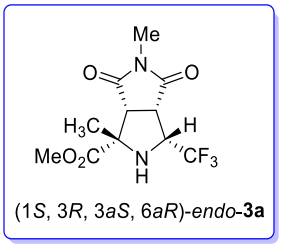
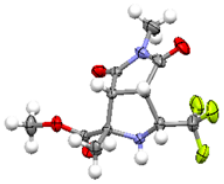
Anexo II

Difracción de Rayos X

ANEXO III.I ILUROS DE AZOMETINO TRIFLUOROMETILADOS EN REACCIONES DE CICLOADICIÓN 1,3-DIPOLAR CATALÍTICA ASIMÉTRICA



(1*S*, 3*R*, 3a*S*, 6a*R*)-*endo*-**3a**



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_symmetry_Int_Tables_number 19

_space_group_name_Hall 'P 2ac 2ab'

loop_

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_symmetry_equiv_pos_as_xyz

1 x,y,z

2 1/2-x,-y,1/2+z

3 -x,1/2+y,1/2-z

4 1/2+x,1/2-y,-z

_cell_length_a 6.60940(10)

_cell_length_b 8.3373(2)

_cell_length_c 24.5995(5)

_cell_angle_alpha 90.00

_cell_angle_beta 90.00

_cell_angle_gamma 90.00

_cell_volume 1355.54

loop_

_atom_site_label

_atom_site_type_symbol

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

O1 O 0.9946(4) 0.4062(3) 0.25028(8)

O2 O 0.5278(2) 0.1057(2) 0.16166(6)

O3 O 0.5929(2) 0.1231(2) 0.03192(6)

O4 O 0.7036(2) -0.10089(16) 0.07201(6)

N1 N 0.7295(3) 0.2644(2) 0.21456(6)

N2 N 0.9026(3) 0.30174(18) 0.08041(7)

C1 C 0.9267(4) 0.3170(3) 0.21599(8)

C2 C 1.0366(3) 0.2457(3) 0.16817(8)

C3 C 1.0587(3) 0.3571(2) 0.11781(9)

C4 C 0.8972(3) 0.1271(2) 0.08603(6)

C5 C 0.8946(3) 0.1130(2) 0.14810(7)

C6 C 0.6936(3) 0.1559(2) 0.17357(7)

C7 C 1.0836(3) 0.0434(3) 0.06192(9)

H7A H 1.0891 0.0631 0.0235

H7B H 1.0745 -0.0699 0.0684

H7C H 1.2037 0.0847 0.0788

C8 C 1.0341(6) 0.5344(3) 0.12765(12)

C9 C 0.7105(3) 0.0548(2) 0.06004(7)

C10 C 0.5346(4) -0.1940(3) 0.05348(13)

H10A H 0.4210 -0.1763 0.0771

H10B H 0.5698 -0.3057 0.0538

H10C H 0.4998 -0.1623 0.0171

C11 C 0.5716(5) 0.3219(4) 0.25113(10)

H11A H 0.4696 0.3769 0.2305

H11B H 0.6295 0.3942 0.2772

H11C H 0.5118 0.2325 0.2697

F1 F 0.8580(4) 0.5762(2) 0.14953(8)

F2 F 1.1825(4) 0.5900(3) 0.15978(10)

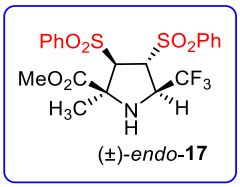
F3 F 1.0504(5) 0.61332(19) 0.08034(9)

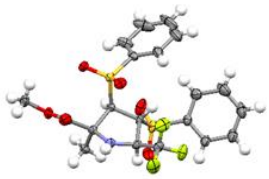
H2N H 0.923(4) 0.327(3) 0.0504(11)

H2 H 1.167(4) 0.210(3) 0.1781(10)

H3 H 1.203(4) 0.346(3) 0.1039(9)

H5 H 0.937(3) 0.018(3) 0.1594(8)





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_symmetry_Int_Tables_number 14

_space_group_name_Hall '-P 2ybc'

loop_

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_symmetry_equiv_pos_as_xyz

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2 -x,1/2+y,1/2-z

3 -x,-y,-z

4 x,1/2-y,1/2+z

_cell_length_a 12.6879(3)

_cell_length_b 16.9089(3)

_cell_length_c 10.7097(2)

_cell_angle_alpha 90

_cell_angle_beta 107.3440(10)

_cell_angle_gamma 90

_cell_volume 2193.17

loop_

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_atom_site_type_symbol

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

C1 C 0.72545(19) 0.16952(14) 0.4334(2)

H1 H 0.7697 0.203 0.3935

C2 C 0.76198(17) 0.08215(13) 0.4273(2)

H2 H 0.6961 0.0486 0.402

C3 C 0.82964(17) 0.06181(12) 0.5690(2)

H3 H 0.9001 0.0374 0.5704

C4 C 0.85023(19) 0.14474(13) 0.6382(2)

C5 C 0.7330(2) -0.09017(15) 0.5440(3)

C6 C 0.8188(3) -0.14315(18) 0.5640(4)

H6 H 0.8869 -0.1338 0.6255

C7 C 0.7986(4) -0.2119(2) 0.4872(6)

H7 H 0.8543 -0.2492 0.4966

C8 C 0.6968(6) -0.2244(3) 0.3980(5)

H8 H 0.6844 -0.2702 0.3475

C9 C 0.6146(5) -0.1715(3) 0.3825(4)

H9 H 0.5461 -0.1814 0.3224

C10 C 0.6310(3) -0.1035(2) 0.4541(3)

H10 H 0.5744 -0.0666 0.4426

C11 C 0.7470(2) 0.03000(16) 0.1683(2)

C12 C 0.7174(3) -0.04826(19) 0.1594(3)

H12 H 0.744 -0.082 0.2304

C13 C 0.6473(3) -0.0759(2) 0.0430(4)

H13 H 0.6248 -0.1284 0.0357

C14 C 0.6108(3) -0.0261(3) -0.0621(3)

H14 H 0.5651 -0.0456 -0.1409

C15 C 0.6406(3) 0.0510(2) -0.0526(3)

H15 H 0.6151 0.0841 -0.1248

C16 C 0.7085(2) 0.08107(19) 0.0632(3)

H16 H 0.7279 0.1343 0.0707

C17 C 0.6057(2) 0.18363(17) 0.3626(3)

C18 C 0.8617(2) 0.14289(14) 0.7840(2)

C19 C 0.9769(3) 0.1062(2) 0.9913(3)

H19A H 0.96 0.1542 1.0291

H19B H 1.0524 0.0918 1.0334

H19C H 0.9292 0.0647 1.0033

C20 C 0.9534(2) 0.18189(16) 0.6173(3)

H20A H 0.9427 0.1886 0.5254

H20B H 1.0157 0.148 0.6536

H20C H 0.9667 0.2325 0.6599

F1 F 0.58542(14) 0.17711(13) 0.23423(17)

F2 F 0.53793(14) 0.13337(13) 0.3941(2)

F3 F 0.57355(16) 0.25553(12) 0.3850(2)

N1 N 0.75168(17) 0.19069(12) 0.5713(2)

H1A H 0.7166 0.2233 0.6061

O1 O 0.88748(17) 0.13849(14) 0.28780(19)

O2 O 0.91577(17) 0.00106(15) 0.3668(2)

O3 O 0.64555(14) 0.03074(11) 0.62544(18)

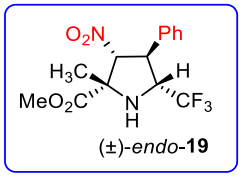
O4 O 0.82038(16) -0.02346(11) 0.76931(17)

O5 O 0.96066(16) 0.11787(11) 0.85302(18)

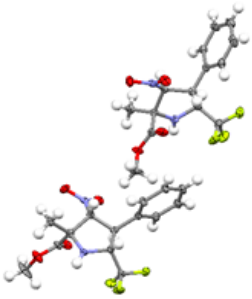
O6 O 0.79056(19) 0.16388(12) 0.82924(19)

S1 S 0.84225(5) 0.06490(4) 0.31329(6)

S2 S 0.75194(5) -0.00409(3) 0.64121(6)



(±)-*endo*-**19**



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_symmetry_equiv_pos_as_xyz

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2 -x,1/2+y,-z

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_cell_length_b 5.9276(6)

_cell_length_c 17.2013(18)

_cell_angle_alpha 90

_cell_angle_beta 99.733(4)

_cell_angle_gamma 90

_cell_volume 1558.13

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_atom_site_type_symbol

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

C1 C 1.0229(3) 0.6927(9) 0.8541(3)

C2 C 1.0254(4) 0.8683(9) 0.9079(3)

H2 H 0.9884 0.9955 0.8952

C3 C 1.0815(4) 0.8602(12) 0.9803(3)

H3 H 1.0829 0.9831 1.016

C4 C 1.1349(4) 0.6767(13) 1.0010(3)

H4 H 1.1733 0.6734 1.0503

C5 C 1.1321(3) 0.4942(11) 0.9484(3)

H5 H 1.1681 0.3657 0.9622

C6 C 1.0759(3) 0.5030(10) 0.8755(3)

H6 H 1.0737 0.3792 0.8401

C7 C 0.9650(3) 0.7103(8) 0.7745(3)

H7 H 0.934 0.8587 0.7712

C8 C 1.0141(3) 0.6918(8) 0.7051(3)

H8 H 1.0574 0.5663 0.717

C9 C 0.9460(3) 0.6191(8) 0.6327(3)

C11 C 0.8957(3) 0.5197(9) 0.7542(3)

H11 H 0.9178 0.3776 0.782

C12 C 0.8960(3) 0.8243(9) 0.5954(3)

C13 C 0.7994(4) 0.9597(10) 0.4854(3)

H13A H 0.8346 1.0964 0.4838

H13B H 0.7519 0.9901 0.5149

H13C H 0.7747 0.9141 0.4315

C14 C 0.9839(3) 0.4801(9) 0.5732(3)

H14A H 0.9364 0.4219 0.5334

H14B H 1.0172 0.3535 0.6001

H14C H 1.0229 0.5744 0.5476

C15 C 0.8099(4) 0.5875(13) 0.7785(3)

F1 F 0.7753(2) 0.7701(8) 0.7425(2)

F2 F 0.8191(2) 0.6276(9) 0.8558(2)

F3 F 0.7507(2) 0.4255(9) 0.7622(2)

N1 N 0.8843(2) 0.4860(7) 0.6700(2)

H1N H 0.8446 0.3956 0.6439

N2 N 1.0632(3) 0.8978(8) 0.6916(3)

O1 O 1.1039(2) 0.8973(7) 0.6359(2)

O2 O 1.0637(3) 1.0606(7) 0.7350(2)

O3 O 0.8935(2) 0.9996(6) 0.6281(2)

O4 O 0.8541(2) 0.7803(6) 0.52369(19)

C16 C 0.6040(3) 0.2803(9) 0.3878(3)

C17 C 0.6542(3) 0.4458(9) 0.4326(3)

H17 H 0.6812 0.5606 0.4065

C18 C 0.6654(3) 0.4451(10) 0.5142(3)

H18 H 0.699 0.5597 0.5439

C19 C 0.6264(4) 0.2730(12) 0.5527(3)

H19 H 0.6353 0.2676 0.6087

C20 C 0.5751(4) 0.1115(11) 0.5088(3)

H20 H 0.5473 -0.0023 0.5346

C21 C 0.5644(3) 0.1161(9) 0.4268(3)

H21 H 0.5292 0.0044 0.397

C22 C 0.5913(3) 0.2813(9) 0.2981(3)

H22 H 0.5571 0.1442 0.2779

C23 C 0.6767(3) 0.2836(8) 0.2650(3)

H23 H 0.7175 0.3924 0.2969

C24 C 0.6537(3) 0.3788(8) 0.1798(3)

C26 C 0.5453(3) 0.4889(9) 0.2580(3)

H26 H 0.5606 0.6229 0.293

C27 C 0.6194(3) 0.1920(10) 0.1206(3)

C29 C 0.7295(3) 0.5005(10) 0.1542(3)

H29A H 0.7513 0.6169 0.193

H29B H 0.7101 0.5712 0.1027

H29C H 0.7764 0.3926 0.1501

C30 C 0.5792(6) 0.1102(15) -0.0140(3)

H30A H 0.5167 0.0904 -0.0131

H30B H 0.6088 -0.0362 -0.0061

H30C H 0.5871 0.1727 -0.0651

C31 C 0.4476(3) 0.4642(11) 0.2411(3)

F4 F 0.4212(2) 0.2992(7) 0.19094(19)

F5 F 0.4089(2) 0.6523(7) 0.2088(2)

F6 F 0.41567(19) 0.4238(8) 0.30653(18)

N4 N 0.7205(3) 0.0575(7) 0.2702(2)

N3 N 0.5797(2) 0.5228(7) 0.1850(2)

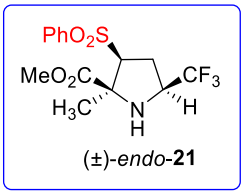
H3N H 0.5578 0.6201 0.1483

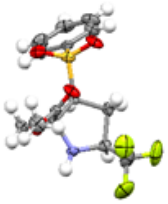
O5 O 0.7873(2) 0.0403(7) 0.2401(2)

O6 O 0.6904(2) -0.0971(7) 0.3027(2)

O7 O 0.5970(2) 0.0074(6) 0.1390(2)

O8 O 0.6160(3) 0.2616(8) 0.0478(2)





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_symmetry_Int_Tables_number 19

_space_group_name_Hall 'P 2ac 2ab'

loop_

_symmetry_equiv_pos_site_id

_symmetry_equiv_pos_as_xyz

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2 1/2-x,-y,1/2+z

3 -x,1/2+y,1/2-z

4 1/2+x,1/2-y,-z

_cell_length_a 10.4529(13)

_cell_length_b 11.2144(14)

_cell_length_c 13.8440(16)

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_cell_angle_gamma 90

_cell_volume 1622.84

loop_

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_atom_site_type_symbol

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

C1 C 0.3171(4) 0.7288(3) 0.1717(3)

C2 C 0.4182(4) 0.7416(4) 0.2329(3)

H2 H 0.4158 0.7985 0.2817

C3 C 0.5240(4) 0.6698(5) 0.2220(4)

H3 H 0.5939 0.6795 0.2628

C4 C 0.5272(5) 0.5848(5) 0.1521(5)

H4 H 0.5983 0.5356 0.1458

C5 C 0.4251(6) 0.5719(5) 0.0909(4)

H5 H 0.4274 0.5141 0.0427

C6 C 0.3196(5) 0.6435(4) 0.1003(3)

H6 H 0.2503 0.6345 0.0588

C7 C 0.0651(3) 0.7249(3) 0.2372(3)

H7 H 0.0971 0.6434 0.2285

C9 C -0.0742(4) 0.6738(4) 0.3668(3)

H9 H -0.0523 0.5923 0.3862

C10 C -0.1515(6) 0.7303(6) 0.4451(4)

N1 N -0.1448(3) 0.6697(3) 0.2764(2)

H1 H -0.2194 0.6383 0.2701

C11 C -0.0734(4) 0.7255(3) 0.1973(3)

C12 C -0.0867(4) 0.6561(4) 0.1041(3)

H12A H -0.0546 0.5767 0.1132

H12B H -0.0387 0.695 0.0541

H12C H -0.1752 0.6526 0.0859

C13 C -0.1266(4) 0.8522(4) 0.1886(3)

C14 C -0.3100(5) 0.9620(4) 0.1436(4)

H14A H -0.3207 0.9895 0.2087

H14B H -0.3924 0.9496 0.1147

H14C H -0.2637 1.0207 0.1071

F1 F -0.1894(4) 0.8388(3) 0.4243(3)

F2 F -0.2578(4) 0.6684(4) 0.4631(2)

F3 F -0.0868(4) 0.7345(5) 0.5271(2)

C8 C 0.0496(4) 0.7429(4) 0.3465(3)

H8A H 0.1213 0.7096 0.3819

H8B H 0.0406 0.8266 0.3627

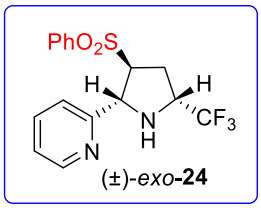
O1 O 0.1380(3) 0.8521(3) 0.0872(2)

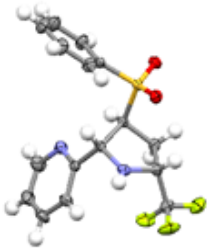
O2 O 0.2152(3) 0.9160(2) 0.2486(2)

O3 O -0.2395(3) 0.8512(2) 0.1438(2)

O4 O -0.0799(3) 0.9400(2) 0.2208(2)

S1 S 0.18132(10) 0.82148(9) 0.18250(9)





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_symmetry_Int_Tables_number 14

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loop_

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_symmetry_equiv_pos_as_xyz

1 x,y,z

2 1/2-x,1/2+y,1/2-z

3 -x,-y,-z

4 1/2+x,1/2-y,1/2+z

_cell_length_a 13.9505(6)

_cell_length_b 5.7490(2)

_cell_length_c 22.6500(9)

_cell_angle_alpha 90

_cell_angle_beta 93.789(2)

_cell_angle_gamma 90

_cell_volume 1812.59

loop_

_atom_site_label

_atom_site_type_symbol

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_atom_site_fract_y

_atom_site_fract_z

C1 C 1.0044(2) 0.3557(6) 0.87072(15)

H2 H 1.0016 0.4634 0.8371

C2 C 1.0116(3) 0.1038(6) 0.84891(16)

H3 H 0.9469 0.037 0.8438

C3 C 1.1205(3) 0.1444(6) 0.93364(16)

H4 H 1.0983 0.135 0.9737

C4 C 1.0987(3) 0.3875(6) 0.90846(17)

H5 H 1.0911 0.4991 0.9399

H6 H 1.1496 0.4401 0.8845

C5 C 1.2269(3) 0.0919(7) 0.9359(2)

C6 C 1.0585(3) 0.0960(6) 0.78951(16)

C7 C 1.0753(4) 0.2575(9) 0.69895(19)

H7 H 1.0608 0.3764 0.672

C8 C 1.1362(4) 0.0849(9) 0.6830(2)

H8 H 1.1614 0.0851 0.646

C9 C 1.1585(4) -0.0861(9) 0.7227(2)

H9 H 1.1988 -0.2068 0.7128

C10 C 1.1220(3) -0.0820(7) 0.7770(2)

H10 H 1.1391 -0.1952 0.8051

C11 C 0.8010(2) 0.3302(6) 0.87051(16)

C12 C 0.7651(3) 0.4849(7) 0.82756(19)

H11 H 0.7974 0.6234 0.8213

C13 C 0.6826(4) 0.4339(9) 0.7945(2)

H12 H 0.6587 0.5379 0.7657

C14 C 0.6352(4) 0.2321(10) 0.8034(2)

H13 H 0.5785 0.1988 0.7811

C15 C 0.6718(3) 0.0752(9) 0.8459(2)

H14 H 0.6397 -0.0641 0.8514

C16 C 0.7542(3) 0.1233(7) 0.8796(2)

H15 H 0.7783 0.0185 0.9082

F1 F 1.26475(19) 0.1072(5) 0.88373(12)

F2 F 1.2479(2) -0.1204(5) 0.95562(14)

F3 F 1.2753(2) 0.2412(6) 0.97094(15)

N1 N 1.0667(2) -0.0216(5) 0.89563(13)

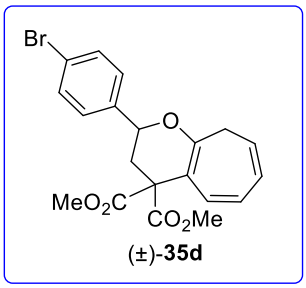
H1 H 1.0674 -0.1702 0.9001

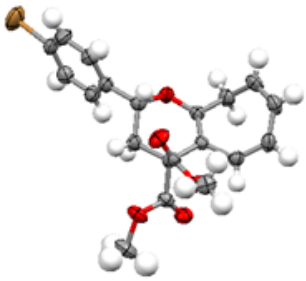
N2 N 1.0356(3) 0.2649(6) 0.75112(14)

O1 O 0.91354(18) 0.2478(4) 0.96479(10)

O2 O 0.90206(19) 0.6511(5) 0.92596(12)

S1 S 0.90538(6) 0.40414(14) 0.91511(4)





data_datos_0m

_symmetry_cell_setting triclinic

_symmetry_space_group_name_H-M 'P -1'

_symmetry_Int_Tables_number 2

_space_group_name_Hall '-P 1'

loop_

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_symmetry_equiv_pos_as_xyz

1 x,y,z

2 -x,-y,-z

_cell_length_a 8.31130(10)

_cell_length_b 9.8001(2)

_cell_length_c 12.3961(2)

_cell_angle_alpha 70.2210(10)

_cell_angle_beta 78.8530(10)

_cell_angle_gamma 77.4320(10)

_cell_volume 919.441

loop_

_atom_site_label

_atom_site_type_symbol

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

Br1 Br 1.29802(4) 0.05592(4) 0.08017(3)

C1 C 1.0759(3) 0.1045(3) 0.1477(2)

C2 C 1.0371(3) 0.2195(3) 0.1931(2)

H2 H 1.1191 0.2697 0.1949

C3 C 0.8737(3) 0.2586(3) 0.2362(2)

H3 H 0.8460 0.3356 0.2677

C4 C 0.7501(3) 0.1857(2) 0.23332(19)

C5 C 0.7937(3) 0.0695(3) 0.1893(2)

H5 H 0.7123 0.0184 0.1881

C6 C 0.9577(3) 0.0274(3) 0.1465(2)

H6 H 0.9866 -0.0519 0.1176

C7 C 0.5695(3) 0.2399(3) 0.2690(2)

H7 H 0.4998 0.1771 0.2593

C8 C 0.5321(3) 0.2475(3) 0.39037(19)

H8A H 0.6058 0.3053 0.4006

H8B H 0.5538 0.1491 0.4439

C9 C 0.3501(3) 0.3166(2) 0.41934(18)

C10 C 0.2903(3) 0.4423(2) 0.31484(17)

C11 C 0.3897(3) 0.4705(2) 0.21215(18)

C12 C 0.3510(3) 0.6048(3) 0.1120(2)

H12A H 0.3315 0.6920 0.1362

H12B H 0.4445 0.6118 0.0510

C13 C 0.2010(3) 0.5956(3) 0.0682(2)

H13 H 0.2112 0.5839 -0.0044

C14 C 0.0528(3) 0.6038(3) 0.1309(2)

H14 H -0.0395 0.6092 0.0966

C15 C 0.0262(3) 0.6048(3) 0.2495(2)

H15 H -0.0716 0.6603 0.2729

C16 C 0.1301(3) 0.5328(2) 0.3287(2)

H16 H 0.0944 0.5425 0.4021

C17 C 0.2328(3) 0.2028(2) 0.45727(18)

C18 C -0.0371(3) 0.1605(3) 0.5501(2)

H18A H -0.0719 0.1547 0.4825

H18B H -0.1300 0.2041 0.5936

H18C H 0.0044 0.0635 0.5969

C19 C 0.3499(3) 0.3719(3) 0.52199(18)

C20 C 0.4374(4) 0.2884(4) 0.7080(2)

H20A H 0.5435 0.3204 0.6885

H20B H 0.4408 0.2014 0.7739

H20C H 0.3533 0.3646 0.7259

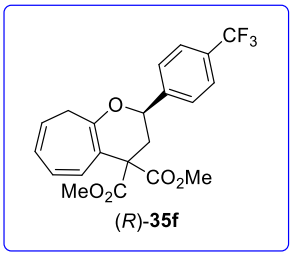
O1 O 0.5360(2) 0.38661(18) 0.18784(13)

O2 O 0.2621(2) 0.08979(19) 0.43504(17)

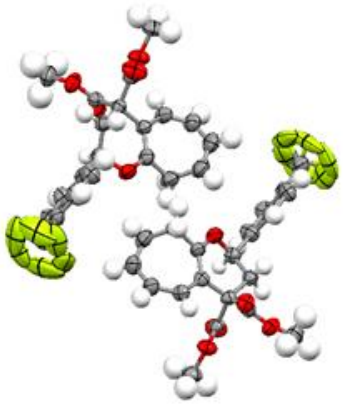
O3 O 0.0925(2) 0.24957(17) 0.51567(14)

O4 O 0.3181(2) 0.49556(18) 0.52330(14)

O5 O 0.3990(2) 0.25617(19) 0.61100(14)



(*R*)-**35f**



data_desordenfin

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_symmetry_Int_Tables_number 1

_space_group_name_Hall 'P 1'

loop_

_symmetry_equiv_pos_site_id

_symmetry_equiv_pos_as_xyz

1 x,y,z

_cell_length_a 8.6119(3)

_cell_length_b 9.9168(3)

_cell_length_c 12.4569(4)

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_cell_angle_beta 77.402(2)

_cell_angle_gamma 77.618(2)

_cell_volume 967.79

loop_

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_atom_site_type_symbol

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

O1 O 0.5531(3) 0.4325(3) 0.6995(3)

O2 O 0.2890(4) 0.1282(3) 0.9382(3)

O3 O 0.1137(3) 0.2809(3) 1.0219(3)

O5 O 0.3976(4) 0.2946(3) 1.1215(3)

O4 O 0.3214(4) 0.5287(3) 1.0366(3)

C1 C 0.3732(6) 0.6454(5) 0.6274(5)

H1A H 0.3474 0.7295 0.6551

H1B H 0.4671 0.6570 0.5677

C2 C 0.2334(6) 0.6322(5) 0.5795(5)

H2 H 0.2496 0.6232 0.5057

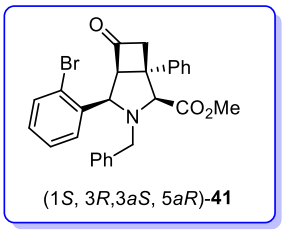
C3 C 0.0875(6) 0.6331(5) 0.6411(5)

H3 H 0.0023 0.6369 0.6049

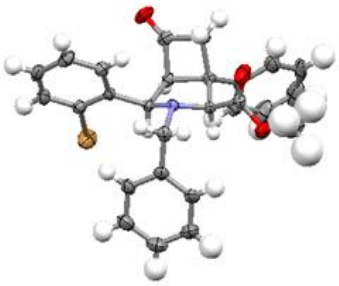
C4 C 0.0519(5) 0.6287(5) 0.7604(5)

H4 H -0.0473 0.6778 0.7845

C5 C 0.1484(5) 0.5600(4) 0.8411(4)



(1*S*, 3*R*,3*aS*, 5*aR*)-**41**



data_02134JavierCorpas

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_symmetry_Int_Tables_number 19

_space_group_name_Hall 'P 2ac 2ab'

loop_

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_symmetry_equiv_pos_as_xyz

1 x,y,z

2 1/2-x,-y,1/2+z

3 -x,1/2+y,1/2-z

4 1/2+x,1/2-y,-z

_cell_length_a 7.3574(3)

_cell_length_b 17.3491(9)

_cell_length_c 18.2869(9)

_cell_angle_alpha 90

_cell_angle_beta 90

_cell_angle_gamma 90

_cell_volume 2334.22

loop_

_atom_site_label

_atom_site_type_symbol

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

Br1 Br 1.12649(5) 0.31329(3) 0.34474(3)

C1 C 0.9095(5) 0.3214(2) 0.4009(2)

C2 C 0.9240(6) 0.3456(2) 0.4729(2)

H2 H 1.039 0.3593 0.4926

C3 C 0.7713(7) 0.3497(2) 0.5151(2)

H3 H 0.7799 0.3668 0.5643

C4 C 0.6051(6) 0.3290(2) 0.4867(2)

H4 H 0.4991 0.3318 0.5163

C5 C 0.5926(5) 0.3042(2) 0.4148(2)

H5 H 0.4776 0.2893 0.3958

C6 C 0.7448(5) 0.3005(2) 0.36993(19)

C7 C 0.7311(5) 0.2740(2) 0.2915(2)

H7 H 0.8279 0.3006 0.2625

C8 C 0.7523(5) 0.1861(2) 0.28064(18)

H8 H 0.8797 0.168 0.2724

C9 C 0.6395(6) 0.1358(2) 0.3312(2)

C10 C 0.4867(6) 0.1273(3) 0.2765(2)

H10A H 0.3774 0.1581 0.2884

H10B H 0.4543 0.0731 0.2655

C11 C 0.6143(6) 0.1657(2) 0.21764(19)

C12 C 0.5511(5) 0.2453(2) 0.1910(2)

H12 H 0.6427 0.2664 0.1559

C13 C 0.5191(5) 0.3749(2) 0.2471(2)

H13A H 0.5033 0.3992 0.2956

H13B H 0.4032 0.381 0.2201

C14 C 0.6660(5) 0.4183(2) 0.2061(2)

C15 C 0.6627(7) 0.4244(3) 0.1305(2)

H15 H 0.5635 0.4031 0.104

C16 C 0.8005(8) 0.4606(3) 0.0931(3)

H16 H 0.7962 0.4639 0.0413

C17 C 0.9449(8) 0.4922(3) 0.1306(3)

H17 H 1.0401 0.5171 0.1046

C18 C 0.9513(7) 0.4876(3) 0.2059(3)

H18 H 1.0504 0.5094 0.232

C19 C 0.8112(6) 0.4507(2) 0.2434(3)

H19 H 0.8154 0.4476 0.2952

C20 C 0.6795(5) 0.1133(2) 0.1570(2)

C21 C 0.8555(7) 0.1167(3) 0.1319(2)

H21 H 0.9381 0.1515 0.1544

C22 C 0.9157(8) 0.0712(3) 0.0748(3)

H22 H 1.0382 0.0749 0.0587

C23 C 0.7995(11) 0.0213(3) 0.0416(3)

H23 H 0.8404 -0.0097 0.0021

C24 C 0.6230(11) 0.0157(3) 0.0654(3)

H24 H 0.5423 -0.0196 0.0426

C25 C 0.5613(7) 0.0619(3) 0.1234(3)

H25 H 0.4389 0.0579 0.1396

C26 C 0.3659(6) 0.2444(2) 0.1547(2)

C27 C 0.2081(8) 0.2686(4) 0.0438(3)

H27A H 0.1652 0.2158 0.0359

H27B H 0.2291 0.2935 -0.0036

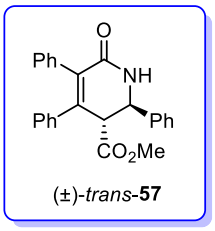
H27C H 0.1162 0.2976 0.0711

N1 N 0.5527(4) 0.29168(18) 0.25797(16)

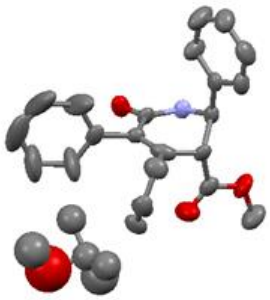
O1 O 0.6702(4) 0.10692(18) 0.38966(16)

O2 O 0.3773(5) 0.2670(2) 0.08526(16)

O3 O 0.2277(4) 0.2253(2) 0.18266(17)



(±)-*trans*-**57**



data_02024JavierCorpas

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_symmetry_Int_Tables_number 14

_space_group_name_Hall '-P 2yn'

loop_

_symmetry_equiv_pos_site_id

_symmetry_equiv_pos_as_xyz

1 x,y,z

2 1/2-x,1/2+y,1/2-z

3 -x,-y,-z

4 1/2+x,1/2-y,1/2+z

_cell_length_a 9.5153(5)

_cell_length_b 18.0720(8)

_cell_length_c 15.6335(9)

_cell_angle_alpha 90

_cell_angle_beta 103.767(2)

_cell_angle_gamma 90

_cell_volume 2611.11

loop_

_atom_site_label

_atom_site_type_symbol

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

C20 C 0.4879(5) 0.7231(2) 0.4023(3)

C21 C 0.5069(8) 0.7657(3) 0.4782(3)

H21 H 0.4451 0.7588 0.5171

C22 C 0.6164(10) 0.8184(3) 0.4971(4)

H22 H 0.6294 0.8475 0.549

C23 C 0.7069(7) 0.8284(3) 0.4401(5)

H23 H 0.7817 0.8644 0.4531

C24 C 0.6878(6) 0.7858(4) 0.3642(6)

H24 H 0.7497 0.7926 0.3253

C25 C 0.5783(7) 0.7331(4) 0.3453(4)

H25 H 0.5654 0.704 0.2934

C1 C 0.4286(6) 0.5899(3) 0.4240(3)

C2 C 0.1736(6) 0.5529(3) 0.3986(4)

H2 H 0.1221 0.5049 0.3816

C3 C 0.1467(6) 0.6029(3) 0.3152(3)

H3 H 0.0439 0.6201 0.3017

C4 C 0.2447(5) 0.6703(3) 0.3341(3)

C5 C 0.3768(6) 0.6631(3) 0.3839(3)

C6 C 0.1163(6) 0.5865(2) 0.4717(4)

C7 C 0.1998(7) 0.5960(4) 0.5535(5)

H7 H 0.3 0.5845 0.5653

C8 C 0.1392(8) 0.6233(5) 0.6225(5)

H8 H 0.1979 0.6271 0.6807

C9 C 0.0002(8) 0.6435(4) 0.6058(5)

H9 H -0.0384 0.6644 0.6511

C10 C -0.0861(7) 0.6339(4) 0.5234(5)

H10 H -0.1855 0.647 0.512

C11 C -0.0308(7) 0.6052(4) 0.4559(5)

H11 H -0.0925 0.5982 0.3991

C12 C 0.1711(7) 0.5604(3) 0.2361(4)

C13 C 0.1033(9) 0.4538(4) 0.1476(5)

H13A H 0.029 0.4703 0.0964

H13B H 0.0871 0.4017 0.1597

H13C H 0.1991 0.4594 0.1354

C14 C 0.1822(5) 0.7420(3) 0.2945(3)

C15 C 0.0956(8) 0.7823(3) 0.3338(4)

H15 H 0.074 0.7639 0.3861

C16 C 0.0370(8) 0.8501(3) 0.2999(5)

H16 H -0.0196 0.8787 0.3303

C17 C 0.0634(7) 0.8750(3) 0.2201(4)

H17 H 0.0225 0.9202 0.1945

C18 C 0.1465(7) 0.8344(3) 0.1811(5)

H18 H 0.1655 0.8513 0.1274

C19 C 0.2068(7) 0.7673(3) 0.2170(4)

H19 H 0.2651 0.7393 0.1873

N1 N 0.3284(5) 0.5377(2) 0.4237(3)

H1 H 0.3572 0.4924 0.4392

O1 O 0.5587(4) 0.5796(2) 0.4572(3)

O2 O 0.2414(7) 0.5809(3) 0.1884(4)

O3 O 0.0956(5) 0.4981(2) 0.2233(3)

O4 O 0.808(2) 0.6371(12) 0.1187(14)

C26 C 0.797(2) 0.7018(11) 0.1674(13)

C27 C 0.6836(12) 0.5981(6) 0.1308(7)

C28 C 0.5457(13) 0.6323(6) 0.1003(8)

C29 C 0.7513(14) 0.6004(7) 0.2211(8)

C30 C 0.704(2) 0.5342(10) 0.0810(14)