(1)	1(1)
C(22B)	29(2)	23(2)	35(2)	-2(1)	5(1)	5(1)
C(23B)	36(2)	20(1)	34(2)	-6(1)	4(1)	4(1)
C(24B)	33(2)	22(2)	39(2)	-7(1)	-3(1)	0(1)
C(25B)	27(2)	21(2)	47(2)	-7(1)	-7(1)	2(1)
N(1C)	25(1)	22(1)	30(1)	-5(1)	3(1)	1(1)
N(2C)	26(1)	24(1)	25(1)	-4(1)	4(1)	1(1)
N(3C)	22(1)	25(1)	31(1)	-6(1)	3(1)	-3(1)
N(4C)	26(1)	35(2)	37(2)	-3(1)	-2(1)	2(1)
C(1C)	34(2)	24(2)	44(2)	-2(1)	6(1)	5(1)
C(2C)	32(2)	34(2)	49(2)	-2(2)	6(2)	7(1)
C(3C)	27(2)	31(2)	37(2)	-1(1)	1(1)	2(1)
C(4C)	29(2)	27(2)	31(2)	-5(1)	1(1)	1(1)
C(5C)	29(2)	23(1)	29(2)	-3(1)	6(1)	1(1)

C(6C)	22(1)	28(2)	26(1)	-5(1)	2(1)	0(1)
C(7C)	26(2)	26(2)	27(2)	-4(1)	3(1)	1(1)
C(8C)	27(2)	32(2)	32(2)	-2(1)	5(1)	2(1)
C(9C)	37(2)	29(2)	42(2)	0(1)	9(2)	-2(1)
C(10C)	45(2)	31(2)	40(2)	4(1)	8(2)	6(2)
C(11C)	37(2)	35(2)	34(2)	0(1)	2(1)	9(1)
C(12C)	30(2)	33(2)	27(2)	-4(1)	4(1)	3(1)
C(13C)	25(1)	29(2)	31(2)	-7(1)	8(1)	-3(1)
C(14C)	31(2)	32(2)	36(2)	-9(1)	8(1)	-7(1)
C(15C)	35(2)	34(2)	48(2)	-12(2)	13(2)	-11(2)
C(16C)	47(2)	22(2)	57(2)	-5(2)	16(2)	-8(2)
C(17C)	38(2)	25(2)	41(2)	-3(1)	12(2)	-1(1)
C(18C)	29(2)	24(2)	35(2)	-5(1)	11(1)	-3(1)
C(19C)	22(1)	32(2)	35(2)	-8(1)	4(1)	-3(1)
C(20C)	28(2)	24(2)	37(2)	-7(1)	9(1)	-2(1)
C(21C)	31(2)	28(2)	42(2)	-9(1)	10(1)	-1(1)
C(22C)	41(2)	25(2)	45(2)	-9(1)	19(2)	-3(1)
C(23C)	53(2)	20(2)	34(2)	-5(1)	18(2)	-2(1)
C(24C)	40(2)	18(1)	32(2)	-3(1)	9(1)	1(1)
C(25C)	31(2)	18(1)	32(2)	-5(1)	9(1)	-1(1)
N(1D)	30(1)	36(2)	26(1)	-8(1)	5(1)	-5(1)
N(2D)	25(1)	41(2)	26(1)	-9(1)	2(1)	-2(1)
N(3D)	29(1)	54(2)	28(1)	-5(1)	5(1)	-7(1)
N(4D)	33(2)	58(2)	29(2)	-5(1)	7(1)	2(1)
C(1D)	47(2)	38(2)	39(2)	-12(2)	13(2)	-2(2)
C(2D)	58(3)	57(3)	33(2)	-12(2)	9(2)	-6(2)
C(3D)	49(2)	72(3)	31(2)	11(2)	8(2)	5(2)
C(4D)	44(2)	44(2)	32(2)	-2(2)	7(2)	-10(2)
C(5D)	33(2)	37(2)	27(2)	-6(1)	4(1)	-3(1)
C(6D)	23(2)	49(2)	26(2)	-6(1)	1(1)	-3(1)
C(7D)	22(2)	50(2)	32(2)	-4(2)	1(1)	2(1)
C(8D)	24(2)	52(2)	33(2)	-3(2)	1(1)	3(2)
C(9D)	29(2)	52(2)	42(2)	3(2)	1(2)	6(2)
C(10D)	31(2)	51(2)	47(2)	-6(2)	-1(2)	8(2)
C(11D)	34(2)	55(2)	35(2)	-10(2)	3(1)	7(2)
C(12D)	24(2)	54(2)	34(2)	-5(2)	2(1)	4(2)

C(13D)	35(2)	52(2)	30(2)	-7(2)	2(1)	-13(2)
C(14D)	52(2)	65(3)	42(2)	-8(2)	11(2)	-24(2)
C(15D)	89(4)	54(3)	52(3)	-10(2)	24(3)	-36(3)
C(16D)	98(4)	43(2)	49(3)	-10(2)	18(3)	-22(3)
C(17D)	70(3)	42(2)	39(2)	-8(2)	11(2)	-11(2)
C(18D)	43(2)	43(2)	30(2)	-7(1)	4(2)	-10(2)
C(19D)	31(2)	48(2)	27(2)	-5(1)	6(1)	-2(2)
C(20D)	29(2)	42(2)	28(2)	-6(1)	3(1)	2(1)
C(21D)	37(2)	51(2)	28(2)	-9(2)	1(1)	7(2)
C(22D)	38(2)	64(3)	33(2)	-14(2)	-7(2)	7(2)
C(23D)	25(2)	63(3)	45(2)	-12(2)	-3(2)	1(2)
C(24D)	28(2)	50(2)	34(2)	-9(2)	4(1)	0(2)
C(25D)	28(2)	40(2)	28(2)	-10(1)	3(1)	-4(1)
C(1S)	118(8)	136(9)	49(4)	-19(5)	10(4)	73(7)
Cl(1S)	93(1)	89(1)	67(1)	5(1)	16(1)	20(1)
Cl(2S)	106(2)	70(1)	88(1)	-2(1)	37(1)	-1(1)
Cl(3S)	104(2)	74(1)	92(1)	2(1)	38(1)	-1(1)
C(1T)	118(8)	136(9)	49(4)	-19(5)	10(4)	73(7)
Cl(1T)	93(1)	89(1)	67(1)	5(1)	16(1)	20(1)
Cl(2T)	106(2)	70(1)	88(1)	-2(1)	37(1)	-1(1)
Cl(3T)	104(2)	74(1)	92(1)	2(1)	38(1)	-1(1)

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**Table S4.** Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **1**.

	x	y	z	U(eq)
H(4A)	3060(40)	2180(30)	-670(20)	34(11)
H(1AA)	234	4313	1808	39
H(1AB)	1449	4758	1954	39
H(2AA)	1627	4224	2862	49
H(2AB)	363	3985	2753	49
H(3AA)	675	2452	2808	59
H(3AB)	1888	2692	2733	59
H(4AA)	1215	1920	1846	43
H(4AB)	90	2357	1814	43
H(5AA)	73	3280	974	30
H(7AA)	-751	1609	577	39
H(8AA)	-1855	1141	-305	47
H(9AA)	-1241	1369	-1188	46
H(10A)	459	2080	-1188	38
H(12A)	1956	3263	-622	29
H(14A)	2859	4887	-181	34
H(15A)	2146	6355	-78	40
H(16A)	830	6468	498	42
H(17A)	279	5139	991	38
H(19A)	2696	2828	1089	26
H(21A)	2791	1091	1366	31
H(22A)	3673	-254	1193	34
H(23A)	4193	-483	284	33
H(24A)	3696	528	-471	31
H(4B)	4290(40)	3530(30)	570(20)	44(12)
H(1BA)	8242	7718	2522	34
H(1BB)	8467	7892	1870	34
H(2BA)	10199	7752	2143	42

H(2BB)	10000	7807	2809	42
H(3BA)	10288	6148	2155	52
H(3BB)	10411	6274	2856	52
H(4BA)	8808	5207	2309	39
H(4BB)	8630	5908	2841	39
H(5BA)	6963	6448	2467	29
H(7BA)	6405	5069	3019	46
H(8BA)	4825	4588	3346	63
H(9BA)	3286	4141	2675	74
H(10B)	3313	4198	1680	63
H(12B)	4213	5039	915	48
H(14B)	4576	6484	433	40
H(15B)	4305	8071	660	39
H(16B)	5362	8904	1472	36
H(17B)	6601	8115	2083	33
H(19B)	7372	5274	1214	33
H(21B)	8217	3777	1573	32
H(22B)	8241	2139	1345	34
H(23B)	6716	1272	817	36
H(24B)	5164	2011	574	39
H(4C)	9940(40)	-840(30)	3940(20)	46(13)
H(1CA)	5505	2437	2370	41
H(1CB)	5644	2568	3070	41
H(2CA)	3937	2061	3063	46
H(2CB)	3759	2169	2366	46
H(3CA)	3918	447	2973	38
H(3CB)	3401	556	2299	38
H(4CA)	5176	-161	2493	35
H(4CB)	5036	630	1997	35
H(5CA)	6837	1395	2221	32
H(6CA)	6837	230	3498	31
H(8CA)	5949	-1430	3241	37
H(9CA)	6020	-3033	3509	43
H(10C)	7656	-3568	3903	46
H(11A)	9199	-2551	3971	42
H(14C)	9667	2028	4119	40



H(15C)	9730	3661	3936	47
H(16C)	8543	4222	3188	50
H(17C)	7268	3141	2604	42
H(19C)	9973	595	3557	36
H(21C)	10668	-29	2676	40
H(22C)	10431	-83	1664	44
H(23C)	8730	-73	1113	42
H(24C)	7291	61	1588	36
H(4D)	8530(40)	520(40)	4590(20)	58(14)
H(1DA)	6462	3647	7196	50
H(1DB)	7726	3875	7266	50
H(2DA)	6814	3371	8171	60
H(2DB)	8015	3163	8145	60
H(3DA)	7524	1550	8008	60
H(3DB)	6343	1751	8089	60
H(4DA)	6677	1115	7100	49
H(4DB)	5804	1865	7125	49
H(5DA)	6105	2739	6276	39
H(6DA)	8368	1528	6467	40
H(8DA)	7597	-196	6625	45
H(9DA)	7712	-1812	6394	50
H(10D)	8235	-2249	5507	53
H(11B)	8606	-1071	4861	50
H(14D)	9396	3527	5270	66
H(15D)	9116	5147	5344	80
H(16D)	7849	5637	5874	77
H(17D)	6857	4492	6326	61
H(19D)	8201	2155	4781	43
H(21D)	6534	1383	4103	47
H(22D)	4705	1065	3981	56
H(23D)	3855	1040	4789	55
H(24D)	4827	1351	5723	45
H(1SA)	6180	4090	4959	118
H(1TA)	5210	2683	4820	118

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**Table S5.** Torsion angles [°] for **1**.

C(5A)-N(1A)-C(1A)-C(2A)	155.8(3)	C(13A)-N(3A)-C(12A)-C(11A)	-74.3(3)
C(4A)-N(1A)-C(1A)-C(2A)	33.9(3)	C(19A)-N(3A)-C(12A)-C(11A)	47.7(3)
N(1A)-C(1A)-C(2A)-C(3A)	-11.1(4)	C(6A)-C(11A)-C(12A)-N(4A)	105.5(3)
C(1A)-C(2A)-C(3A)-C(4A)	-15.1(4)	C(10A)-C(11A)-C(12A)-N(4A)	-73.3(3)
C(5A)-N(1A)-C(4A)-C(3A)	-165.8(3)	C(6A)-C(11A)-C(12A)-N(3A)	-15.0(4)
C(1A)-N(1A)-C(4A)-C(3A)	-42.8(3)	C(10A)-C(11A)-C(12A)-N(3A)	166.3(3)
C(2A)-C(3A)-C(4A)-N(1A)	35.6(4)	C(19A)-N(3A)-C(13A)-C(14A)	164.4(3)
C(1A)-N(1A)-C(5A)-N(2A)	-175.9(2)	C(12A)-N(3A)-C(13A)-C(14A)	-76.6(3)
C(4A)-N(1A)-C(5A)-N(2A)	-58.2(3)	C(19A)-N(3A)-C(13A)-C(18A)	-16.7(4)
C(1A)-N(1A)-C(5A)-C(18A)	61.1(3)	C(12A)-N(3A)-C(13A)-C(18A)	102.4(3)
C(4A)-N(1A)-C(5A)-C(18A)	178.8(3)	C(18A)-C(13A)-C(14A)-C(15A)	-0.8(5)
C(6A)-N(2A)-C(5A)-N(1A)	159.5(2)	N(3A)-C(13A)-C(14A)-C(15A)	178.2(3)
C(19A)-N(2A)-C(5A)-N(1A)	-77.2(3)	C(13A)-C(14A)-C(15A)-C(16A)	-1.1(5)
C(6A)-N(2A)-C(5A)-C(18A)	-76.0(3)	C(14A)-C(15A)-C(16A)-C(17A)	1.4(5)
C(19A)-N(2A)-C(5A)-C(18A)	47.3(3)	C(15A)-C(16A)-C(17A)-C(18A)	0.3(5)
C(19A)-N(2A)-C(6A)-C(11A)	-18.2(4)	C(16A)-C(17A)-C(18A)-C(13A)	-2.2(5)
C(5A)-N(2A)-C(6A)-C(11A)	104.3(3)	C(16A)-C(17A)-C(18A)-C(5A)	-177.7(3)
C(19A)-N(2A)-C(6A)-C(7A)	160.6(3)	C(14A)-C(13A)-C(18A)-C(17A)	2.4(4)
C(5A)-N(2A)-C(6A)-C(7A)	-77.0(3)	N(3A)-C(13A)-C(18A)-C(17A)	-176.5(3)
C(11A)-C(6A)-C(7A)-C(8A)	-0.5(5)	C(14A)-C(13A)-C(18A)-C(5A)	178.0(3)
N(2A)-C(6A)-C(7A)-C(8A)	-179.3(3)	N(3A)-C(13A)-C(18A)-C(5A)	-0.9(4)
C(6A)-C(7A)-C(8A)-C(9A)	1.1(5)	N(1A)-C(5A)-C(18A)-C(17A)	-78.0(4)
C(7A)-C(8A)-C(9A)-C(10A)	-0.5(6)	N(2A)-C(5A)-C(18A)-C(17A)	160.6(3)
C(8A)-C(9A)-C(10A)-C(11A)	-0.7(5)	N(1A)-C(5A)-C(18A)-C(13A)	106.6(3)
C(7A)-C(6A)-C(11A)-C(10A)	-0.6(4)	N(2A)-C(5A)-C(18A)-C(13A)	-14.8(4)
N(2A)-C(6A)-C(11A)-C(10A)	178.1(3)	C(13A)-N(3A)-C(19A)-N(2A)	51.2(3)
C(7A)-C(6A)-C(11A)-C(12A)	-179.4(3)	C(12A)-N(3A)-C(19A)-N(2A)	-70.8(3)
N(2A)-C(6A)-C(11A)-C(12A)	-0.7(4)	C(13A)-N(3A)-C(19A)-C(20A)	176.5(2)
C(9A)-C(10A)-C(11A)-C(6A)	1.3(5)	C(12A)-N(3A)-C(19A)-C(20A)	54.4(3)
C(9A)-C(10A)-C(11A)-C(12A)	-180.0(3)	C(6A)-N(2A)-C(19A)-N(3A)	55.0(3)
C(25A)-N(4A)-C(12A)-N(3A)	45.7(3)	C(5A)-N(2A)-C(19A)-N(3A)	-68.8(3)
C(25A)-N(4A)-C(12A)-C(11A)	-75.8(3)	C(6A)-N(2A)-C(19A)-C(20A)	-67.7(3)
C(13A)-N(3A)-C(12A)-N(4A)	165.5(2)	C(5A)-N(2A)-C(19A)-C(20A)	168.6(2)
C(19A)-N(3A)-C(12A)-N(4A)	-72.6(3)	N(3A)-C(19A)-C(20A)-C(21A)	158.4(3)

N(2A)-C(19A)-C(20A)-C(21A)	-77.3(3)	N(2B)-C(6B)-C(7B)-C(8B)	-179.3(3)
N(3A)-C(19A)-C(20A)-C(25A)	-15.5(4)	C(6B)-C(7B)-C(8B)-C(9B)	0.3(5)
N(2A)-C(19A)-C(20A)-C(25A)	108.9(3)	C(7B)-C(8B)-C(9B)-C(10B)	-0.7(6)
C(25A)-C(20A)-C(21A)-C(22A)	2.4(4)	C(8B)-C(9B)-C(10B)-C(11B)	0.1(6)
C(19A)-C(20A)-C(21A)-C(22A)	-171.5(3)	C(9B)-C(10B)-C(11B)-C(6B)	0.8(5)
C(20A)-C(21A)-C(22A)-C(23A)	0.9(5)	C(9B)-C(10B)-C(11B)-C(12B)	-178.0(3)
C(21A)-C(22A)-C(23A)-C(24A)	-3.3(5)	C(7B)-C(6B)-C(11B)-C(10B)	-1.2(5)
C(22A)-C(23A)-C(24A)-C(25A)	2.4(5)	N(2B)-C(6B)-C(11B)-C(10B)	178.7(3)
C(12A)-N(4A)-C(25A)-C(20A)	-4.5(4)	C(7B)-C(6B)-C(11B)-C(12B)	177.6(3)
C(12A)-N(4A)-C(25A)-C(24A)	173.6(3)	N(2B)-C(6B)-C(11B)-C(12B)	-2.5(4)
C(21A)-C(20A)-C(25A)-N(4A)	174.8(3)	C(25B)-N(4B)-C(12B)-N(3B)	51.7(5)
C(19A)-C(20A)-C(25A)-N(4A)	-11.3(4)	C(25B)-N(4B)-C(12B)-C(11B)	-69.8(5)
C(21A)-C(20A)-C(25A)-C(24A)	-3.3(4)	C(13B)-N(3B)-C(12B)-N(4B)	166.1(3)
C(19A)-C(20A)-C(25A)-C(24A)	170.5(3)	C(19B)-N(3B)-C(12B)-N(4B)	-71.7(4)
C(23A)-C(24A)-C(25A)-N(4A)	-177.2(3)	C(13B)-N(3B)-C(12B)-C(11B)	-70.8(3)
C(23A)-C(24A)-C(25A)-C(20A)	0.9(4)	C(19B)-N(3B)-C(12B)-C(11B)	51.4(3)
C(5B)-N(1B)-C(1B)-C(2B)	154.6(3)	C(10B)-C(11B)-C(12B)-N(4B)	-77.5(4)
C(4B)-N(1B)-C(1B)-C(2B)	33.9(3)	C(6B)-C(11B)-C(12B)-N(4B)	103.7(4)
N(1B)-C(1B)-C(2B)-C(3B)	-11.3(4)	C(10B)-C(11B)-C(12B)-N(3B)	162.0(3)
C(1B)-C(2B)-C(3B)-C(4B)	-14.7(4)	C(6B)-C(11B)-C(12B)-N(3B)	-16.8(4)
C(5B)-N(1B)-C(4B)-C(3B)	-164.6(3)	C(19B)-N(3B)-C(13B)-C(14B)	170.9(3)
C(1B)-N(1B)-C(4B)-C(3B)	-43.4(3)	C(12B)-N(3B)-C(13B)-C(14B)	-70.3(4)
C(2B)-C(3B)-C(4B)-N(1B)	35.6(4)	C(19B)-N(3B)-C(13B)-C(18B)	-10.6(5)
C(4B)-N(1B)-C(5B)-N(2B)	-56.1(3)	C(12B)-N(3B)-C(13B)-C(18B)	108.2(4)
C(1B)-N(1B)-C(5B)-N(2B)	-172.5(3)	C(18B)-C(13B)-C(14B)-C(15B)	-1.4(5)
C(4B)-N(1B)-C(5B)-C(18B)	-178.6(3)	N(3B)-C(13B)-C(14B)-C(15B)	177.2(3)
C(1B)-N(1B)-C(5B)-C(18B)	65.0(3)	C(13B)-C(14B)-C(15B)-C(16B)	2.1(6)
C(6B)-N(2B)-C(5B)-N(1B)	162.7(3)	C(14B)-C(15B)-C(16B)-C(17B)	-1.9(5)
C(19B)-N(2B)-C(5B)-N(1B)	-74.3(3)	C(15B)-C(16B)-C(17B)-C(18B)	1.1(5)
C(6B)-N(2B)-C(5B)-C(18B)	-72.4(3)	C(16B)-C(17B)-C(18B)-C(13B)	-0.4(5)
C(19B)-N(2B)-C(5B)-C(18B)	50.6(3)	C(16B)-C(17B)-C(18B)-C(5B)	-172.6(3)
C(19B)-N(2B)-C(6B)-C(7B)	165.2(3)	C(14B)-C(13B)-C(18B)-C(17B)	0.5(5)
C(5B)-N(2B)-C(6B)-C(7B)	-73.2(4)	N(3B)-C(13B)-C(18B)-C(17B)	-177.9(3)
C(19B)-N(2B)-C(6B)-C(11B)	-14.7(4)	C(14B)-C(13B)-C(18B)-C(5B)	172.8(3)
C(5B)-N(2B)-C(6B)-C(11B)	106.9(3)	N(3B)-C(13B)-C(18B)-C(5B)	-5.6(5)
C(11B)-C(6B)-C(7B)-C(8B)	0.6(5)	N(1B)-C(5B)-C(18B)-C(17B)	-81.3(4)

N(2B)-C(5B)-C(18B)-C(17B)	157.1(3)	C(1C)-N(1C)-C(5C)-N(2C)	-177.5(3)
N(1B)-C(5B)-C(18B)-C(13B)	106.7(3)	C(4C)-N(1C)-C(5C)-C(18C)	179.7(3)
N(2B)-C(5B)-C(18B)-C(13B)	-15.0(4)	C(1C)-N(1C)-C(5C)-C(18C)	61.5(4)
C(6B)-N(2B)-C(19B)-N(3B)	52.9(3)	C(25C)-N(2C)-C(5C)-N(1C)	166.2(2)
C(5B)-N(2B)-C(19B)-N(3B)	-70.3(3)	C(6C)-N(2C)-C(5C)-N(1C)	-71.2(3)
C(6B)-N(2B)-C(19B)-C(20B)	-70.8(3)	C(25C)-N(2C)-C(5C)-C(18C)	-70.9(3)
C(5B)-N(2B)-C(19B)-C(20B)	166.1(2)	C(6C)-N(2C)-C(5C)-C(18C)	51.7(3)
C(13B)-N(3B)-C(19B)-N(2B)	48.1(4)	C(25C)-N(2C)-C(6C)-N(3C)	52.1(3)
C(12B)-N(3B)-C(19B)-N(2B)	-73.1(3)	C(5C)-N(2C)-C(6C)-N(3C)	-70.7(3)
C(13B)-N(3B)-C(19B)-C(20B)	172.8(3)	C(25C)-N(2C)-C(6C)-C(7C)	-71.8(3)
C(12B)-N(3B)-C(19B)-C(20B)	51.6(4)	C(5C)-N(2C)-C(6C)-C(7C)	165.4(2)
N(2B)-C(19B)-C(20B)-C(21B)	-73.9(4)	C(13C)-N(3C)-C(6C)-N(2C)	49.0(3)
N(3B)-C(19B)-C(20B)-C(21B)	162.0(3)	C(19C)-N(3C)-C(6C)-N(2C)	-72.7(3)
N(2B)-C(19B)-C(20B)-C(25B)	109.4(4)	C(13C)-N(3C)-C(6C)-C(7C)	175.5(2)
N(3B)-C(19B)-C(20B)-C(25B)	-14.7(5)	C(19C)-N(3C)-C(6C)-C(7C)	53.8(3)
C(25B)-C(20B)-C(21B)-C(22B)	1.3(5)	N(2C)-C(6C)-C(7C)-C(8C)	-77.6(4)
C(19B)-C(20B)-C(21B)-C(22B)	-175.5(3)	N(3C)-C(6C)-C(7C)-C(8C)	157.4(3)
C(20B)-C(21B)-C(22B)-C(23B)	1.1(5)	N(2C)-C(6C)-C(7C)-C(12C)	108.0(3)
C(21B)-C(22B)-C(23B)-C(24B)	-2.1(5)	N(3C)-C(6C)-C(7C)-C(12C)	-17.0(4)
C(22B)-C(23B)-C(24B)-C(25B)	0.9(6)	C(12C)-C(7C)-C(8C)-C(9C)	1.2(5)
C(12B)-N(4B)-C(25B)-C(24B)	166.7(4)	C(6C)-C(7C)-C(8C)-C(9C)	-173.4(3)
C(12B)-N(4B)-C(25B)-C(20B)	-12.7(6)	C(7C)-C(8C)-C(9C)-C(10C)	1.2(5)
C(23B)-C(24B)-C(25B)-N(4B)	-177.9(4)	C(8C)-C(9C)-C(10C)-C(11C)	-2.2(6)
C(23B)-C(24B)-C(25B)-C(20B)	1.5(6)	C(9C)-C(10C)-C(11C)-C(12C)	0.8(6)
C(21B)-C(20B)-C(25B)-N(4B)	176.8(4)	C(19C)-N(4C)-C(12C)-C(11C)	173.7(3)
C(19B)-C(20B)-C(25B)-N(4B)	-6.5(6)	C(19C)-N(4C)-C(12C)-C(7C)	-5.3(5)
C(21B)-C(20B)-C(25B)-C(24B)	-2.5(6)	C(10C)-C(11C)-C(12C)-N(4C)	-177.4(3)
C(19B)-C(20B)-C(25B)-C(24B)	174.2(3)	C(10C)-C(11C)-C(12C)-C(7C)	1.6(5)
C(5C)-N(1C)-C(1C)-C(2C)	160.6(3)	C(8C)-C(7C)-C(12C)-N(4C)	176.4(3)
C(4C)-N(1C)-C(1C)-C(2C)	37.1(3)	C(6C)-C(7C)-C(12C)-N(4C)	-9.1(5)
N(1C)-C(1C)-C(2C)-C(3C)	-12.2(4)	C(8C)-C(7C)-C(12C)-C(11C)	-2.6(5)
C(1C)-C(2C)-C(3C)-C(4C)	-16.0(4)	C(6C)-C(7C)-C(12C)-C(11C)	171.8(3)
C(5C)-N(1C)-C(4C)-C(3C)	-171.6(3)	C(6C)-N(3C)-C(13C)-C(18C)	-13.1(4)
C(1C)-N(1C)-C(4C)-C(3C)	-47.3(3)	C(19C)-N(3C)-C(13C)-C(18C)	105.5(3)
C(2C)-C(3C)-C(4C)-N(1C)	38.6(3)	C(6C)-N(3C)-C(13C)-C(14C)	168.2(3)
C(4C)-N(1C)-C(5C)-N(2C)	-59.2(3)	C(19C)-N(3C)-C(13C)-C(14C)	-73.2(4)

C(18C)-C(13C)-C(14C)-C(15C)	0.8(5)	C(6C)-N(2C)-C(25C)-C(24C)	165.0(3)
N(3C)-C(13C)-C(14C)-C(15C)	179.6(3)	C(5C)-N(2C)-C(25C)-C(24C)	-74.1(3)
C(13C)-C(14C)-C(15C)-C(16C)	-0.8(5)	C(6C)-N(2C)-C(25C)-C(20C)	-15.5(4)
C(14C)-C(15C)-C(16C)-C(17C)	-0.1(6)	C(5C)-N(2C)-C(25C)-C(20C)	105.3(3)
C(15C)-C(16C)-C(17C)-C(18C)	1.1(6)	C(4D)-N(1D)-C(1D)-C(2D)	42.4(4)
C(14C)-C(13C)-C(18C)-C(17C)	0.1(5)	C(5D)-N(1D)-C(1D)-C(2D)	165.5(3)
N(3C)-C(13C)-C(18C)-C(17C)	-178.5(3)	N(1D)-C(1D)-C(2D)-C(3D)	-22.7(4)
C(14C)-C(13C)-C(18C)-C(5C)	176.8(3)	C(1D)-C(2D)-C(3D)-C(4D)	-4.5(5)
N(3C)-C(13C)-C(18C)-C(5C)	-1.9(5)	C(5D)-N(1D)-C(4D)-C(3D)	-170.6(3)
C(16C)-C(17C)-C(18C)-C(13C)	-1.1(5)	C(1D)-N(1D)-C(4D)-C(3D)	-46.7(4)
C(16C)-C(17C)-C(18C)-C(5C)	-177.8(3)	C(2D)-C(3D)-C(4D)-N(1D)	30.7(4)
N(1C)-C(5C)-C(18C)-C(13C)	102.3(3)	C(4D)-N(1D)-C(5D)-N(2D)	-57.8(4)
N(2C)-C(5C)-C(18C)-C(13C)	-17.9(4)	C(1D)-N(1D)-C(5D)-N(2D)	-175.5(3)
N(1C)-C(5C)-C(18C)-C(17C)	-81.1(4)	C(4D)-N(1D)-C(5D)-C(18D)	-179.5(3)
N(2C)-C(5C)-C(18C)-C(17C)	158.7(3)	C(1D)-N(1D)-C(5D)-C(18D)	62.8(4)
C(12C)-N(4C)-C(19C)-N(3C)	44.9(4)	C(25D)-N(2D)-C(5D)-N(1D)	164.7(3)
C(12C)-N(4C)-C(19C)-C(20C)	-76.5(4)	C(6D)-N(2D)-C(5D)-N(1D)	-72.1(3)
C(13C)-N(3C)-C(19C)-N(4C)	168.4(3)	C(25D)-N(2D)-C(5D)-C(18D)	-72.8(4)
C(6C)-N(3C)-C(19C)-N(4C)	-70.1(3)	C(6D)-N(2D)-C(5D)-C(18D)	50.4(4)
C(13C)-N(3C)-C(19C)-C(20C)	-69.0(3)	C(25D)-N(2D)-C(6D)-N(3D)	56.7(4)
C(6C)-N(3C)-C(19C)-C(20C)	52.6(3)	C(5D)-N(2D)-C(6D)-N(3D)	-68.3(3)
N(4C)-C(19C)-C(20C)-C(21C)	-78.9(4)	C(25D)-N(2D)-C(6D)-C(7D)	-66.4(4)
N(3C)-C(19C)-C(20C)-C(21C)	159.4(3)	C(5D)-N(2D)-C(6D)-C(7D)	168.6(3)
N(4C)-C(19C)-C(20C)-C(25C)	102.0(3)	C(13D)-N(3D)-C(6D)-N(2D)	48.1(4)
N(3C)-C(19C)-C(20C)-C(25C)	-19.7(4)	C(19D)-N(3D)-C(6D)-N(2D)	-74.0(3)
C(25C)-C(20C)-C(21C)-C(22C)	0.9(5)	C(13D)-N(3D)-C(6D)-C(7D)	171.5(3)
C(19C)-C(20C)-C(21C)-C(22C)	-178.2(3)	C(19D)-N(3D)-C(6D)-C(7D)	49.3(4)
C(20C)-C(21C)-C(22C)-C(23C)	-1.9(5)	N(2D)-C(6D)-C(7D)-C(8D)	-69.5(4)
C(21C)-C(22C)-C(23C)-C(24C)	1.4(5)	N(3D)-C(6D)-C(7D)-C(8D)	167.1(3)
C(22C)-C(23C)-C(24C)-C(25C)	0.0(5)	N(2D)-C(6D)-C(7D)-C(12D)	109.9(4)
C(23C)-C(24C)-C(25C)-C(20C)	-1.0(5)	N(3D)-C(6D)-C(7D)-C(12D)	-13.5(4)
C(23C)-C(24C)-C(25C)-N(2C)	178.5(3)	C(12D)-C(7D)-C(8D)-C(9D)	1.9(5)
C(21C)-C(20C)-C(25C)-C(24C)	0.5(5)	C(6D)-C(7D)-C(8D)-C(9D)	-178.6(3)
C(19C)-C(20C)-C(25C)-C(24C)	179.6(3)	C(7D)-C(8D)-C(9D)-C(10D)	0.1(5)
C(21C)-C(20C)-C(25C)-N(2C)	-178.9(3)	C(8D)-C(9D)-C(10D)-C(11D)	-0.9(5)
C(19C)-C(20C)-C(25C)-N(2C)	0.2(5)	C(9D)-C(10D)-C(11D)-C(12D)	-0.5(6)

C(19D)-N(4D)-C(12D)-C(11D)	159.0(3)	N(2D)-C(5D)-C(18D)-C(13D)	-17.5(5)
C(19D)-N(4D)-C(12D)-C(7D)	-21.5(5)	C(12D)-N(4D)-C(19D)-N(3D)	59.8(4)
C(10D)-C(11D)-C(12D)-N(4D)	-178.0(3)	C(12D)-N(4D)-C(19D)-C(20D)	-61.4(4)
C(10D)-C(11D)-C(12D)-C(7D)	2.6(5)	C(13D)-N(3D)-C(19D)-N(4D)	162.9(3)
C(8D)-C(7D)-C(12D)-N(4D)	177.3(3)	C(6D)-N(3D)-C(19D)-N(4D)	-74.1(3)
C(6D)-C(7D)-C(12D)-N(4D)	-2.2(5)	C(13D)-N(3D)-C(19D)-C(20D)	-74.2(4)
C(8D)-C(7D)-C(12D)-C(11D)	-3.2(5)	C(6D)-N(3D)-C(19D)-C(20D)	48.7(4)
C(6D)-C(7D)-C(12D)-C(11D)	177.3(3)	N(4D)-C(19D)-C(20D)-C(25D)	105.2(4)
C(6D)-N(3D)-C(13D)-C(14D)	168.9(3)	N(3D)-C(19D)-C(20D)-C(25D)	-14.1(5)
C(19D)-N(3D)-C(13D)-C(14D)	-72.1(4)	N(4D)-C(19D)-C(20D)-C(21D)	-74.1(5)
C(6D)-N(3D)-C(13D)-C(18D)	-14.1(5)	N(3D)-C(19D)-C(20D)-C(21D)	166.6(3)
C(19D)-N(3D)-C(13D)-C(18D)	104.9(4)	C(25D)-C(20D)-C(21D)-C(22D)	-1.6(6)
C(18D)-C(13D)-C(14D)-C(15D)	-0.4(6)	C(19D)-C(20D)-C(21D)-C(22D)	177.7(4)
N(3D)-C(13D)-C(14D)-C(15D)	176.7(4)	C(20D)-C(21D)-C(22D)-C(23D)	1.5(7)
C(13D)-C(14D)-C(15D)-C(16D)	0.0(8)	C(21D)-C(22D)-C(23D)-C(24D)	0.4(7)
C(14D)-C(15D)-C(16D)-C(17D)	0.0(8)	C(22D)-C(23D)-C(24D)-C(25D)	-2.1(7)
C(15D)-C(16D)-C(17D)-C(18D)	0.6(8)	C(21D)-C(20D)-C(25D)-C(24D)	0.0(6)
C(16D)-C(17D)-C(18D)-C(13D)	-1.0(6)	C(19D)-C(20D)-C(25D)-C(24D)	-179.3(4)
C(16D)-C(17D)-C(18D)-C(5D)	-176.0(4)	C(21D)-C(20D)-C(25D)-N(2D)	176.8(3)
C(14D)-C(13D)-C(18D)-C(17D)	0.9(6)	C(19D)-C(20D)-C(25D)-N(2D)	-2.5(6)
N(3D)-C(13D)-C(18D)-C(17D)	-176.0(4)	C(23D)-C(24D)-C(25D)-C(20D)	1.9(6)
C(14D)-C(13D)-C(18D)-C(5D)	176.0(4)	C(23D)-C(24D)-C(25D)-N(2D)	-175.0(4)
N(3D)-C(13D)-C(18D)-C(5D)	-0.9(5)	C(6D)-N(2D)-C(25D)-C(20D)	-17.7(5)
N(1D)-C(5D)-C(18D)-C(17D)	-82.2(4)	C(5D)-N(2D)-C(25D)-C(20D)	105.1(4)
N(2D)-C(5D)-C(18D)-C(17D)	157.4(3)	C(6D)-N(2D)-C(25D)-C(24D)	159.2(3)
N(1D)-C(5D)-C(18D)-C(13D)	102.8(4)	C(5D)-N(2D)-C(25D)-C(24D)	-78.1(4)

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Symmetry transformations used to generate equivalent atoms:

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! Optimized Parameters !

! (Angstroms and Degrees) !

! Name	Definition	Value	Derivative Info.	!
! R1	R(1,2)	1.5538	-DE/DX = -0.0001	!
! R2	R(1,13)	1.5197	-DE/DX = 0.0	!
! R3	R(1,25)	1.4133	-DE/DX = 0.0	!
! R4	R(1,53)	1.0973	-DE/DX = 0.0	!
! R5	R(2,3)	2.3613	-DE/DX = 0.0	!
! R6	R(2,4)	1.423	-DE/DX = 0.0	!
! R7	R(2,11)	1.4169	-DE/DX = 0.0	!
! R8	R(3,4)	1.3948	-DE/DX = 0.0	!
! R9	R(3,16)	1.3824	-DE/DX = 0.0	!
! R10	R(3,30)	1.0874	-DE/DX = 0.0	!
! R11	R(4,5)	1.397	-DE/DX = 0.0	!
! R12	R(4,12)	2.5869	-DE/DX = 0.0	!
! R13	R(5,13)	1.3962	-DE/DX = 0.0	!
! R14	R(5,15)	3.5605	-DE/DX = 0.0	!
! R15	R(5,16)	3.3038	-DE/DX = 0.0	!
! R16	R(5,21)	1.3952	-DE/DX = 0.0	!
! R17	R(6,7)	1.4086	-DE/DX = 0.0	!
! R18	R(6,11)	1.4205	-DE/DX = 0.0	!
! R19	R(6,12)	1.4873	-DE/DX = 0.0	!
! R20	R(7,8)	1.3938	-DE/DX = 0.0	!
! R21	R(7,31)	1.0867	-DE/DX = 0.0	!
! R22	R(8,9)	1.3951	-DE/DX = 0.0	!

! R23	R(8,32)	1.0859	-DE/DX = 0.0	!
! R24	R(9,10)	1.3918	-DE/DX = 0.0	!
! R25	R(9,33)	1.0861	-DE/DX = 0.0	!
! R26	R(10,11)	1.4003	-DE/DX = 0.0	!
! R27	R(10,34)	1.0852	-DE/DX = 0.0	!
! R28	R(12,14)	1.3548	-DE/DX = 0.0	!
! R29	R(12,35)	1.0879	-DE/DX = 0.0	!
! R30	R(13,24)	1.3876	-DE/DX = 0.0	!
! R31	R(14,15)	1.3769	-DE/DX = 0.0	!
! R32	R(14,36)	1.0138	-DE/DX = 0.0	!
! R33	R(15,16)	1.4465	-DE/DX = 0.0	!
! R34	R(15,17)	1.4237	-DE/DX = 0.0	!
! R35	R(16,20)	1.4456	-DE/DX = 0.0	!
! R36	R(17,18)	1.3706	-DE/DX = 0.0	!
! R37	R(17,37)	1.0901	-DE/DX = 0.0	!
! R38	R(18,19)	1.4289	-DE/DX = 0.0	!
! R39	R(18,38)	1.0849	-DE/DX = 0.0	!
! R40	R(19,20)	1.3651	-DE/DX = 0.0	!
! R41	R(19,39)	1.0863	-DE/DX = 0.0	!
! R42	R(20,40)	1.0871	-DE/DX = 0.0	!
! R43	R(21,22)	1.398	-DE/DX = 0.0	!
! R44	R(21,41)	1.0837	-DE/DX = 0.0	!
! R45	R(22,23)	1.3986	-DE/DX = 0.0	!
! R46	R(22,42)	1.0864	-DE/DX = 0.0	!
! R47	R(23,24)	1.4007	-DE/DX = 0.0	!
! R48	R(23,43)	1.0855	-DE/DX = 0.0	!
! R49	R(24,44)	1.0866	-DE/DX = 0.0	!
! R50	R(25,26)	1.4678	-DE/DX = 0.0	!



! R51	R(25,29)	1.4618	-DE/DX = 0.0	!
! R52	R(26,27)	1.5389	-DE/DX = 0.0	!
! R53	R(26,45)	1.095	-DE/DX = 0.0	!
! R54	R(26,46)	1.0997	-DE/DX = 0.0	!
! R55	R(27,28)	1.5385	-DE/DX = 0.0	!
! R56	R(27,47)	1.0956	-DE/DX = 0.0	!
! R57	R(27,48)	1.0936	-DE/DX = 0.0	!
! R58	R(28,29)	1.5335	-DE/DX = 0.0	!
! R59	R(28,49)	1.0935	-DE/DX = 0.0	!
! R60	R(28,50)	1.096	-DE/DX = 0.0	!
! R61	R(29,51)	1.1012	-DE/DX = 0.0	!
! R62	R(29,52)	1.0977	-DE/DX = 0.0	!
! A1	A(2,1,13)	100.4722	-DE/DX = 0.0	!
! A2	A(2,1,25)	118.0229	-DE/DX = 0.0	!
! A3	A(2,1,53)	105.823	-DE/DX = 0.0	!
! A4	A(13,1,25)	114.6692	-DE/DX = 0.0	!
! A5	A(13,1,53)	110.7256	-DE/DX = 0.0	!
! A6	A(25,1,53)	106.7597	-DE/DX = 0.0	!
! A7	A(1,2,3)	135.3236	-DE/DX = 0.0	!
! A8	A(1,2,4)	108.6712	-DE/DX = 0.0	!
! A9	A(1,2,11)	121.2776	-DE/DX = 0.0	!
! A10	A(3,2,11)	98.8668	-DE/DX = 0.0	!
! A11	A(4,2,11)	109.2217	-DE/DX = 0.0	!
! A12	A(2,3,16)	143.0287	-DE/DX = 0.0	!
! A13	A(2,3,30)	87.3905	-DE/DX = 0.0	!
! A14	A(4,3,16)	122.3951	-DE/DX = 0.0	!
! A15	A(4,3,30)	115.5214	-DE/DX = 0.0	!
! A16	A(16,3,30)	121.8549	-DE/DX = 0.0	!

! A17	A(2,4,5)	109.8818	-DE/DX = 0.0	!
! A18	A(2,4,12)	94.343	-DE/DX = 0.0	!
! A19	A(3,4,5)	126.934	-DE/DX = 0.0	!
! A20	A(3,4,12)	101.0475	-DE/DX = 0.0	!
! A21	A(5,4,12)	104.1313	-DE/DX = 0.0	!
! A22	A(4,5,13)	110.1656	-DE/DX = 0.0	!
! A23	A(4,5,15)	53.4313	-DE/DX = 0.0	!
! A24	A(4,5,16)	41.21	-DE/DX = 0.0	!
! A25	A(4,5,21)	128.2094	-DE/DX = 0.0	!
! A26	A(13,5,15)	152.2145	-DE/DX = 0.0	!
! A27	A(13,5,16)	151.2967	-DE/DX = 0.0	!
! A28	A(13,5,21)	121.6116	-DE/DX = 0.0	!
! A29	A(15,5,21)	78.8364	-DE/DX = 0.0	!
! A30	A(16,5,21)	87.0073	-DE/DX = 0.0	!
! A31	A(7,6,11)	117.1495	-DE/DX = 0.0	!
! A32	A(7,6,12)	115.9622	-DE/DX = 0.0	!
! A33	A(11,6,12)	125.7949	-DE/DX = 0.0	!
! A34	A(6,7,8)	122.4395	-DE/DX = 0.0	!
! A35	A(6,7,31)	118.3003	-DE/DX = 0.0	!
! A36	A(8,7,31)	119.2602	-DE/DX = 0.0	!
! A37	A(7,8,9)	119.4161	-DE/DX = 0.0	!
! A38	A(7,8,32)	119.968	-DE/DX = 0.0	!
! A39	A(9,8,32)	120.6094	-DE/DX = 0.0	!
! A40	A(8,9,10)	119.6416	-DE/DX = 0.0	!
! A41	A(8,9,33)	120.503	-DE/DX = 0.0	!
! A42	A(10,9,33)	119.8418	-DE/DX = 0.0	!
! A43	A(9,10,11)	121.1189	-DE/DX = 0.0	!
! A44	A(9,10,34)	120.625	-DE/DX = 0.0	!

! A45	A(11,10,34)	118.25	-DE/DX = 0.0	!
! A46	A(2,11,6)	121.5568	-DE/DX = 0.0	!
! A47	A(2,11,10)	118.1837	-DE/DX = 0.0	!
! A48	A(6,11,10)	120.1905	-DE/DX = 0.0	!
! A49	A(4,12,6)	76.8897	-DE/DX = 0.0	!
! A50	A(4,12,14)	87.1771	-DE/DX = 0.0	!
! A51	A(4,12,35)	137.3894	-DE/DX = 0.0	!
! A52	A(6,12,14)	132.1305	-DE/DX = 0.0	!
! A53	A(6,12,35)	112.4718	-DE/DX = 0.0	!
! A54	A(14,12,35)	109.7063	-DE/DX = 0.0	!
! A55	A(1,13,5)	110.7704	-DE/DX = 0.0	!
! A56	A(1,13,24)	128.8171	-DE/DX = 0.0	!
! A57	A(5,13,24)	120.3808	-DE/DX = 0.0	!
! A58	A(12,14,15)	136.4193	-DE/DX = 0.0	!
! A59	A(12,14,36)	112.0182	-DE/DX = 0.0	!
! A60	A(15,14,36)	111.5581	-DE/DX = 0.0	!
! A61	A(5,15,14)	71.1854	-DE/DX = 0.0	!
! A62	A(5,15,17)	140.8569	-DE/DX = 0.0	!
! A63	A(14,15,16)	123.8626	-DE/DX = 0.0	!
! A64	A(14,15,17)	116.3582	-DE/DX = 0.0	!
! A65	A(16,15,17)	119.6924	-DE/DX = 0.0	!
! A66	A(3,16,5)	43.8472	-DE/DX = 0.0	!
! A67	A(3,16,15)	124.0664	-DE/DX = 0.0	!
! A68	A(3,16,20)	120.2332	-DE/DX = 0.0	!
! A69	A(5,16,20)	143.4173	-DE/DX = 0.0	!
! A70	A(15,16,20)	115.6559	-DE/DX = 0.0	!
! A71	A(15,17,18)	121.3345	-DE/DX = 0.0	!
! A72	A(15,17,37)	118.4649	-DE/DX = 0.0	!

! A73	A(18,17,37)	120.1178	-DE/DX = 0.0	!
! A74	A(17,18,19)	119.231	-DE/DX = 0.0	!
! A75	A(17,18,38)	120.4263	-DE/DX = 0.0	!
! A76	A(19,18,38)	120.3142	-DE/DX = 0.0	!
! A77	A(18,19,20)	120.6139	-DE/DX = 0.0	!
! A78	A(18,19,39)	119.4847	-DE/DX = 0.0	!
! A79	A(20,19,39)	119.8923	-DE/DX = 0.0	!
! A80	A(16,20,19)	122.072	-DE/DX = 0.0	!
! A81	A(16,20,40)	117.4249	-DE/DX = 0.0	!
! A82	A(19,20,40)	120.4215	-DE/DX = 0.0	!
! A83	A(5,21,22)	117.4793	-DE/DX = 0.0	!
! A84	A(5,21,41)	120.8959	-DE/DX = 0.0	!
! A85	A(22,21,41)	121.6234	-DE/DX = 0.0	!
! A86	A(21,22,23)	121.5093	-DE/DX = 0.0	!
! A87	A(21,22,42)	118.9752	-DE/DX = 0.0	!
! A88	A(23,22,42)	119.5154	-DE/DX = 0.0	!
! A89	A(22,23,24)	119.9881	-DE/DX = 0.0	!
! A90	A(22,23,43)	120.0015	-DE/DX = 0.0	!
! A91	A(24,23,43)	120.0077	-DE/DX = 0.0	!
! A92	A(13,24,23)	119.012	-DE/DX = 0.0	!
! A93	A(13,24,44)	120.0815	-DE/DX = 0.0	!
! A94	A(23,24,44)	120.9037	-DE/DX = 0.0	!
! A95	A(1,25,26)	123.5487	-DE/DX = 0.0	!
! A96	A(1,25,29)	122.8919	-DE/DX = 0.0	!
! A97	A(26,25,29)	112.5071	-DE/DX = 0.0	!
! A98	A(25,26,27)	103.6051	-DE/DX = 0.0	!
! A99	A(25,26,45)	112.096	-DE/DX = 0.0	!
! A100	A(25,26,46)	110.7799	-DE/DX = 0.0	!

! A101	A(27,26,45)	111.7069	-DE/DX = 0.0	!
! A102	A(27,26,46)	111.4993	-DE/DX = 0.0	!
! A103	A(45,26,46)	107.2238	-DE/DX = 0.0	!
! A104	A(26,27,28)	103.6335	-DE/DX = 0.0	!
! A105	A(26,27,47)	109.7762	-DE/DX = 0.0	!
! A106	A(26,27,48)	112.5034	-DE/DX = 0.0	!
! A107	A(28,27,47)	109.6758	-DE/DX = 0.0	!
! A108	A(28,27,48)	113.3405	-DE/DX = 0.0	!
! A109	A(47,27,48)	107.8537	-DE/DX = 0.0	!
! A110	A(27,28,29)	102.4651	-DE/DX = 0.0	!
! A111	A(27,28,49)	113.2633	-DE/DX = 0.0	!
! A112	A(27,28,50)	110.2766	-DE/DX = 0.0	!
! A113	A(29,28,49)	112.6867	-DE/DX = 0.0	!
! A114	A(29,28,50)	109.9759	-DE/DX = 0.0	!
! A115	A(49,28,50)	108.1012	-DE/DX = 0.0	!
! A116	A(25,29,28)	102.7427	-DE/DX = 0.0	!
! A117	A(25,29,51)	112.987	-DE/DX = 0.0	!
! A118	A(25,29,52)	110.7988	-DE/DX = 0.0	!
! A119	A(28,29,51)	110.1297	-DE/DX = 0.0	!
! A120	A(28,29,52)	112.7115	-DE/DX = 0.0	!
! A121	A(51,29,52)	107.5367	-DE/DX = 0.0	!
! D1	D(13,1,2,3)	-23.5241	-DE/DX = 0.0	!
! D2	D(13,1,2,4)	-0.6891	-DE/DX = 0.0	!
! D3	D(13,1,2,11)	127.037	-DE/DX = 0.0	!
! D4	D(25,1,2,3)	-148.918	-DE/DX = 0.0	!
! D5	D(25,1,2,4)	-126.083	-DE/DX = 0.0	!
! D6	D(25,1,2,11)	1.6431	-DE/DX = 0.0	!
! D7	D(53,1,2,3)	91.7181	-DE/DX = 0.0	!

! D8	D(53,1,2,4)	114.553	-DE/DX = 0.0	!
! D9	D(53,1,2,11)	-117.7208	-DE/DX = 0.0	!
! D10	D(2,1,13,5)	1.6706	-DE/DX = 0.0	!
! D11	D(2,1,13,24)	179.5946	-DE/DX = 0.0	!
! D12	D(25,1,13,5)	129.308	-DE/DX = 0.0	!
! D13	D(25,1,13,24)	-52.768	-DE/DX = 0.0	!
! D14	D(53,1,13,5)	-109.8239	-DE/DX = 0.0	!
! D15	D(53,1,13,24)	68.1002	-DE/DX = 0.0	!
! D16	D(2,1,25,26)	73.1474	-DE/DX = 0.0	!
! D17	D(2,1,25,29)	-94.2352	-DE/DX = 0.0	!
! D18	D(13,1,25,26)	-44.9534	-DE/DX = 0.0	!
! D19	D(13,1,25,29)	147.664	-DE/DX = 0.0	!
! D20	D(53,1,25,26)	-167.9801	-DE/DX = 0.0	!
! D21	D(53,1,25,29)	24.6373	-DE/DX = 0.0	!
! D22	D(1,2,3,16)	109.6266	-DE/DX = 0.0	!
! D23	D(1,2,3,30)	-105.4971	-DE/DX = 0.0	!
! D24	D(11,2,3,16)	-45.2137	-DE/DX = 0.0	!
! D25	D(11,2,3,30)	99.6626	-DE/DX = 0.0	!
! D26	D(1,2,4,5)	-0.496	-DE/DX = 0.0	!
! D27	D(1,2,4,12)	106.2322	-DE/DX = 0.0	!
! D28	D(11,2,4,5)	-134.779	-DE/DX = 0.0	!
! D29	D(11,2,4,12)	-28.0507	-DE/DX = 0.0	!
! D30	D(1,2,11,6)	-105.7782	-DE/DX = 0.0	!
! D31	D(1,2,11,10)	77.2378	-DE/DX = 0.0	!
! D32	D(3,2,11,6)	53.7497	-DE/DX = 0.0	!
! D33	D(3,2,11,10)	-123.2343	-DE/DX = 0.0	!
! D34	D(4,2,11,6)	21.7025	-DE/DX = 0.0	!
! D35	D(4,2,11,10)	-155.2814	-DE/DX = 0.0	!

! D36	D(16,3,4,5)	77.9573	-DE/DX = 0.0	!
! D37	D(16,3,4,12)	-39.2994	-DE/DX = 0.0	!
! D38	D(30,3,4,5)	-107.4453	-DE/DX = 0.0	!
! D39	D(30,3,4,12)	135.2981	-DE/DX = 0.0	!
! D40	D(2,3,16,5)	-65.3424	-DE/DX = 0.0	!
! D41	D(2,3,16,15)	-25.18	-DE/DX = 0.0	!
! D42	D(2,3,16,20)	157.3565	-DE/DX = 0.0	!
! D43	D(4,3,16,5)	-28.5002	-DE/DX = 0.0	!
! D44	D(4,3,16,15)	11.6623	-DE/DX = 0.0	!
! D45	D(4,3,16,20)	-165.8012	-DE/DX = 0.0	!
! D46	D(30,3,16,5)	157.2408	-DE/DX = 0.0	!
! D47	D(30,3,16,15)	-162.5968	-DE/DX = 0.0	!
! D48	D(30,3,16,20)	19.9398	-DE/DX = 0.0	!
! D49	D(2,4,5,13)	1.6231	-DE/DX = 0.0	!
! D50	D(2,4,5,15)	155.9195	-DE/DX = 0.0	!
! D51	D(2,4,5,16)	-175.7282	-DE/DX = 0.0	!
! D52	D(2,4,5,21)	-177.0478	-DE/DX = 0.0	!
! D53	D(3,4,5,13)	145.7184	-DE/DX = 0.0	!
! D54	D(3,4,5,15)	-59.9852	-DE/DX = 0.0	!
! D55	D(3,4,5,16)	-31.6329	-DE/DX = 0.0	!
! D56	D(3,4,5,21)	-32.9524	-DE/DX = 0.0	!
! D57	D(12,4,5,13)	-98.4025	-DE/DX = 0.0	!
! D58	D(12,4,5,15)	55.8939	-DE/DX = 0.0	!
! D59	D(12,4,5,16)	84.2462	-DE/DX = 0.0	!
! D60	D(12,4,5,21)	82.9267	-DE/DX = 0.0	!
! D61	D(2,4,12,6)	30.6458	-DE/DX = 0.0	!
! D62	D(2,4,12,14)	165.1608	-DE/DX = 0.0	!
! D63	D(2,4,12,35)	-78.4113	-DE/DX = 0.0	!

! D64	D(3,4,12,6)	-84.705	-DE/DX = 0.0	!
! D65	D(3,4,12,14)	49.81	-DE/DX = 0.0	!
! D66	D(3,4,12,35)	166.2378	-DE/DX = 0.0	!
! D67	D(5,4,12,6)	142.4123	-DE/DX = 0.0	!
! D68	D(5,4,12,14)	-83.0727	-DE/DX = 0.0	!
! D69	D(5,4,12,35)	33.3551	-DE/DX = 0.0	!
! D70	D(4,5,13,1)	-2.1212	-DE/DX = 0.0	!
! D71	D(4,5,13,24)	179.7537	-DE/DX = 0.0	!
! D72	D(15,5,13,1)	-50.4732	-DE/DX = 0.0	!
! D73	D(15,5,13,24)	131.4017	-DE/DX = 0.0	!
! D74	D(16,5,13,1)	1.5133	-DE/DX = 0.0	!
! D75	D(16,5,13,24)	-176.6118	-DE/DX = 0.0	!
! D76	D(21,5,13,1)	176.6525	-DE/DX = 0.0	!
! D77	D(21,5,13,24)	-1.4727	-DE/DX = 0.0	!
! D78	D(4,5,15,14)	-90.1496	-DE/DX = 0.0	!
! D79	D(4,5,15,17)	160.9195	-DE/DX = 0.0	!
! D80	D(13,5,15,14)	-29.2978	-DE/DX = 0.0	!
! D81	D(13,5,15,17)	-138.2286	-DE/DX = 0.0	!
! D82	D(21,5,15,14)	111.1972	-DE/DX = 0.0	!
! D83	D(21,5,15,17)	2.2664	-DE/DX = 0.0	!
! D84	D(4,5,16,3)	37.6319	-DE/DX = 0.0	!
! D85	D(4,5,16,20)	117.0817	-DE/DX = 0.0	!
! D86	D(13,5,16,3)	32.4498	-DE/DX = 0.0	!
! D87	D(13,5,16,20)	111.8996	-DE/DX = 0.0	!
! D88	D(21,5,16,3)	-143.4063	-DE/DX = 0.0	!
! D89	D(21,5,16,20)	-63.9565	-DE/DX = 0.0	!
! D90	D(4,5,21,22)	179.9674	-DE/DX = 0.0	!
! D91	D(4,5,21,41)	0.3888	-DE/DX = 0.0	!



! D92	D(13,5,21,22)	1.4324	-DE/DX = 0.0	!
! D93	D(13,5,21,41)	-178.1461	-DE/DX = 0.0	!
! D94	D(15,5,21,22)	-158.1894	-DE/DX = 0.0	!
! D95	D(15,5,21,41)	22.2321	-DE/DX = 0.0	!
! D96	D(16,5,21,22)	179.0969	-DE/DX = 0.0	!
! D97	D(16,5,21,41)	-0.4817	-DE/DX = 0.0	!
! D98	D(11,6,7,8)	0.5985	-DE/DX = 0.0	!
! D99	D(11,6,7,31)	-179.4317	-DE/DX = 0.0	!
! D100	D(12,6,7,8)	169.3483	-DE/DX = 0.0	!
! D101	D(12,6,7,31)	-10.6819	-DE/DX = 0.0	!
! D102	D(7,6,11,2)	-178.842	-DE/DX = 0.0	!
! D103	D(7,6,11,10)	-1.9177	-DE/DX = 0.0	!
! D104	D(12,6,11,2)	13.6469	-DE/DX = 0.0	!
! D105	D(12,6,11,10)	-169.4288	-DE/DX = 0.0	!
! D106	D(7,6,12,4)	168.5756	-DE/DX = 0.0	!
! D107	D(7,6,12,14)	94.7672	-DE/DX = 0.0	!
! D108	D(7,6,12,35)	-55.2519	-DE/DX = 0.0	!
! D109	D(11,6,12,4)	-23.7826	-DE/DX = 0.0	!
! D110	D(11,6,12,14)	-97.591	-DE/DX = 0.0	!
! D111	D(11,6,12,35)	112.3899	-DE/DX = 0.0	!
! D112	D(6,7,8,9)	0.0818	-DE/DX = 0.0	!
! D113	D(6,7,8,32)	179.1635	-DE/DX = 0.0	!
! D114	D(31,7,8,9)	-179.8877	-DE/DX = 0.0	!
! D115	D(31,7,8,32)	-0.806	-DE/DX = 0.0	!
! D116	D(7,8,9,10)	0.5469	-DE/DX = 0.0	!
! D117	D(7,8,9,33)	179.2036	-DE/DX = 0.0	!
! D118	D(32,8,9,10)	-178.5287	-DE/DX = 0.0	!
! D119	D(32,8,9,33)	0.128	-DE/DX = 0.0	!

! D120	D(8,9,10,11)	-1.9054	-DE/DX = 0.0	!
! D121	D(8,9,10,34)	177.1759	-DE/DX = 0.0	!
! D122	D(33,9,10,11)	179.4289	-DE/DX = 0.0	!
! D123	D(33,9,10,34)	-1.4898	-DE/DX = 0.0	!
! D124	D(9,10,11,2)	179.6482	-DE/DX = 0.0	!
! D125	D(9,10,11,6)	2.6215	-DE/DX = 0.0	!
! D126	D(34,10,11,2)	0.5456	-DE/DX = 0.0	!
! D127	D(34,10,11,6)	-176.4811	-DE/DX = 0.0	!
! D128	D(4,12,14,15)	-38.7577	-DE/DX = 0.0	!
! D129	D(4,12,14,36)	140.3843	-DE/DX = 0.0	!
! D130	D(6,12,14,15)	30.7043	-DE/DX = 0.0	!
! D131	D(6,12,14,36)	-150.1537	-DE/DX = 0.0	!
! D132	D(35,12,14,15)	-178.6687	-DE/DX = 0.0	!
! D133	D(35,12,14,36)	0.4733	-DE/DX = 0.0	!
! D134	D(1,13,24,23)	-177.3549	-DE/DX = 0.0	!
! D135	D(1,13,24,44)	2.0518	-DE/DX = 0.0	!
! D136	D(5,13,24,23)	0.395	-DE/DX = 0.0	!
! D137	D(5,13,24,44)	179.8017	-DE/DX = 0.0	!
! D138	D(12,14,15,5)	58.5262	-DE/DX = 0.0	!
! D139	D(12,14,15,16)	13.3295	-DE/DX = 0.0	!
! D140	D(12,14,15,17)	-163.2633	-DE/DX = 0.0	!
! D141	D(36,14,15,5)	-120.6186	-DE/DX = 0.0	!
! D142	D(36,14,15,16)	-165.8153	-DE/DX = 0.0	!
! D143	D(36,14,15,17)	17.5919	-DE/DX = 0.0	!
! D144	D(14,15,16,3)	19.8499	-DE/DX = 0.0	!
! D145	D(14,15,16,20)	-162.5812	-DE/DX = 0.0	!
! D146	D(17,15,16,3)	-163.6647	-DE/DX = 0.0	!
! D147	D(17,15,16,20)	13.9042	-DE/DX = 0.0	!

! D148	D(5,15,17,18)	-99.9029	-DE/DX = 0.0	!
! D149	D(5,15,17,37)	83.403	-DE/DX = 0.0	!
! D150	D(14,15,17,18)	167.885	-DE/DX = 0.0	!
! D151	D(14,15,17,37)	-8.8092	-DE/DX = 0.0	!
! D152	D(16,15,17,18)	-8.8583	-DE/DX = 0.0	!
! D153	D(16,15,17,37)	174.4476	-DE/DX = 0.0	!
! D154	D(3,16,20,19)	167.5686	-DE/DX = 0.0	!
! D155	D(3,16,20,40)	-9.1573	-DE/DX = 0.0	!
! D156	D(5,16,20,19)	115.5472	-DE/DX = 0.0	!
! D157	D(5,16,20,40)	-61.1787	-DE/DX = 0.0	!
! D158	D(15,16,20,19)	-10.1004	-DE/DX = 0.0	!
! D159	D(15,16,20,40)	173.1736	-DE/DX = 0.0	!
! D160	D(15,17,18,19)	-0.9216	-DE/DX = 0.0	!
! D161	D(15,17,18,38)	-178.9896	-DE/DX = 0.0	!
! D162	D(37,17,18,19)	175.7185	-DE/DX = 0.0	!
! D163	D(37,17,18,38)	-2.3495	-DE/DX = 0.0	!
! D164	D(17,18,19,20)	5.046	-DE/DX = 0.0	!
! D165	D(17,18,19,39)	-176.0539	-DE/DX = 0.0	!
! D166	D(38,18,19,20)	-176.8838	-DE/DX = 0.0	!
! D167	D(38,18,19,39)	2.0163	-DE/DX = 0.0	!
! D168	D(18,19,20,16)	0.7964	-DE/DX = 0.0	!
! D169	D(18,19,20,40)	177.4262	-DE/DX = 0.0	!
! D170	D(39,19,20,16)	-178.0993	-DE/DX = 0.0	!
! D171	D(39,19,20,40)	-1.4695	-DE/DX = 0.0	!
! D172	D(5,21,22,23)	-0.3684	-DE/DX = 0.0	!
! D173	D(5,21,22,42)	179.7413	-DE/DX = 0.0	!
! D174	D(41,21,22,23)	179.2069	-DE/DX = 0.0	!
! D175	D(41,21,22,42)	-0.6834	-DE/DX = 0.0	!

! D176	D(21,22,23,24)	-0.6616	-DE/DX = 0.0	!
! D177	D(21,22,23,43)	179.9392	-DE/DX = 0.0	!
! D178	D(42,22,23,24)	179.2281	-DE/DX = 0.0	!
! D179	D(42,22,23,43)	-0.171	-DE/DX = 0.0	!
! D180	D(22,23,24,13)	0.6459	-DE/DX = 0.0	!
! D181	D(22,23,24,44)	-178.7558	-DE/DX = 0.0	!
! D182	D(43,23,24,13)	-179.955	-DE/DX = 0.0	!
! D183	D(43,23,24,44)	0.6433	-DE/DX = 0.0	!
! D184	D(1,25,26,27)	-165.1491	-DE/DX = 0.0	!
! D185	D(1,25,26,45)	-44.5549	-DE/DX = 0.0	!
! D186	D(1,25,26,46)	75.1718	-DE/DX = 0.0	!
! D187	D(29,25,26,27)	3.399	-DE/DX = 0.0	!
! D188	D(29,25,26,45)	123.9932	-DE/DX = 0.0	!
! D189	D(29,25,26,46)	-116.2801	-DE/DX = 0.0	!
! D190	D(1,25,29,28)	-170.9991	-DE/DX = 0.0	!
! D191	D(1,25,29,51)	70.3676	-DE/DX = 0.0	!
! D192	D(1,25,29,52)	-50.3798	-DE/DX = 0.0	!
! D193	D(26,25,29,28)	20.366	-DE/DX = 0.0	!
! D194	D(26,25,29,51)	-98.2673	-DE/DX = 0.0	!
! D195	D(26,25,29,52)	140.9854	-DE/DX = 0.0	!
! D196	D(25,26,27,28)	-25.7691	-DE/DX = 0.0	!
! D197	D(25,26,27,47)	91.3204	-DE/DX = 0.0	!
! D198	D(25,26,27,48)	-148.5729	-DE/DX = 0.0	!
! D199	D(45,26,27,28)	-146.6265	-DE/DX = 0.0	!
! D200	D(45,26,27,47)	-29.537	-DE/DX = 0.0	!
! D201	D(45,26,27,48)	90.5697	-DE/DX = 0.0	!
! D202	D(46,26,27,28)	93.417	-DE/DX = 0.0	!
! D203	D(46,26,27,47)	-149.4936	-DE/DX = 0.0	!

