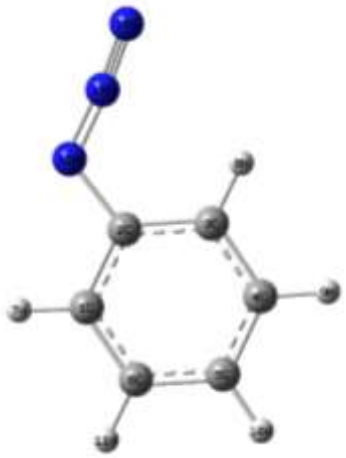
6. Anexos.

6.1. Anexo I.

En este anexo se regogen la totalidad de los parámetros geométricos obtenidos en la optimizacion de los componenetes de la reacion principal registrados con el método M062X/6-31+G(d,p) en fase gas. Además, se recogen las representaciones de dichos componentes y la codificacion correspomdiente, es decir, el numero que identifica a cada átomo.

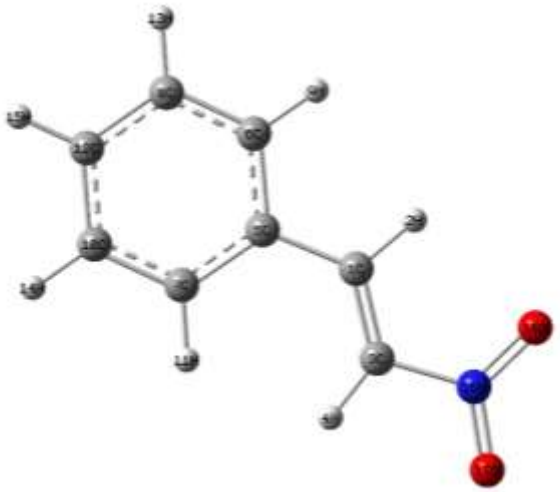
Los parámetros adjuntados incluyen distancias de enlace (R), angulos entre los átomos (A) y planos diedricos entre los átomos (D).

-Reactivo 1: Fenilazida (dipolo).



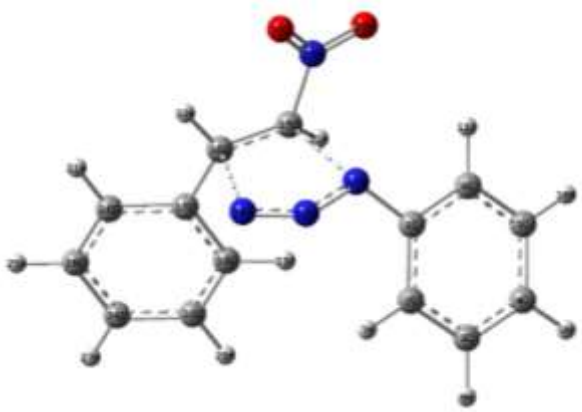
NºR	Átomos	d(A)	NºA	Átomos	A()
R1	R(1,2)	1.3966	A1	A(2,1,6)	119.645
R2	R(1,6)	1.3898	A2	A(2,1,7)	118.819
R3	R(1,7)	1.0847	A3	A(6,1,7)	121.536
R4	R(2,3)	1.3974	A4	A(1,2,3)	120.349
R5	R(2,12)	1.4218	A5	A(1,2,12)	115.845
R6	R(3,4)	1.3931	A6	A(3,2,12)	123.806
R7	R(3,8)	1.0865	A7	A(2,3,4)	119.404
R8	R(4,5)	1.3931	A8	A(2,3,8)	120.619
R9	R(4,9)	1.0853	A9	A(4,3,8)	119.977
R10	R(5,6)	1.3956	A10	A(3,4,5)	120.608
R11	R(5,10)	1.0847	A11	A(3,4,9)	119.262
R12	R(6,11)	1.0853	A12	A(5,4,9)	120.130
R13	R(12,13)	1.2351	A13	A(4,5,6)	119.517
R14	R(13,14)	1.1292	A14	A(4,5,10)	120.198
			A15	A(6,5,10)	120.285
			A16	A(1,6,5)	120.478
			A17	A(1,6,11)	119.434
			A18	A(5,6,11)	120.088
			A19	A(2,12,13)	116.207
			A20	A(12,13,14)	174.538

-Reactivo 2: Nitroestireno (dipolarófilo).



NºR	Átomos	d(A)	NºA	Átomos	A()	NºD	Átomos	D ()
1	R(1,2)	1.0879	A1	A(2,1,3)	116.67	D1	D(2,1,3,4)	179.997
R2	R(1,3)	1.3341	A2	A(2,1,5)	117.18	D2	D(2,1,3,16)	-0.003
R3	R(1,5)	1.4648	A3	A(3,1,5)	126.15	D3	D(5,1,3,4)	0.000
R4	R(3,4)	1.0803	A4	A(1,3,4)	128.48	D4	D(5,1,3,16)	-180.000
R5	R(3,16)	1.4561	A5	A(1,3,16)	119.89	D5	D(2,1,5,6)	-0.025
R6	R(5,6)	1.4009	A6	A(4,3,16)	111.63	D6	D(2,1,5,7)	179.974
R7	R(5,7)	1.4037	A7	A(1,5,6)	118.22	D7	D(3,1,5,6)	179.972
R8	R(6,8)	1.3922	A8	A(1,5,7)	122.92	D8	D(3,1,5,7)	-0.029
R9	R(6,9)	1.0864	A9	A(6,5,7)	118.87	D9	D(1,3,16,17)	-179.994
R10	R(7,10)	1.3884	A10	A(5,6,8)	120.75	D10	D(1,3,16,18)	0.006
R11	R(7,11)	1.0854	A11	A(5,6,9)	119.26	D11	D(4,3,16,17)	0.006
R12	R(8,12)	1.3926	A12	A(8,6,9)	119.99	D12	D(4,3,16,18)	-179.994
R13	R(8,13)	1.0849	A13	A(5,7,10)	120.38	D13	D(1,5,6,8)	-179.999
R14	R(10,12)	1.3971	A14	A(5,7,11)	12.02	D14	D(1,5,6,9)	0.001
R15	R(10,14)	1.0850	A15	A(10,7,11)	11.94	D15	D(7,5,6,8)	0.002
R16	R(12,15)	1.0851	A16	A(6,8,12)	119.87	D16	D(7,5,6,9)	-179.999
R17	R(16,17)	1.2212	A17	A(6,8,13)	119.89	D17	D(1,5,7,10)	179.999
R18	R(16,18)	1.2199	A18	A(12,8,13)	120.24	D18	D(1,5,7,11)	-0.004
			A19	A(7,10,12)	120.23	D19	D(6,5,7,10)	-0.002
			A20	A(7,10,14)	119.74	D20	D(6,5,7,11)	179.996
			A21	A(12,10,14)	120.03	D21	D(5,6,8,12)	-0.001
			A22	A(8,12,10)	119.91	D22	D(5,6,8,13)	180.000
			A23	A(8,12,15)	120.11	D23	D(9,6,8,12)	180.000
			A24	A(10,12,15)	119.98	D24	D(9,6,8,13)	0.000
			A25	A(3,16,17)	115.74	D25	D(5,7,10,12)	0.000
			A26	A(3,16,18)	119.33	D26	D(5,7,10,14)	179.999
			A27	A(17,16,18)	124.93	D27	D(11,7,10,12)	-179.997
						D28	D(11,7,10,14)	0.0019
						D29	D(6,8,12,10)	-0.0005
						D30	D(6,8,12,15)	-180.000
						D31	D(13,8,12,10)	179.999
						D32	D(13,8,12,15)	0.0002
						D33	D(7,10,12,8)	0.0007
						D34	D(7,10,12,15)	180.000
						D35	D(14,10,12,8)	-179.998
						D36	D(14,10,12,15)	0.0006

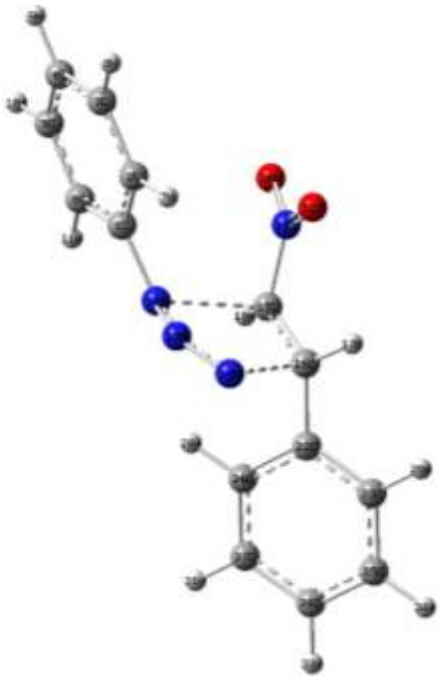
-Estado de Transición vía 1,4 aproximación *endo*: TS-14n.



NºR	Átomos	d(A)	NºA	Átomos	A()	NºD	Átomos	D ()
R1	R(1,2)	1.3984	A1	A(2,1,6)	120.84	D1	D(6,1,2,3)	0.57
R2	R(1,6)	1.3971	A2	A(2,1,12)	123.25	D2	D(6,1,2,7)	179.70
R3	R(1,12)	1.4183	A3	A(6,1,12)	115.85	D3	D(12,1,2,3)	177.76
R4	R(2,3)	1.3918	A4	A(1,2,3)	119.17	D4	D(12,1,2,7)	-3.11
R5	R(2,7)	1.0863	A5	A(1,2,7)	120.08	D5	D(2,1,6,5)	0.49
R6	R(3,4)	1.3948	A6	A(3,2,7)	120.74	D6	D(2,1,6,11)	-179.94
R7	R(3,8)	1.0852	A7	A(2,3,4)	120.46	D7	D(12,1,6,5)	-176.91
R8	R(4,5)	1.395	A8	A(2,3,8)	119.40	D8	D(12,1,6,11)	2.67
R9	R(4,9)	1.0848	A9	A(4,3,8)	120.14	D9	D(2,1,12,13)	6.98
R10	R(5,6)	1.3912	A10	A(3,4,5)	119.82	D10	D(6,1,12,13)	-175.69
R11	R(5,10)	1.085	A11	A(3,4,9)	120.04	D11	D(1,2,3,4)	-1.08
R12	R(6,11)	1.0861	A12	A(5,4,9)	120.14	D12	D(1,2,3,8)	179.15
R13	R(11,29)	2.657	A13	A(4,5,6)	120.42	D13	D(7,2,3,4)	179.80
R14	R(12,13)	1.2713	A14	A(4,5,10)	120.14	D14	D(7,2,3,8)	0.02
R15	R(12,15)	2.0694	A15	A(6,5,10)	119.43	D15	D(2,3,4,5)	0.53
R16	R(12,28)	2.5894	A16	A(1,6,5)	119.27	D16	D(2,3,4,9)	-179.76
R17	R(12,31)	2.4299	A17	A(1,6,11)	119.09	D17	D(8,3,4,5)	-17.97
R18	R(13,14)	1.1614	A18	A(5,6,11)	121.64	D18	D(8,3,4,9)	0.02
R19	R(13,15)	2.5607	A19	A(1,12,13)	118.65	D19	D(3,4,5,6)	0.55
R20	R(13,16)	2.5561	A20	A(12,13,14)	137.64	D20	D(3,4,5,10)	179.82
R21	R(14,16)	2.0893	A21	A(16,15,28)	118.59	D21	D(9,4,5,6)	-179.17
R22	R(14,32)	2.3736	A22	A(16,15,31)	124.76	D22	D(9,4,5,10)	0.10
R23	R(15,16)	1.3856	A23	A(28,15,31)	111.46	D23	D(4,5,6,1)	-1.04
R24	R(15,28)	1.4622	A24	A(15,16,17)	120.41	D24	D(4,5,6,11)	179.39
R25	R(15,31)	1.0828	A25	A(15,16,32)	117.16	D25	D(10,5,6,1)	179.68
R26	R(16,17)	1.4763	A26	A(17,16,32)	118.34	D26	D(10,5,6,11)	0.11
R27	R(16,32)	1.0861	A27	A(16,17,18)	119.75	D27	D(1,12,13,14)	-133.23
R28	R(17,18)	1.3988	A28	A(16,17,19)	121.31	D28	D(28,15,16,17)	160.77
R29	R(17,19)	1.4021	A29	A(18,17,19)	118.93	D29	D(28,15,16,32)	3.89
R30	R(18,20)	1.3926	A30	A(17,18,20)	120.55	D30	D(31,15,16,17)	8.48
R31	R(18,21)	1.0865	A31	A(17,18,21)	119.38	D31	D(31,15,16,32)	-148.40
R32	R(19,22)	1.3911	A32	A(20,18,21)	120.07	D32	D(16,15,28,29)	-161.83
R33	R(19,23)	1.0888	A33	A(17,19,22)	120.46	D33	D(16,15,28,30)	19.58
R34	R(20,24)	1.3936	A34	A(17,19,23)	120.13	D34	D(31,15,28,29)	-6.07
R35	R(20,25)	1.0853	A35	A(22,19,23)	119.41	D35	D(31,15,28,30)	175.34

R36	R(22,24)	1.3952	A36	A(18,20,24)	120.16	D36	D(15,16,17,18)	-150.57
R37	R(22,26)	1.0854	A37	A(18,20,25)	119.72	D37	D(15,16,17,19)	30.77
R38	R(24,27)	1.0852	A38	A(24,20,25)	120.12	D38	D(32,16,17,18)	6.05
R39	R(28,29)	1.221	A39	A(19,22,24)	120.20	D39	D(32,16,17,19)	-172.62
R40	R(28,30)	1.2178	A40	A(19,22,26)	119.67	D40	D(16,17,18,20)	-179.82
			A41	A(24,22,26)	120.12	D41	D(16,17,18,21)	0.53
			A42	A(20,24,22)	119.69	D42	D(19,17,18,20)	-1.13
			A43	A(20,24,27)	120.18	D43	D(19,17,18,21)	179.23
			A44	A(22,24,27)	120.14	D44	D(16,17,19,22)	179.90
			A45	A(15,28,29)	116.33	D45	D(16,17,19,23)	0.69
			A46	A(15,28,30)	118.45	D46	D(18,17,19,22)	1.23
			A47	A(29,28,30)	125.21	D47	D(18,17,19,23)	-177.98
						D48	D(17,18,20,24)	0.36
						D49	D(17,18,20,25)	-179.67
						D50	D(21,18,20,24)	-179.99
						D51	D(21,18,20,25)	-0.03
						D52	D(17,19,22,24)	-0.58
						D53	D(17,19,22,26)	179.89
						D54	D(23,19,22,24)	178.64
						D55	D(23,19,22,26)	-0.89
						D56	D(18,20,24,22)	0.31
						D57	D(18,20,24,27)	179.94
						D58	D(25,20,24,22)	-17.97
						D59	D(25,20,24,27)	-0.03
						D60	D(19,22,24,20)	-0.20
						D61	D(19,22,24,27)	-179.83
						D62	D(26,22,24,20)	179.33
						D63	D(26,22,24,27)	-0.30

-Estado de Transición vía 1,4 aproximación *exo*: TS-14x.

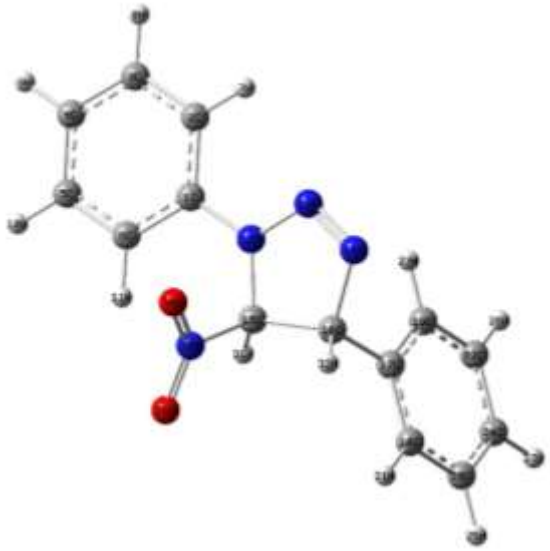


NºR	Átomos	d(A)	NºA	Átomos	A()	NºD	Átomos	D ()
R1	R(1,2)	1.3982	A1	A(2,1,6)	120.86	D1	D(6,1,2,3)	0.12
R2	R(1,6)	1.3956	A2	A(2,1,12)	122.59	D2	D(6,1,2,7)	-178.61
R3	R(1,12)	1.4193	A3	A(6,1,12)	116.39	D3	D(12,1,2,3)	176.46
R4	R(2,3)	1.3904	A4	A(1,2,3)	119.14	D4	D(12,1,2,7)	-3.33
R5	R(2,7)	1.0861	A5	A(1,2,7)	119.95	D5	D(2,1,6,5)	-0.37
R6	R(3,4)	1.3951	A6	A(3,2,7)	120.91	D6	D(2,1,6,11)	179.34
R7	R(3,8)	1.0849	A7	A(2,3,4)	120.36	D7	D(12,1,6,5)	-175.93
R8	R(4,5)	1.3944	A8	A(2,3,8)	119.49	D8	D(12,1,6,11)	0.38
R9	R(4,9)	1.085	A9	A(4,3,8)	120.15	D9	D(2,1,12,13)	22.88
R10	R(5,6)	1.3905	A10	A(3,4,5)	120.06	D10	D(2,1,12,15)	-9.03
R11	R(5,10)	1.0849	A11	A(3,4,9)	119.93	D11	D(2,1,12,18)	-118.92
R12	R(6,11)	1.0852	A12	A(5,4,9)	120.00	D12	D(2,1,12,19)	-7.83
R13	R(12,13)	1.2736	A13	A(4,5,6)	120.12	D13	D(6,1,12,13)	-161.64
R14	R(12,15)	2.1085	A14	A(4,5,10)	12.02	D14	D(6,1,12,15)	85.21
R15	R(12,18)	2.4503	A15	A(6,5,10)	119.68	D15	D(6,1,12,18)	56.55
R16	R(12,19)	2.6444	A16	A(1,6,5)	119.45	D16	D(6,1,12,19)	97.16
R17	R(13,14)	1.1634	A17	A(1,6,11)	119.10	D17	D(1,2,3,4)	-1.13
R18	R(13,15)	2.5651	A18	A(5,6,11)	121.46	D18	D(1,2,3,8)	179.65
R19	R(13,16)	2.548	A19	A(1,12,13)	118.85	D19	D(7,2,3,4)	178.66
R20	R(14,15)	2.6912	A20	A(1,12,15)	116.24	D20	D(7,2,3,8)	-0.56
R21	R(14,16)	2.0506	A21	A(1,12,18)	113.64	D21	D(2,3,4,5)	0.27
R22	R(14,17)	2.3367	A22	A(1,12,19)	85.09	D22	D(2,3,4,9)	-17.95

R23	R(14,22)	2.7223	A23	A(13,12,18)	115.92	D23	D(8,3,4,5)	179.48
R24	R(15,16)	1.3895	A24	A(13,12,19)	102.16	D24	D(8,3,4,9)	-0.29
R25	R(15,18)	1.0808	A25	A(18,12,19)	48.81	D25	D(3,4,5,6)	0.56
R26	R(15,19)	1.4531	A26	A(12,13,14)	137.37	D26	D(3,4,5,10)	-179.65
R27	R(16,17)	1.0852	A27	A(12,13,16)	85.45	D27	D(9,4,5,6)	-179.67
R28	R(16,22)	1.4779	A28	A(13,14,17)	116.43	D28	D(9,4,5,10)	0.12
R29	R(19,20)	1.2202	A29	A(13,14,22)	112.59	D29	D(4,5,6,1)	-0.51
R30	R(19,21)	1.224	A30	A(15,14,17)	49.15	D30	D(4,5,6,11)	179.79
R31	R(22,23)	1.3985	A31	A(15,14,22)	54.64	D31	D(10,5,6,1)	179.70
R32	R(22,24)	1.4015	A32	A(17,14,22)	51.04	D32	D(10,5,6,11)	0.00
R33	R(23,25)	1.3925	A33	A(12,15,14)	54.86	D33	D(1,12,13,14)	-137.63
R34	R(23,26)	1.0865	A34	A(12,15,16)	102.05	D34	D(1,12,13,16)	-132.55
R35	R(24,27)	1.3911	A35	A(13,15,18)	118.04	D35	D(18,12,13,14)	3.33
R36	R(24,28)	1.0879	A36	A(13,15,19)	100.38	D36	D(18,12,13,16)	8.41
R37	R(25,29)	1.3937	A37	A(14,15,18)	131.36	D37	D(19,12,13,14)	-46.56
R38	R(25,30)	1.0853	A38	A(14,15,19)	107.61	D38	D(19,12,13,16)	-41.48
R39	R(27,29)	1.3951	A39	A(16,15,18)	125.05	D39	D(1,12,15,14)	13.08
R40	R(27,31)	1.0854	A40	A(16,15,19)	118.14	D40	D(1,12,15,16)	142.03
R41	R(29,32)	1.0852	A41	A(18,15,19)	112.13	D41	D(1,12,19,20)	-50.18
			A42	A(13,16,17)	106.42	D42	D(1,12,19,21)	83.18
			A43	A(13,16,22)	109.55	D43	D(13,12,19,20)	-168.67
			A44	A(15,16,17)	116.98	D44	D(13,12,19,21)	-35.31
			A45	A(15,16,22)	120.07	D45	D(18,12,19,20)	77.40
			A46	A(17,16,22)	118.07	D46	D(18,12,19,21)	-149.24
			A47	A(12,19,20)	108.64	D47	D(12,13,14,17)	31.01
			A48	A(12,19,21)	101.63	D48	D(12,13,14,22)	-25.37
			A49	A(15,19,20)	116.85	D49	D(12,13,16,17)	127.60
			A50	A(15,19,21)	118.13	D50	D(12,13,16,22)	-103.69
			A51	A(20,19,21)	124.94	D51	D(17,14,15,12)	-161.84
			A52	A(14,22,23)	119.28	D52	D(17,14,15,18)	13.69
			A53	A(14,22,24)	100.30	D53	D(17,14,15,19)	-79.44
			A54	A(16,22,23)	119.91	D54	D(22,14,15,12)	132.09
			A55	A(16,22,24)	121.02	D55	D(22,14,15,18)	70.79
			A56	A(23,22,24)	11.91	D56	D(22,14,15,19)	-145.51
			A57	A(22,23,25)	120.48	D57	D(13,14,22,23)	-179.80
			A58	A(22,23,26)	119.42	D58	D(13,14,22,24)	-47.89
			A59	A(25,23,26)	120.10	D59	D(15,14,22,23)	136.50
			A60	A(22,24,27)	120.39	D60	D(15,14,22,24)	-91.59
			A61	A(22,24,28)	119.73	D61	D(17,14,22,23)	73.73
			A62	A(27,24,28)	11.99	D62	D(17,14,22,24)	-154.36
			A63	A(23,25,29)	120.13	D63	D(12,15,16,17)	-109.21
			A64	A(23,25,30)	119.75	D64	D(12,15,16,22)	95.97
			A65	A(29,25,30)	120.12	D65	D(18,15,16,17)	145.91
			A66	A(24,27,29)	120.18	D66	D(18,15,16,22)	-8.91
			A67	A(24,27,31)	119.74	D67	D(19,15,16,17)	-0.79
			A68	A(29,27,31)	120.08	D68	D(19,15,16,22)	-162.69
			A69	A(25,29,27)	119.74	D69	D(13,15,19,20)	-122.89
			A70	A(25,29,32)	120.15	D70	D(13,15,19,21)	53.91

A71	A(27,29,32)	120.11	D71	D(14,15,19,20)	-148.05
			D72	D(14,15,19,21)	28.76
			D73	D(16,15,19,20)	160.31
			D74	D(16,15,19,21)	-22.88
			D75	D(18,15,19,20)	3.29
			D76	D(18,15,19,21)	-179.90
			D77	D(13,16,22,23)	-129.53
			D78	D(13,16,22,24)	49.26
			D79	D(15,16,22,23)	146.99
			D80	D(15,16,22,24)	-34.22
			D81	D(17,16,22,23)	-0.76
			D82	D(17,16,22,24)	1.71
			D83	D(14,22,23,25)	124.44
			D84	D(14,22,23,26)	-55.95
			D85	D(16,22,23,25)	-179.85
			D86	D(16,22,23,26)	-0.24
			D87	D(24,22,23,25)	1.34
			D88	D(24,22,23,26)	-179.05
			D89	D(14,22,24,27)	-133.39
			D90	D(14,22,24,28)	45.41
			D91	D(16,22,24,27)	179.85
			D92	D(16,22,24,28)	-1.34
			D93	D(23,22,24,27)	-1.35
			D94	D(23,22,24,28)	177.46
			D95	D(22,23,25,29)	-0.48
			D96	D(22,23,25,30)	179.59
			D97	D(26,23,25,29)	179.92
			D98	D(26,23,25,30)	-0.02
			D99	D(22,24,27,29)	0.49
			D100	D(22,24,27,31)	179.92
			D101	D(28,24,27,29)	-178.31
			D102	D(28,24,27,31)	1.11
			D103	D(23,25,29,27)	-0.39
			D104	D(23,25,29,32)	-179.88
			D105	D(30,25,29,27)	179.54
			D106	D(30,25,29,32)	0.01
			D107	D(24,27,29,25)	0.38
			D108	D(24,27,29,32)	17.99
			D109	D(31,27,29,25)	-179.04
			D110	D(31,27,29,32)	0.45

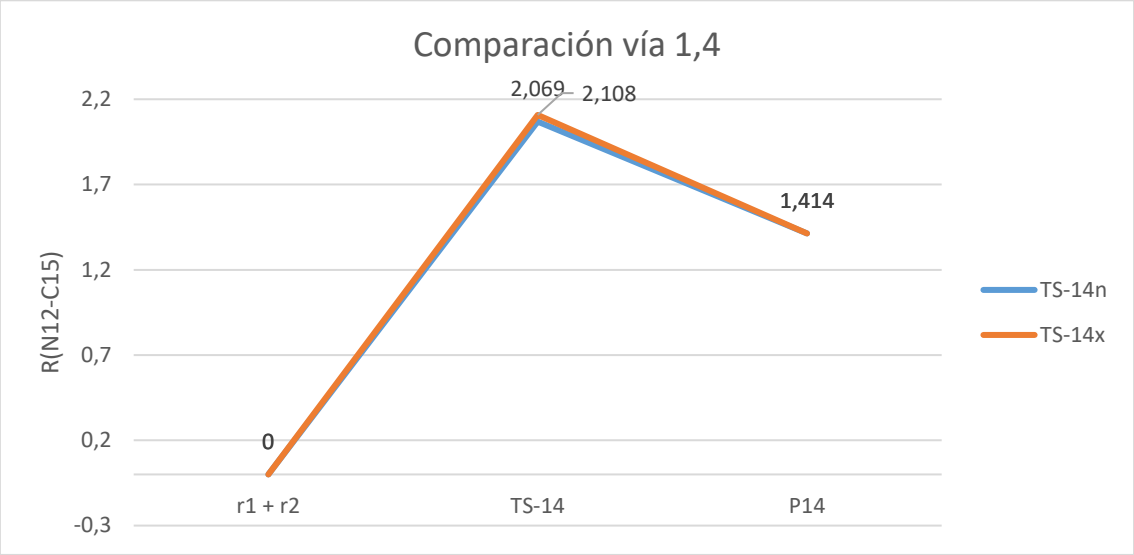
-Producto vía 1,4: P14.



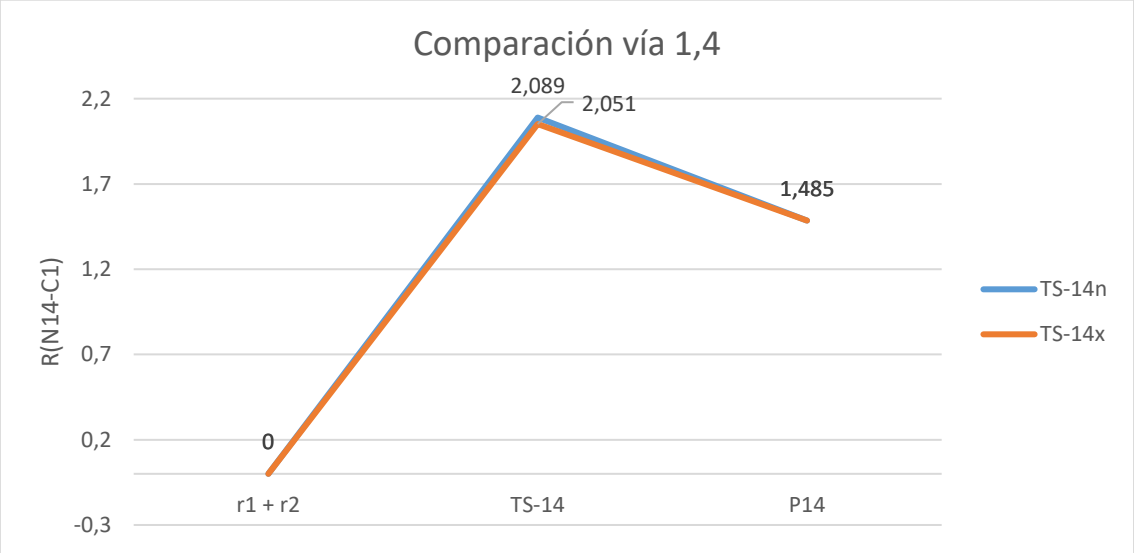
NºR	Átomos	d(A)	NºA	Átomos	A()	NºD	Átomos	D ()
R1	R(1,2)	1.3988	A1	A(2,1,6)	120.35	D1	D(6,1,2,3)	-0.12
R2	R(1,6)	1.3972	A2	A(2,1,12)	120.17	D2	D(6,1,2,7)	179.61
R3	R(1,12)	1.4083	A3	A(6,1,12)	119.47	D3	D(12,1,2,3)	179.18
R4	R(2,3)	1.3897	A4	A(1,2,3)	119.24	D4	D(12,1,2,7)	-1.10
R5	R(2,7)	1.083	A5	A(1,2,7)	119.72	D5	D(2,1,6,5)	0.41
R6	R(3,4)	1.3954	A6	A(3,2,7)	121.04	D6	D(2,1,6,11)	-179.28
R7	R(3,8)	1.0853	A7	A(2,3,4)	120.97	D7	D(12,1,6,5)	-178.88
R8	R(4,5)	1.3912	A8	A(2,3,8)	119.01	D8	D(12,1,6,11)	0.14
R9	R(4,9)	1.0845	A9	A(4,3,8)	120.03	D9	D(2,1,12,13)	12.06
R10	R(5,6)	1.3934	A10	A(3,4,5)	119.29	D10	D(2,1,12,15)	177.60
R11	R(5,10)	1.0851	A11	A(3,4,9)	120.37	D11	D(6,1,12,13)	-168.64
R12	R(6,11)	1.086	A12	A(5,4,9)	120.34	D12	D(6,1,12,15)	-3.11
R13	R(12,13)	1.3762	A13	A(4,5,6)	120.62	D13	D(1,2,3,4)	-0.23
R14	R(12,15)	1.4139	A14	A(4,5,10)	120.30	D14	D(1,2,3,8)	179.82
R15	R(13,14)	1.2359	A15	A(6,5,10)	119.07	D15	D(7,2,3,4)	-179.94
R16	R(14,16)	1.4847	A16	A(1,6,5)	119.54	D16	D(7,2,3,8)	0.11
R17	R(15,16)	1.5427	A17	A(1,6,11)	121.08	D17	D(2,3,4,5)	0.26
R18	R(15,28)	1.5376	A18	A(5,6,11)	119.38	D18	D(2,3,4,9)	-179.96
R19	R(15,31)	1.0899	A19	A(1,12,13)	121.20	D19	D(8,3,4,5)	-179.79
R20	R(16,17)	1.512	A20	A(1,12,15)	126.18	D20	D(8,3,4,9)	-0.01
R21	R(16,32)	1.0933	A21	A(13,12,15)	111.26	D21	D(3,4,5,6)	0.04
R22	R(17,18)	1.3952	A22	A(12,13,14)	112.23	D22	D(3,4,5,10)	179.56
R23	R(17,19)	1.3969	A23	A(13,14,16)	110.59	D23	D(9,4,5,6)	-17.97
R24	R(18,20)	1.3936	A24	A(12,15,16)	100.92	D24	D(9,4,5,10)	-0.21
R25	R(18,21)	1.0869	A25	A(12,15,28)	111.39	D25	D(4,5,6,1)	-0.38
R26	R(19,22)	1.3924	A26	A(12,15,31)	115.52	D26	D(4,5,6,11)	179.33
R27	R(19,23)	1.087	A27	A(16,15,28)	109.01	D27	D(10,5,6,1)	-179.90
R28	R(20,24)	1.3933	A28	A(16,15,31)	115.13	D28	D(10,5,6,11)	-0.02
R29	R(20,25)	1.0852	A29	A(28,15,31)	104.92	D29	D(1,12,13,14)	176.18
R30	R(22,24)	1.3946	A30	A(14,16,15)	103.03	D30	D(15,12,13,14)	8.67
R31	R(22,26)	1.0852	A31	A(14,16,17)	111.06	D31	D(1,12,15,16)	179.89
R32	R(24,27)	1.0852	A32	A(14,16,32)	108.33	D32	D(1,12,15,28)	-6.45
R33	R(28,29)	1.2167	A33	A(15,16,17)	112.62	D33	D(1,12,15,31)	55.04

R34	R(28,30)	1,2105	A34	A(15,16,32)	111.40	D34	D(13,12,15,16)	-13.36
			A35	A(17,16,32)	110.13	D35	D(13,12,15,28)	102.22
			A36	A(16,17,18)	119.74	D36	D(13,12,15,31)	-138.21
			A37	A(16,17,19)	120.47	D37	D(12,13,14,16)	1.06
			A38	A(18,17,19)	119.74	D38	D(13,14,16,15)	-9.19
			A39	A(17,18,20)	120.19	D39	D(13,14,16,17)	111.62
			A40	A(17,18,21)	119.74	D40	D(13,14,16,32)	-127.31
			A41	A(20,18,21)	120.07	D41	D(12,15,16,14)	12.94
			A42	A(17,19,22)	120.01	D42	D(12,15,16,17)	-106.80
			A43	A(17,19,23)	119.93	D43	D(12,15,16,32)	128.89
			A44	A(22,19,23)	120.06	D44	D(28,15,16,14)	-104.40
			A45	A(18,20,24)	119.99	D45	D(28,15,16,17)	135.86
			A46	A(18,20,25)	119.79	D46	D(28,15,16,32)	0.12
			A47	A(24,20,25)	120.22	D47	D(31,15,16,14)	138.05
			A48	A(19,22,24)	120.15	D48	D(31,15,16,17)	18.31
			A49	A(19,22,26)	119.73	D49	D(31,15,16,32)	-106.00
			A50	A(24,22,26)	120.11	D50	D(12,15,28,29)	1.50
			A51	A(20,24,22)	119.92	D51	D(12,15,28,30)	-32.39
			A52	A(20,24,27)	120.05	D52	D(16,15,28,29)	-99.08
			A53	A(22,24,27)	120.03	D53	D(16,15,28,30)	78.11
			A54	A(15,28,29)	115.70	D54	D(31,15,28,29)	24.74
			A55	A(15,28,30)	117.54	D55	D(31,15,28,30)	-158.07
			A56	A(29,28,30)	126.69	D56	D(14,16,17,18)	1.42
						D57	D(14,16,17,19)	-40.27
						D58	D(15,16,17,18)	-102.78
						D59	D(15,16,17,19)	74.70
						D60	D(32,16,17,18)	22.23
						D61	D(32,16,17,19)	-160.28
						D62	D(16,17,18,20)	177.35
						D63	D(16,17,18,21)	-2.63
						D64	D(19,17,18,20)	-0.16
						D65	D(19,17,18,21)	179.86
						D66	D(16,17,19,22)	-177.33
						D67	D(16,17,19,23)	3.48
						D68	D(18,17,19,22)	0.16
						D69	D(18,17,19,23)	-179.03
						D70	D(17,18,20,24)	0.04
						D71	D(17,18,20,25)	179.79
						D72	D(21,18,20,24)	-179.98
						D73	D(21,18,20,25)	-0.23
						D74	D(17,19,22,24)	-0.05
						D75	D(17,19,22,26)	-179.73
						D76	D(23,19,22,24)	17.91
						D77	D(23,19,22,26)	-0.55
						D78	D(18,20,24,22)	0.07
						D79	D(18,20,24,27)	17.98
						D80	D(25,20,24,22)	-179.68
						D81	D(25,20,24,27)	0.00
						D82	D(19,22,24,20)	-0.01
						D83	D(19,22,24,27)	-179.78
						D84	D(26,22,24,20)	179.62
						D85	D(26,22,24,27)	-0.10

A continuación se presentan algunas representaciones de las comparaciones de los principales valores expuestos en el trabajo. En primer lugar la comparación de los valores del enlace N12-C15, para la vía 1,4.



A continuación el enlace N14-C16.



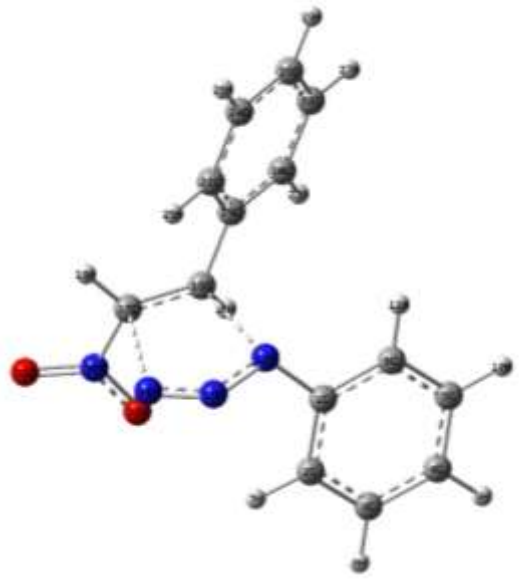
-Estado de Transición vía 1,5 aproximación *endo*: TS-15n.

NºR	Átomos	d(A)	NºA	Átomos	A()	NºD	Átomos	D ()
R1	R(1,2)	1.398	A1	A(2,1,6)	120.63	D1	D(6,1,2,3)	0.1658
R2	R(1,6)	1.3953	A2	A(2,1,12)	122.80	D2	D(6,1,2,7)	-179.3032
R3	R(1,12)	1.4145	A3	A(6,1,12)	116.26	D3	D(12,1,2,3)	173.6361
R4	R(2,3)	1.3905	A4	A(1,2,3)	119.33	D4	D(12,1,2,7)	-5.8328
R5	R(2,7)	1.0865	A5	A(1,2,7)	119.85	D5	D(2,1,6,5)	0.3406
R6	R(3,4)	1.3959	A6	A(3,2,7)	120.82	D6	D(2,1,6,11)	-179.7426
R7	R(3,8)	1.0853	A7	A(2,3,4)	120.37	D7	D(12,1,6,5)	-17.3541
R8	R(4,5)	1.3941	A8	A(2,3,8)	119.52	D8	D(12,1,6,11)	6.3758
R9	R(4,9)	1.085	A9	A(4,3,8)	120.10	D9	D(2,1,12,13)	27.0779
R10	R(5,6)	1.3921	A10	A(3,4,5)	119.93	D10	D(2,1,12,15)	-89.7307
R11	R(5,10)	1.0852	A11	A(3,4,9)	119.99	D11	D(2,1,12,32)	120.0802
R12	R(6,11)	1.0857	A12	A(5,4,9)	120.09	D12	D(6,1,12,13)	-159.1861
R13	R(12,13)	1.2693	A13	A(4,5,6)	120.17	D13	D(6,1,12,15)	84.0052
R14	R(12,15)	2.0948	A14	A(4,5,10)	120.16	D14	D(6,1,12,32)	53.6557
R15	R(12,32)	2.3456	A15	A(6,5,10)	119.67	D15	D(1,2,3,4)	-0.0065
R16	R(13,14)	1.1606	A16	A(1,6,5)	119.56	D16	D(1,2,3,8)	179.9957
R17	R(13,15)	2.5916	A17	A(1,6,11)	118.90	D17	D(7,2,3,4)	178.8136
R18	R(13,16)	2.5561	A18	A(5,6,11)	121.53	D18	D(7,2,3,8)	-0.5406
R19	R(14,16)	2.1248	A19	A(1,12,13)	119.91	D19	D(2,3,4,5)	0.6276
R20	R(14,28)	2.6987	A20	A(1,12,15)	115.81	D20	D(2,3,4,9)	-17.9666
R21	R(14,31)	2.4521	A21	A(1,12,32)	113.78	D21	D(8,3,4,5)	179.9781
R22	R(15,16)	1.3902	A22	A(13,12,32)	117.73	D22	D(8,3,4,9)	-0.3155
R23	R(15,17)	1.473	A23	A(12,13,14)	138.01	D23	D(3,4,5,6)	-0.1141
R24	R(15,32)	1.0856	A24	A(12,13,16)	82.81	D24	D(3,4,5,10)	179.4615
R25	R(16,28)	1.4519	A25	A(14,13,15)	86.16	D25	D(9,4,5,6)	-179.8202
R26	R(16,31)	1.0797	A26	A(13,14,28)	106.11	D26	D(9,4,5,10)	-0.2446
R27	R(17,18)	1.4003	A27	A(13,14,31)	117.02	D27	D(4,5,6,1)	-0.3654
R28	R(17,19)	1.4026	A28	A(28,14,31)	47.98	D28	D(4,5,6,11)	179.72
R29	R(18,20)	1.3917	A29	A(12,15,16)	100.00	D29	D(10,5,6,1)	-179.9431
R30	R(18,21)	1.0867	A30	A(12,15,17)	99.23	D30	D(10,5,6,11)	0.1423

R31	R(19,22)	1.3912	A31	A(13,15,17)	104.21	D31	D(1,12,13,14)	-142.9848
R32	R(19,23)	1.0868	A32	A(13,15,32)	110.70	D32	D(1,12,13,16)	-13.7086
R33	R(20,24)	1.394	A33	A(16,15,17)	120.94	D33	D(32,12,13,14)	2.9125
R34	R(20,25)	1.0852	A34	A(16,15,32)	117.43	D34	D(32,12,13,16)	8.8114
R35	R(22,24)	1.3949	A35	A(17,15,32)	118.12	D35	D(1,12,15,16)	149.8904
R36	R(22,26)	1.0854	A36	A(13,16,28)	103.45	D36	D(1,12,15,17)	25.9947
R37	R(24,27)	1.0853	A37	A(13,16,31)	11.40	D37	D(12,13,14,28)	-24.8918
R38	R(28,29)	1.2204	A38	A(14,16,15)	101.85	D38	D(12,13,14,31)	25.6999
R39	R(28,30)	1.2232	A39	A(15,16,28)	118.10	D39	D(15,13,14,28)	-38.5981
			A40	A(15,16,31)	125.03	D40	D(15,13,14,31)	11.9936
			A41	A(28,16,31)	111.77	D41	D(14,13,15,17)	-108.0184
			A42	A(15,17,18)	119.31	D42	D(14,13,15,32)	12.4001
			A43	A(15,17,19)	121.70	D43	D(12,13,16,28)	-98.5189
			A44	A(18,17,19)	118.82	D44	D(12,13,16,31)	139.8755
			A45	A(17,18,20)	120.69	D45	D(13,14,28,29)	-170.2221
			A46	A(17,18,21)	119.29	D46	D(13,14,28,30)	-35.3543
			A47	A(20,18,21)	120.02	D47	D(31,14,28,29)	77.6781
			A48	A(17,19,22)	120.47	D48	D(31,14,28,30)	-147.4541
			A49	A(17,19,23)	120.19	D49	D(12,15,16,14)	-16.4022
			A50	A(22,19,23)	119.34	D50	D(12,15,16,28)	87.2524
			A51	A(18,20,24)	120.04	D51	D(12,15,16,31)	-120.1401
			A52	A(18,20,25)	119.77	D52	D(17,15,16,14)	90.8008
			A53	A(24,20,25)	120.19	D53	D(17,15,16,28)	-165.5446
			A54	A(19,22,24)	120.21	D54	D(17,15,16,31)	-12.9372
			A55	A(19,22,26)	119.69	D55	D(32,15,16,14)	-110.7177
			A56	A(24,22,26)	120.10	D56	D(32,15,16,28)	-7.0631
			A57	A(20,24,22)	119.76	D57	D(32,15,16,31)	145.5443
			A58	A(20,24,27)	120.13	D58	D(12,15,17,18)	-89.2293
			A59	A(22,24,27)	120.11	D59	D(12,15,17,19)	85.8229
			A60	A(14,28,29)	107.15	D60	D(13,15,17,18)	-118.4645
			A61	A(14,28,30)	105.20	D61	D(13,15,17,19)	56.5877
			A62	A(16,28,29)	116.68	D62	D(16,15,17,18)	163.1518
			A63	A(16,28,30)	118.33	D63	D(16,15,17,19)	-2.1796
			A64	A(29,28,30)	124.98	D64	D(32,15,17,18)	4.8142
						D65	D(32,15,17,19)	-179.8664
						D66	D(13,16,28,29)	117.3853
						D67	D(13,16,28,30)	-61.1267
						D68	D(15,16,28,29)	-161.7779
						D69	D(15,16,28,30)	19.7101
						D70	D(31,16,28,29)	-5.7121
						D71	D(31,16,28,30)	175.7759
						D72	D(15,17,18,20)	-175.6741
						D73	D(15,17,18,21)	-3.6273
						D74	D(19,17,18,20)	0.4786
						D75	D(19,17,18,21)	-178.8227

D76	D(15,17,19,22)	-175.9542
D77	D(15,17,19,23)	3.0429
D78	D(18,17,19,22)	-0.8786
D79	D(18,17,19,23)	178.1185
D80	D(17,18,20,24)	0.0173
D81	D(17,18,20,25)	-179.6635
D82	D(21,18,20,24)	179.3136
D83	D(21,18,20,25)	-0.3673
D84	D(17,19,22,24)	0.7851
D85	D(17,19,22,26)	-179.8075
D86	D(23,19,22,24)	-178.2204
D87	D(23,19,22,26)	0.1187
D88	D(18,20,24,22)	-0.0123
D89	D(18,20,24,27)	-179.9276
D90	D(25,20,24,22)	179.5565
D91	D(25,20,24,27)	-0.0248
D92	D(19,22,24,20)	-0.2769
D93	D(19,22,24,27)	179.5277
D94	D(26,22,24,20)	-179.6818
D95	D(26,22,24,27)	0.1228

-Estado de Transición vía 1,5 aproximación *exo*: TS-15x.



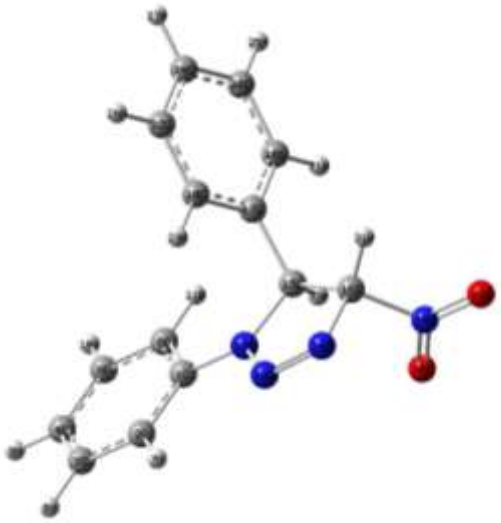
NºR	Átomos	d(A)	NºA	Átomos	A()	NºD	Átomos	D ()
R1	R(1,2)	1.40	A1	A(2,1,6)	121.11	D1	D(6,1,2,3)	1.59
R2	R(1,6)	1.39	A2	A(2,1,12)	122.39	D2	D(6,1,2,7)	-177.27
R3	R(1,12)	1.42	A3	A(6,1,12)	116.35	D3	D(12,1,2,3)	176.92
R4	R(2,3)	1.39	A4	A(1,2,3)	119.02	D4	D(12,1,2,7)	-1.95

R5	R(2,7)	1.09	A5	A(1,2,7)	119.88	D5	D(2,1,6,5)	-0.54
R6	R(3,4)	1.40	A6	A(3,2,7)	121.09	D6	D(2,1,6,11)	17.99
R7	R(3,8)	1.09	A7	A(2,3,4)	120.39	D7	D(12,1,6,5)	-176.13
R8	R(4,5)	1.39	A8	A(2,3,8)	119.49	D8	D(12,1,6,11)	4.34
R9	R(4,9)	1.09	A9	A(4,3,8)	120.11	D9	D(2,1,12,13)	2.78
R10	R(5,6)	1.39	A10	A(3,4,5)	120.05	D10	D(2,1,12,15)	-92.72
R11	R(5,10)	1.09	A11	A(3,4,9)	119.93	D11	D(2,1,12,16)	-88.08
R12	R(6,11)	1.09	A12	A(5,4,9)	120.02	D12	D(6,1,12,13)	-15.67
R13	R(12,13)	1.27	A13	A(4,5,6)	120.15	D13	D(6,1,12,15)	82.81
R14	R(12,15)	2.03	A14	A(4,5,10)	120.20	D14	D(6,1,12,16)	87.45
R15	R(12,16)	2.31	A15	A(6,5,10)	119.68	D15	D(1,2,3,4)	-1.46
R16	R(13,14)	1.16	A16	A(1,6,5)	119.26	D16	D(1,2,3,8)	17.95
R17	R(13,15)	2.58	A17	A(1,6,11)	119.04	D17	D(7,2,3,4)	177.38
R18	R(13,17)	2.55	A18	A(5,6,11)	121.70	D18	D(7,2,3,8)	-1.63
R19	R(14,17)	2.18	A19	A(1,12,13)	119.34	D19	D(2,3,4,5)	0.30
R20	R(14,18)	2.57	A20	A(1,12,15)	116.08	D20	D(2,3,4,9)	-179.53
R21	R(14,30)	2.61	A21	A(1,12,16)	88.40	D21	D(8,3,4,5)	179.30
R22	R(15,16)	1.09	A22	A(13,12,16)	113.17	D22	D(8,3,4,9)	-0.52
R23	R(15,17)	1.39	A23	A(12,13,14)	139.21	D23	D(3,4,5,6)	0.78
R24	R(15,19)	1.48	A24	A(12,13,17)	82.02	D24	D(3,4,5,10)	-179.97
R25	R(17,18)	1.08	A25	A(14,13,15)	89.09	D25	D(9,4,5,6)	-179.40
R26	R(17,30)	1.45	A26	A(13,14,18)	113.46	D26	D(9,4,5,10)	-0.15
R27	R(19,20)	1.40	A27	A(13,14,30)	103.37	D27	D(4,5,6,1)	-0.66
R28	R(19,21)	1.40	A28	A(18,14,30)	48.22	D28	D(4,5,6,11)	178.86
R29	R(20,22)	1.39	A29	A(12,15,17)	102.12	D29	D(10,5,6,1)	-179.91
R30	R(20,23)	1.09	A30	A(12,15,19)	100.40	D30	D(10,5,6,11)	-0.39
R31	R(21,24)	1.39	A31	A(13,15,16)	104.86	D31	D(1,12,13,14)	-138.66
R32	R(21,25)	1.09	A32	A(13,15,19)	114.22	D32	D(1,12,13,17)	-126.50
R33	R(22,26)	1.39	A33	A(16,15,17)	116.50	D33	D(16,12,13,14)	-36.78
R34	R(22,27)	1.09	A34	A(16,15,19)	117.03	D34	D(16,12,13,17)	-24.62
R35	R(24,26)	1.40	A35	A(17,15,19)	120.86	D35	D(1,12,15,17)	127.26
R36	R(24,28)	1.09	A36	A(13,17,18)	118.11	D36	D(1,12,15,19)	-107.79
R37	R(26,29)	1.09	A37	A(13,17,30)	97.26	D37	D(12,13,14,18)	-2.70
R38	R(30,31)	1.22	A38	A(14,17,15)	101.63	D38	D(12,13,14,30)	4.73
R39	R(30,32)	1,23	A39	A(15,17,18)	125.27	D39	D(15,13,14,18)	-10.86
			A40	A(15,17,30)	117.64	D40	D(15,13,14,30)	3.91
			A41	A(18,17,30)	112.85	D41	D(14,13,15,16)	-123.60
			A42	A(15,19,20)	119.46	D42	D(14,13,15,19)	106.99
			A43	A(15,19,21)	121.34	D43	D(12,13,17,18)	-12.48
			A44	A(20,19,21)	119.19	D44	D(12,13,17,30)	11.44
			A45	A(19,20,22)	120.43	D45	D(13,14,30,31)	171.78
			A46	A(19,20,23)	119.41	D46	D(13,14,30,32)	40.11
			A47	A(22,20,23)	120.16	D47	D(18,14,30,31)	-78.56
			A48	A(19,21,24)	120.34	D48	D(18,14,30,32)	149.77
			A49	A(19,21,25)	119.82	D49	D(12,15,17,14)	6.81
			A50	A(24,21,25)	119.82	D50	D(12,15,17,18)	115.77
			A51	A(20,22,26)	120.05	D51	D(12,15,17,30)	-89.11
			A52	A(20,22,27)	119.78	D52	D(16,15,17,14)	103.91
			A53	A(26,22,27)	120.17	D53	D(16,15,17,18)	-147.13
			A54	A(21,24,26)	120.17	D54	D(16,15,17,30)	7.98
			A55	A(21,24,28)	119.77	D55	D(19,15,17,14)	-103.28
			A56	A(26,24,28)	120.06	D56	D(19,15,17,18)	5.68

A57	A(22,26,24)	119.80
A58	A(22,26,29)	120.13
A59	A(24,26,29)	120.07
A60	A(14,30,31)	111.37
A61	A(14,30,32)	97.10
A62	A(17,30,31)	117.40
A63	A(17,30,32)	117.87
A64	A(31,30,32)	124.70

D57	D(19,15,17,30)	160.80
D58	D(12,15,19,20)	10.34
D59	D(12,15,19,21)	-75.55
D60	D(13,15,19,20)	130.15
D61	D(13,15,19,21)	-48.84
D62	D(16,15,19,20)	7.12
D63	D(16,15,19,21)	-171.86
D64	D(17,15,19,20)	-145.56
D65	D(17,15,19,21)	35.46
D66	D(13,17,30,31)	124.44
D67	D(13,17,30,32)	-53.71
D68	D(15,17,30,31)	-158.37
D69	D(15,17,30,32)	23.49
D70	D(18,17,30,31)	-0.25
D71	D(18,17,30,32)	-17.84
D72	D(15,19,20,22)	179.96
D73	D(15,19,20,23)	0.36
D74	D(21,19,20,22)	-1.03
D75	D(21,19,20,23)	179.36
D76	D(15,19,21,24)	-18.00
D77	D(15,19,21,25)	1.08
D78	D(20,19,21,24)	1.03
D79	D(20,19,21,25)	-177.90
D80	D(19,20,22,26)	0.39
D81	D(19,20,22,27)	-179.55
D82	D(23,20,22,26)	180.00
D83	D(23,20,22,27)	0.06
D84	D(19,21,24,26)	-0.40
D85	D(19,21,24,28)	-179.93
D86	D(25,21,24,26)	178.54
D87	D(25,21,24,28)	-1.00
D88	D(20,22,26,24)	0.26
D89	D(20,22,26,29)	179.94
D90	D(27,22,26,24)	-179.81
D91	D(27,22,26,29)	-0.12
D92	D(21,24,26,22)	-0.25
D93	D(21,24,26,29)	-179.94
D94	D(28,24,26,22)	179.28
D95	D(28,24,26,29)	-0.40

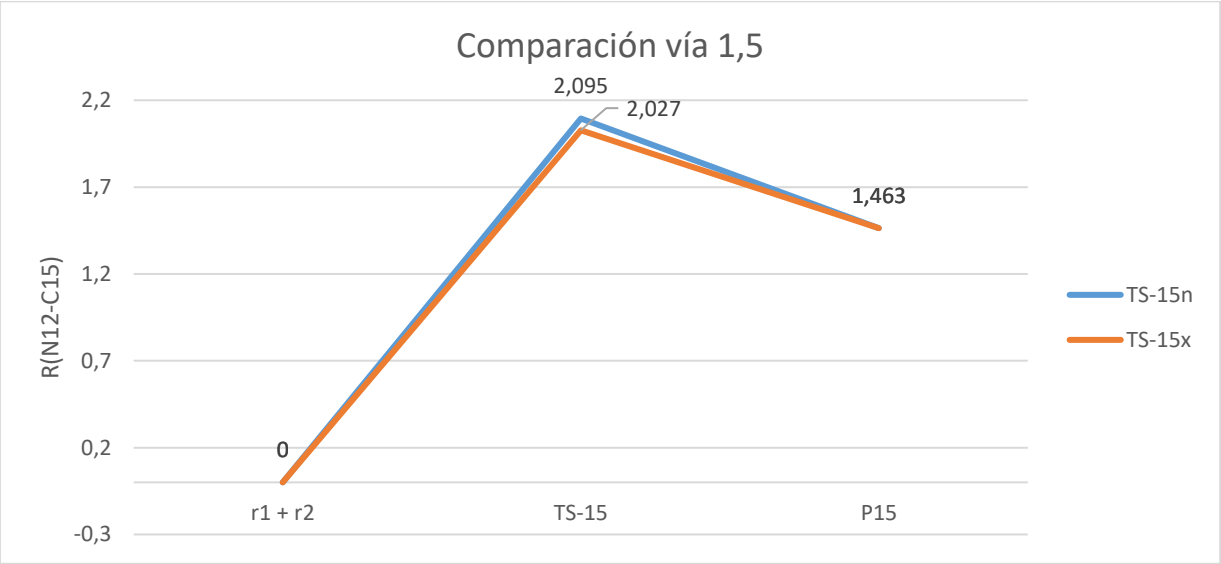
-Producto vía 1,5: P15.



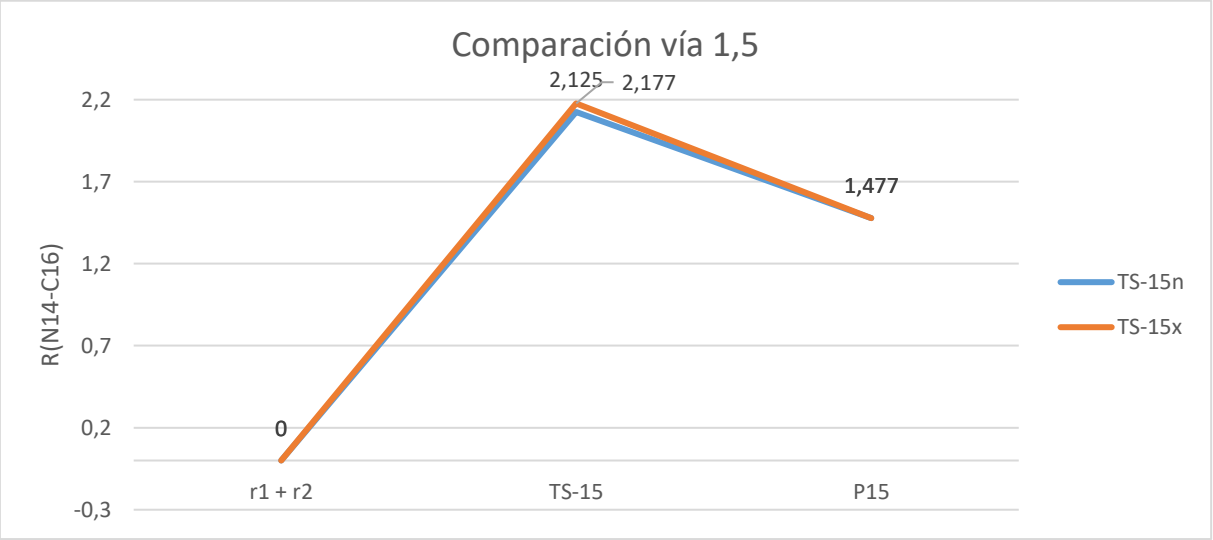
NºR	Átomos	d(A)	NºA	Átomos	A(º)	NºD	Átomos	D (º)
R1	R(1,2)	1.400	A1	A(2,1,6)	120.26	D1	D(6,1,2,3)	0.0046
R2	R(1,6)	1.398	A2	A(2,1,12)	120.32	D2	D(6,1,2,7)	179.5836
R3	R(1,12)	1.407	A3	A(6,1,12)	119.42	D3	D(12,1,2,3)	-179.8469
R4	R(2,3)	1.390	A4	A(1,2,3)	119.30	D4	D(12,1,2,7)	-0.2680
R5	R(2,7)	1.083	A5	A(1,2,7)	119.73	D5	D(2,1,6,5)	-0.1293
R6	R(3,4)	1.396	A6	A(3,2,7)	120.97	D6	D(2,1,6,11)	179.2298
R7	R(3,8)	1.085	A7	A(2,3,4)	120.96	D7	D(12,1,6,5)	179.7235
R8	R(4,5)	1.391	A8	A(2,3,8)	118.98	D8	D(12,1,6,11)	-0.9173
R9	R(4,9)	1.085	A9	A(4,3,8)	120.06	D9	D(2,1,12,13)	0.0381
R10	R(5,6)	1.393	A10	A(3,4,5)	119.24	D10	D(2,1,12,15)	-179.8033
R11	R(5,10)	1.085	A11	A(3,4,9)	120.38	D11	D(6,1,12,13)	-179.8147
R12	R(6,11)	1.085	A12	A(5,4,9)	120.38	D12	D(6,1,12,15)	0.3439
R13	R(12,13)	1.334	A13	A(4,5,6)	120.70	D13	D(1,2,3,4)	0.0668
R14	R(12,15)	1.463	A14	A(4,5,10)	120.25	D14	D(1,2,3,8)	179.8377
R15	R(13,14)	1.250	A15	A(6,5,10)	119.05	D15	D(7,2,3,4)	-179.5068
R16	R(14,16)	1.477	A16	A(1,6,5)	119.54	D16	D(7,2,3,8)	0.2640
R17	R(15,16)	1.534	A17	A(1,6,11)	120.68	D17	D(2,3,4,5)	-0.0123
R18	R(15,17)	1.514	A18	A(5,6,11)	119.78	D18	D(2,3,4,9)	179.9082
R19	R(15,32)	1.095	A19	A(1,12,13)	121.48	D19	D(8,3,4,5)	-179.7807
R20	R(16,28)	1.517	A20	A(1,12,15)	126.45	D20	D(8,3,4,9)	0.1397
R21	R(16,31)	1.089	A21	A(13,12,15)	112.07	D21	D(3,4,5,6)	-0.1151
R22	R(17,18)	1.395	A22	A(12,13,14)	113.85	D22	D(3,4,5,10)	-179.9598
R23	R(17,19)	1.396	A23	A(13,14,16)	108.94	D23	D(9,4,5,6)	179.9645
R24	R(18,20)	1.394	A24	A(12,15,16)	98.86	D24	D(9,4,5,10)	0.1198
R25	R(18,21)	1.088	A25	A(12,15,17)	113.24	D25	D(4,5,6,1)	0.1855
R26	R(19,22)	1.393	A26	A(12,15,32)	109.84	D26	D(4,5,6,11)	-179.1795
R27	R(19,23)	1.087	A27	A(16,15,17)	112.53	D27	D(10,5,6,1)	-179.968
R28	R(20,24)	1.394	A28	A(16,15,32)	110.48	D28	D(10,5,6,11)	0.6670
R29	R(20,25)	1.085	A29	A(17,15,32)	111.29	D29	D(1,12,13,14)	177.2869
R30	R(22,24)	1.395	A30	A(14,16,15)	105.67	D30	D(15,12,13,14)	-2.8508
R31	R(22,26)	1.085	A31	A(14,16,28)	105.79	D31	D(1,12,15,16)	-173.7031
R32	R(24,27)	1.085	A32	A(14,16,31)	111.64	D32	D(1,12,15,17)	67.0288
R33	R(28,29)	1.212	A33	A(15,16,28)	112.04	D33	D(1,12,15,32)	-58.0725
R34	R(28,30)	1.216	A34	A(15,16,31)	115.71	D34	D(13,12,15,16)	6.4428
			A35	A(28,16,31)	105.65	D35	D(13,12,15,17)	-112.8252
			A36	A(15,17,18)	119.54	D36	D(13,12,15,32)	122.0734

A37	A(15,17,19)	120.65	D37	D(12,13,14,16)	-2.6028
A38	A(18,17,19)	119.77	D38	D(13,14,16,15)	6.6266
A39	A(17,18,20)	120.19	D39	D(13,14,16,28)	-112.3443
A40	A(17,18,21)	119.78	D40	D(13,14,16,31)	133.2103
A41	A(20,18,21)	120.03	D41	D(12,15,16,14)	-7.3936
A42	A(17,19,22)	120.00	D42	D(12,15,16,28)	107.3415
A43	A(17,19,23)	119.80	D43	D(12,15,16,31)	-131.4625
A44	A(22,19,23)	120.20	D44	D(17,15,16,14)	112.4010
A45	A(18,20,24)	119.97	D45	D(17,15,16,28)	-132.8640
A46	A(18,20,25)	119.82	D46	D(17,15,16,31)	-116.6790
A47	A(24,20,25)	120.21	D47	D(32,15,16,14)	-122.5321
A48	A(19,22,24)	120.17	D48	D(32,15,16,28)	-7797.0000
A49	A(19,22,26)	119.73	D49	D(32,15,16,31)	113.3990
A50	A(24,22,26)	120.11	D50	D(12,15,17,18)	-149.2379
A51	A(20,24,22)	119.90	D51	D(12,15,17,19)	32.9789
A52	A(20,24,27)	120.05	D52	D(16,15,17,18)	99.6946
A53	A(22,24,27)	120.05	D53	D(16,15,17,19)	-78.0887
A54	A(16,28,29)	116.73	D54	D(32,15,17,18)	-24.9242
A55	A(16,28,30)	116.88	D55	D(32,15,17,19)	157.2926
A56	A(29,28,30)	126.37	D56	D(14,16,28,29)	-101.2566
			D57	D(14,16,28,30)	77.0911
			D58	D(15,16,28,29)	144.0758
			D59	D(15,16,28,30)	-37.5764
			D60	D(31,16,28,29)	17.2474
			D61	D(31,16,28,30)	-164.4048
			D62	D(15,17,18,20)	-177.6072
			D63	D(15,17,18,21)	2.6462
			D64	D(19,17,18,20)	0.1958
			D65	D(19,17,18,21)	-179.5508
			D66	D(15,17,19,22)	177.6256
			D67	D(15,17,19,23)	-3.2109
			D68	D(18,17,19,22)	-0.1524
			D69	D(18,17,19,23)	179.0111
			D70	D(17,18,20,24)	-0.1033
			D71	D(17,18,20,25)	-179.7785
			D72	D(21,18,20,24)	179.6427
			D73	D(21,18,20,25)	-0.0325
			D74	D(17,19,22,24)	0.0169
			D75	D(17,19,22,26)	179.7505
			D76	D(23,19,22,24)	-179.1432
			D77	D(23,19,22,26)	0.5903
			D78	D(18,20,24,22)	-0.0328
			D79	D(18,20,24,27)	-179.7382
			D80	D(25,20,24,22)	179.6411
			D81	D(25,20,24,27)	-0.0642
			D82	D(19,22,24,20)	0.0760
			D83	D(19,22,24,27)	179.7813
			D84	D(26,22,24,20)	-179.6565
			D85	D(26,22,24,27)	0.0488

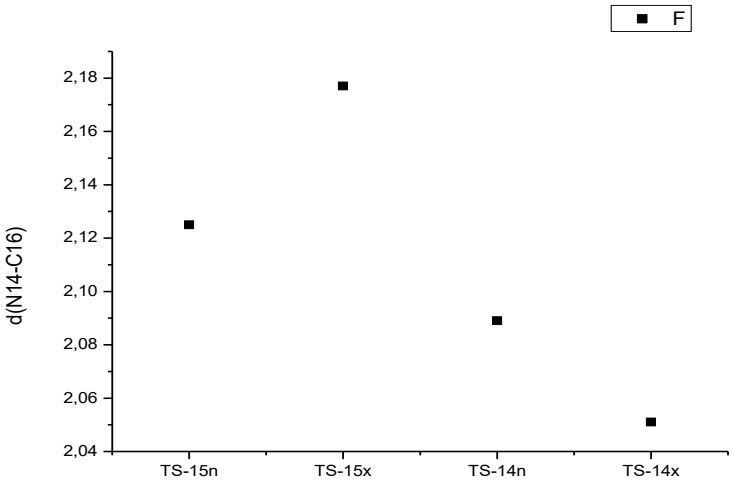
A continuación se continúan con las representaciones de las comparaciones de los principales valores expuestos en el trabajo. En primer lugar la comparación de los valores del enlace N12-C15, para la vía 1,5.



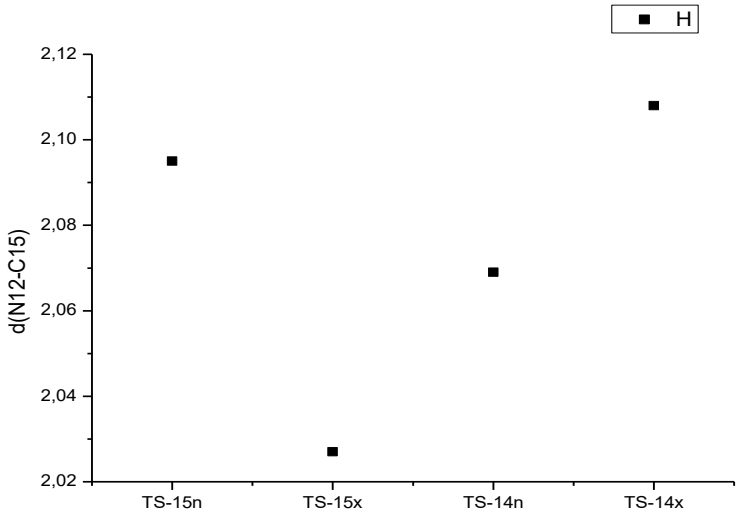
Para el enlace N14-C16.



Finalmente se comparan los resultados obtenidos entre las diferentes vías. Para el enlace N14-C16.



Para el enlace N12-C15.



6.2. Anexo II.

A continuación se adjuntan los resultados obtenidos en las cargas y los calculo realizados para obtener las GEDTs para los diferentes niveles y disolventes.

-Para el método M062X/6-31+G(d,p) en fase gas.

TS-14n

TS-14n

átomo	Nº	NBO dipolo	átomo	Nº	NBO dispola
C	1	0.1084	C	15	-0.0924
C	2	-0.2694	C	16	-0.2857
C	3	-0.2362	C	17	-0.0729
C	4	-0.2512	C	18	-0.2216
C	5	-0.2334	C	19	-0.2390
C	6	-0.2493	C	20	-0.2388
H	7	0.2620	H	21	0.2536
H	8	0.2589	C	22	-0.2388
H	9	0.2575	H	23	0.2451
H	10	0.2607	C	24	-0.2468
H	11	0.2781	H	25	0.2562
N	12	-0.2909	H	26	0.2555
N	13	0.1651	H	27	0.2550
N	14	-0.0058	N	28	0.5277
			O	29	-0.4049
			O	30	-0.3995
			H	31	0.2862
			H	32	0.3065
	Suma (NBOs)	0.05471		Suma (NBOs)	-0.05469

GEDT 2E-05

TS-14x

TS-14x

átomo	Nº	NBO dipolo	átomo	Nº	NBO dispola
C	1	0.09127	C	15	-0.08913
C	2	-0.24396	C	16	-0.28151
C	3	-0.23551	H	17	0.3064
C	4	-0.23722	H	18	0.28937
C	5	-0.23883	N	19	0.51275
C	6	-0.22765	O	20	-0.39385
H	7	0.26522	O	21	-0.42029
H	8	0.25938	C	22	-0.07464
H	9	0.25653	C	23	-0.22184
H	10	0.25788	C	24	-0.23749
H	11	0.26213	C	25	-0.2396
N	12	-0.29406	H	26	0.25296

N	13	0.16364	C	27	-0.23923
N	14	-0.01414	H	28	0.25159
			C	29	-0.24606
			H	30	0.25573
			H	31	0.25547
			H	32	0.25472
	Suma (NBOs)	0.06468		Suma (NBOs)	-0.06465
		GEDT	3E-05		

TS-15n

TS-15n

átomo	Nº	NBO dipolo	átomo	Nº	NBO dispola
C	1	0.10962	C	15	-0.19484
C	2	-0.24872	C	16	-0.17347
C	3	-0.23494	C	17	-0.0929
C	4	-0.24654	C	18	-0.21226
C	5	-0.24106	C	19	-0.23197
C	6	-0.24119	C	20	-0.23812
H	7	0.25883	H	21	0.25455
H	8	0.25817	C	22	-0.24207
H	9	0.25639	H	23	0.25097
H	10	0.25785	C	24	-0.23738
H	11	0.26662	H	25	0.25761
N	12	-0.29046	H	26	0.25674
N	13	0.17343	H	27	0.25585
N	14	-0.0203	N	28	0.51602
			O	29	-0.39883
			O	30	-0.42079
			H	31	0.28814
			H	32	0.30502
	Suma (NBOs)	0.0577		Suma (NBOs)	-0.05773
		GEDT	-3E-05		

TS-15x

TS-15x

átomo	Nº	NBO dipolo	átomo	Nº	NBO dispola
C	1	0.10451	C	15	-0.19614
C	2	-0.24265	H	16	0.30001
C	3	-0.23608	C	17	-0.1814
C	4	-0.24461	H	18	0.28844
C	5	-0.24169	C	19	-0.07466
C	6	-0.24408	C	20	-0.22691
H	7	0.26977	C	21	-0.22645
H	8	0.26059	C	22	-0.24244

H	9	0.25699	H	23	0.25442
H	10	0.25766	C	24	-0.23889
H	11	0.26803	H	25	0.25094
N	12	-0.29032	C	26	-0.2431
N	13	0.18043	H	27	0.25646
N	14	-0.00721	H	28	0.25712
			H	29	0.25576
			N	30	0.51622
			O	31	-0.39453
			O	32	-0.44618
	Suma (NBOs)	0.09134		Suma (NBOs)	-0.09133
			GEDT	1E-05	

-Para el método M062X/6-311+G(d,p) en agua.

TS-14n

TS-14n

átomo	Nº	NBO dipolo	átomo	Nº	NBO dispola
N	12	-0.30703	N	28	0.51726
N	13	0.16967	C	15	-0.04174
N	14	-0.02494	C	16	-0.23255
C	1	0.111460	C	17	-0.08196
C	2	-0.234040	C	18	-0.19256
C	6	-0.220700	C	19	-0.20967
C	5	-0.197320	C	20	-0.20643
C	3	-0.196200	C	22	-0.20351
C	4	-0.213550	C	24	-0.21078
H	7	0.235790	H	21	0.22598
H	8	0.229820	H	23	0.21892
H	9	0.227730	H	25	0.22589
H	10	0.228950	H	26	0.22608
H	11	0.240350	H	27	0.22504
			H	31	0.25696
			H	32	0.27176
			O	29	-0.41888
			O	30	-0.41978
	Suma (NBOs)	0.04999		Suma (NBOs)	-0.04997
			GEDT	2E-05	

TS-14x

TS-14x

átomo	Nº	NBO dipolo	átomo	Nº	NBO dispola
N	12	-0.300580	N	19	0.50013
N	13	0.165900	C	15	-0.0353

N	14	-0.032880	C	16	-0.22574
C	1	0.095510	C	22	-0.08389
C	2	-0.220250	C	23	-0.19247
C	3	-0.203030	C	24	-0.20744
C	4	-0.203530	C	25	-0.20718
C	5	-0.205020	C	27	-0.20466
C	6	-0.198680	C	29	-0.21036
H	7	0.236060	H	17	0.27062
H	8	0.229760	H	18	0.25931
H	9	0.227490	H	26	0.22606
H	10	0.229300	H	28	0.22381
H	11	0.237320	H	30	0.22584
			H	31	0.22588
			H	32	0.22486
			O	20	-0.41573
			O	21	-0.43107
	Suma (NBOs)	0.05737		Suma (NBOs)	-0.05733
			GEDT	4E-05	

TS-15n

TS-15n					
átomo	Nº	NBO dipolo	átomo	Nº	NBO dispola
C	1	0.10604	C	15	-0.13025
C	2	-0.2188	C	16	-0.13043
C	3	-0.20059	C	17	-0.10749
C	4	-0.20978	C	18	-0.1782
C	5	-0.2045	C	19	-0.19375
C	6	-0.20521	C	20	-0.20698
H	7	0.2322	C	22	-0.20581
H	8	0.22853	C	24	-0.19792
H	9	0.22657	H	21	0.22668
H	10	0.22813	H	23	0.22293
H	11	0.23594	H	25	0.22709
N	12	-0.30418	H	26	0.22695
N	13	0.17838	H	27	0.22566
N	14	-0.03736	H	31	0.25822
			H	32	0.26884
			N	28	0.50899
			O	29	-0.42901
			O	30	-0.44089
	Suma (NBOs)	0.05537		Suma (NBOs)	-0.05537
			GEDT	-1.5959E-16	

TS-15x

TS-15x					
átomo	Nº	NBO dipolo	átomo	Nº	NBO dispola
C	1	0.10977	C	15	-0.13321
C	2	-0.21819	C	17	-0.13875
C	3	-0.20088	C	19	-0.08756
C	4	-0.20844	C	20	-0.19082
C	5	-0.20269	C	21	-0.19729
C	6	-0.21025	C	22	-0.20746
H	7	0.23621	C	24	-0.20471
H	8	0.2291	C	26	-0.20588
H	9	0.22734	H	16	0.26402
H	10	0.22893	H	18	0.25937
H	11	0.23789	H	23	0.22709
N	12	-0.30235	H	25	0.22283
N	13	0.18737	H	27	0.22665
N	14	-0.02071	H	28	0.2264
			H	29	0.22531
			N	30	0.50989
			O	31	-0.42749
			O	32	-0.4615
	Suma (NBOs)	0.0931		Suma (NBOs)	-0.09311
		GEDT	-1E-05		

-Para el método M062X/6-311+G(d,p) en ACN.

TS-14n

TS-14n					
átomo	Nº	NBO dipolo	átomo	Nº	NBO dispola
C	1	0.11506	C	15	-0.04105
C	2	-0.23591	C	16	-0.23446
C	3	-0.20573	C	17	-0.0836
C	4	-0.22269	C	18	-0.19978
C	5	-0.20671	C	19	-0.21512
C	6	-0.22526	C	20	-0.21584
H	7	0.24345	C	22	-0.21321
H	8	0.23637	C	24	-0.21967
H	9	0.23404	H	21	0.23392
H	10	0.23567	H	23	0.23133
H	11	0.24484	H	25	0.2323
N	12	-0.30687	H	26	0.23227
N	13	0.17102	H	27	0.23129
N	14	-0.03768	H	31	0.2681
			H	32	0.27781
			N	28	0.51515

			O	29	-0.41864
			O	30	-0.42036
	Suma (NBOs)	0.0396		Suma (NBOs)	-0.03956
		GEDT	4E-05		

TS-14x

TS-14x

átomo	Nº	NBO dipolo	átomo	Nº	NBO dispola
C	1	0.09453	C	15	-0.03522
C	2	-0.2246	C	16	-0.22751
C	3	-0.21076	C	22	-0.08522
C	4	-0.21101	C	23	-0.19937
C	5	-0.21307	C	24	-0.21222
C	6	-0.20409	C	25	-0.21591
H	7	0.24368	C	27	-0.21358
H	8	0.23657	C	29	-0.21894
H	9	0.23405	H	17	0.27733
H	10	0.23603	H	18	0.26875
H	11	0.24414	H	26	0.23421
N	12	-0.30142	H	28	0.23213
N	13	0.16567	H	30	0.23245
N	14	-0.0439	H	31	0.23245
			H	32	0.23134
			N	19	0.49829
			O	20	-0.41458
			O	21	-0.43023
	Suma (NBOs)	0.04582		Suma (NBOs)	-0.04583
		GEDT	-1E-05		

TS-15n

TS-15n

átomo	Nº	NBO dipolo	átomo	Nº	NBO dispola
C	1	0.10543	C	15	-0.13141
C	2	-0.22702	C	16	-0.13096
C	3	-0.20965	C	17	-0.10798
C	4	-0.2178	C	18	-0.18581
C	5	-0.21275	C	19	-0.19746
C	6	-0.21082	C	20	-0.21796
H	7	0.24129	C	22	-0.21614
H	8	0.23606	C	24	-0.20691
H	9	0.23358	H	21	0.23483
H	10	0.23539	H	23	0.23317
H	11	0.24345	H	25	0.2341
N	12	-0.30544	H	26	0.23353

N	13	0.1789	H	27	0.23252
N	14	-0.04645	H	31	0.26816
			H	32	0.27552
			N	28	0.50638
			O	29	-0.42797
			O	30	-0.43979
	Suma (NBOs)	0.04417		Suma (NBOs)	-0.04418
			GEDT	-1E-05	

TS-15x

TS-15x					
átomo	Nº	NBO dipolo	átomo	Nº	NBO dispola
C	1	0.11031	C	15	-0.13464
C	2	-0.22373	C	17	-0.13834
C	3	-0.20854	C	19	-0.0859
C	4	-0.21654	C	20	-0.19708
C	5	-0.21079	C	21	-0.20373
C	6	-0.21631	C	22	-0.21724
H	7	0.2431	C	24	-0.21405
H	8	0.23613	C	26	-0.21499
H	9	0.23398	H	16	0.27122
H	10	0.23579	H	18	0.26829
H	11	0.24523	H	23	0.23504
N	12	-0.30357	H	25	0.23282
N	13	0.18698	H	27	0.23296
N	14	-0.03056	H	28	0.2327
			H	29	0.23166
			N	30	0.50743
			O	31	-0.4268
			O	32	-0.46082
	Suma (NBOs)	0.08148		Suma (NBOs)	-0.08147
			GEDT	1E-05	

-Para el método M062X/6-311+G(d,p) en cloroformo.

TS-14n

TS-14n					
átomo	Nº	NBO dipolo	átomo	Nº	NBO dispola
C	1	0.11535	C	15	-0.04084
C	2	-0.23659	C	16	-0.23608
C	3	-0.20213	C	17	-0.08033
C	4	-0.2191	C	18	-0.1946
C	5	-0.20153	C	19	-0.21368
C	6	-0.22252	C	20	-0.20962

H	7	0.23863	C	22	-0.20805
H	8	0.23137	C	24	-0.21504
H	9	0.22945	H	21	0.22853
H	10	0.2315	H	23	0.22438
H	11	0.24481	H	25	0.22773
N	12	-0.30587	H	26	0.22732
N	13	0.16846	H	27	0.22666
N	14	-0.02789	H	31	0.26173
			H	32	0.27508
			N	28	0.5145
			O	29	-0.41627
			O	30	-0.41537
	Suma (NBOs)	0.04394		Suma (NBOs)	-0.04395

GEDT -1E-05

TS-14x

TS-14x

átomo	Nº	NBO dipolo	átomo	Nº	NBO dispola
C	1	0.0957	C	15	-0.03555
C	2	-0.22012	C	16	-0.22899
C	3	-0.204	C	22	-0.08219
C	4	-0.20557	C	23	-0.19454
C	5	-0.20729	C	24	-0.20983
C	6	-0.20123	C	25	-0.21022
H	7	0.23955	C	27	-0.20834
H	8	0.23152	C	29	-0.21426
H	9	0.22882	H	17	0.27395
H	10	0.23056	H	18	0.26242
H	11	0.23799	H	26	0.22846
N	12	-0.3039	H	28	0.22649
N	13	0.16394	H	30	0.22764
N	14	-0.03483	H	31	0.22739
			H	32	0.22658
			N	19	0.49741
			O	20	-0.40943
			O	21	-0.42815
	Suma (NBOs)	0.05114		Suma (NBOs)	-0.05116

GEDT -2E-05

TS-15n

TS-15n					
átomo	Nº	NBO dipolo	átomo	Nº	NBO dispola
C	1	0.10791	C	15	-0.13401
C	2	-0.22174	C	16	-0.13036
C	3	-0.20284	C	17	-0.10538
C	4	-0.21325	C	18	-0.18154
C	5	-0.20819	C	19	-0.19777
C	6	-0.20906	C	20	-0.20901
H	7	0.23484	C	22	-0.21087
H	8	0.23051	C	24	-0.20219
H	9	0.22826	H	21	0.22859
H	10	0.22996	H	23	0.22655
H	11	0.23916	H	25	0.22928
N	12	-0.30379	H	26	0.22842
N	13	0.17691	H	27	0.22754
N	14	-0.04044	H	31	0.26269
			H	32	0.27142
			N	28	0.50583
			O	29	-0.42167
			O	30	-0.43574
	Suma (NBOs)	0.04824		Suma (NBOs)	-0.04822
		GEDT	2E-05		

TS-15x

TS-15x					
átomo	Nº	NBO dipolo	átomo	Nº	NBO dispola
C	1	0.1112	C	15	-0.13674
C	2	-0.21885	C	17	-0.13836
C	3	-0.20337	C	19	-0.08545
C	4	-0.21255	C	20	-0.19489
C	5	-0.20764	C	21	-0.19962
C	6	-0.21504	C	22	-0.21175
H	7	0.24084	C	24	-0.20807
H	8	0.23177	C	26	-0.21038
H	9	0.22905	H	16	0.26805
H	10	0.23045	H	18	0.26357
H	11	0.24205	H	23	0.2297
N	12	-0.30306	H	25	0.22625
N	13	0.18504	H	27	0.2284
N	14	-0.02525	H	28	0.22837
			H	29	0.22727
			N	30	0.50709
			O	31	-0.41968
			O	32	-0.45838

	Suma (NBOs)	0.08464		Suma (NBOs)	-0.08462
		GEDT	2E-05		

-Para el método M062X/6-311+G(d.p) en tolueno.

TS-14n

TS-14n

átomo	Nº	NBO dipolo	átomo	Nº	NBO dispola
N	12	-0.30563	N	28	0.51061
N	13	0.16573	C	15	-0.03987
N	14	-0.02027	C	16	-0.23841
C	1	0.1163	C	17	-0.07755
C	2	-0.23664	C	18	-0.1911
C	6	-0.19906	C	19	-0.2123
C	5	-0.21645	C	20	-0.20498
C	3	-0.19736	C	22	-0.20387
C	4	-0.22041	C	24	-0.2118
H	7	0.23448	H	21	0.22392
H	8	0.22693	H	23	0.21976
H	9	0.22538	H	25	0.22367
H	10	0.22766	H	26	0.22307
H	11	0.24411	H	27	0.2226
			H	31	0.25575
			H	32	0.27179
			O	29	-0.40949
			O	30	-0.40657
	Suma (NBOs)	0.04477		Suma (NBOs)	-0.04477
		GEDT	0		

TS-14x

TS-14x

átomo	Nº	NBO dipolo	átomo	Nº	NBO dispola
C	1	0.09763	C	15	-0.03484
C	2	-0.21572	C	16	-0.23145
C	3	-0.19999	C	22	-0.07933
C	4	-0.20227	C	23	-0.19131
C	5	-0.20345	C	24	-0.20813
C	6	-0.19733	C	25	-0.20579
H	7	0.23554	C	27	-0.20412
H	8	0.22702	C	29	-0.21114
H	9	0.22432	H	17	0.27049
H	10	0.22583	H	18	0.25595
H	11	0.23295	H	26	0.22364
N	12	-0.30608	H	28	0.22232

N	13	0.16206	H	30	0.22343
N	14	-0.02783	H	31	0.22305
			H	32	0.22244
			N	19	0.49364
			O	20	-0.39933
			O	21	-0.42221
	Suma (NBOs)	0.05268		Suma (NBOs)	-0.05269
			GEDT	-1E-05	

TS-15n

TS-15n

átomo	Nº	NBO dipolo	átomo	Nº	NBO dispola
C	1	0.11032	C	15	-0.13757
C	2	-0.21891	C	16	-0.12914
C	3	-0.19851	C	17	-0.10243
C	4	-0.21057	C	18	-0.17943
C	5	-0.20477	C	19	-0.19764
C	6	-0.20744	C	20	-0.20355
H	7	0.23034	C	22	-0.20689
H	8	0.22605	C	24	-0.19989
H	9	0.22400	H	21	0.22394
H	10	0.22558	H	23	0.22189
H	11	0.23573	H	25	0.22518
N	12	-0.30249	H	26	0.22421
N	13	0.17434	H	27	0.22337
N	14	-0.03533	H	31	0.25675
			H	32	0.26790
			N	28	0.50163
			O	29	-0.40960
			O	30	-0.42704
	Suma (NBOs)	0.04834		Suma (NBOs)	-0.04831
			GEDT	3E-05	

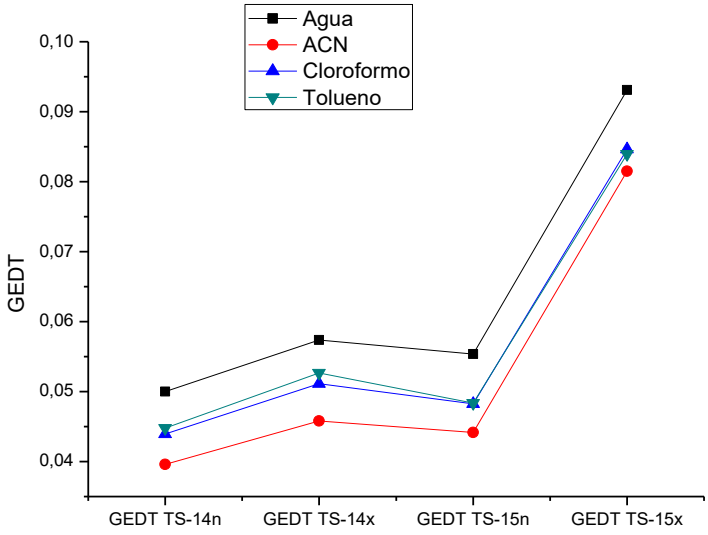
TS-15x

TS-15x

átomo	Nº	NBO dipolo	átomo	Nº	NBO dispola
C	1	0.11238	C	15	-0.13977
C	2	-0.21451	C	17	-0.13810
C	3	-0.19967	C	19	-0.08258
C	4	-0.20962	C	20	-0.19348
C	5	-0.20499	C	21	-0.19695
C	6	-0.21343	C	22	-0.20778
H	7	0.23806	C	24	-0.20363
H	8	0.22776	C	26	-0.20753
H	9	0.22477	H	16	0.26441

H	10	0.22585	H	18	0.25826
H	11	0.23903	H	23	0.22519
N	12	-0.30351	H	25	0.22160
N	13	0.18228	H	27	0.22425
N	14	-0.02047	H	28	0.22436
			H	29	0.22329
			N	30	0.50366
			O	31	-0.40605
			O	32	-0.45312
	Suma (NBOs)	0.08393		Suma (NBOs)	-0.08397
		GEDT	-4E-05		

A continuación, algunas representaciones gráficas referentes a los datos presentados. En este caso para los diferentes disolventes en el método M062X/6-311+G(d,p).



6.3. Anexo III.

En este anexo se regogen la totalidad de los parámetros geométricos obtenidos en la optimizacion de los componenetes de la reacion entre metilazida y nitropropeno, registrados con el método M062X/6-31+G(d,p) en fase gas. Además, se recogen las representaciones de dichos componentes y la codificacion correspomdiente, es decir, el numero que identifica a cada átomo.

Los parámetros adjuntados incluyen distancias de enlace (R), angulos entre los átomos (A) y planos diedricos entre los átomos (D).

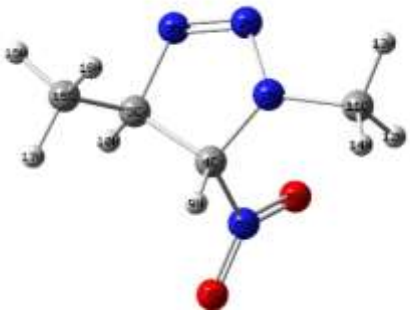
-Reactivo 1 (dipolo).

-Reactivo 2 (dipolarófilo).

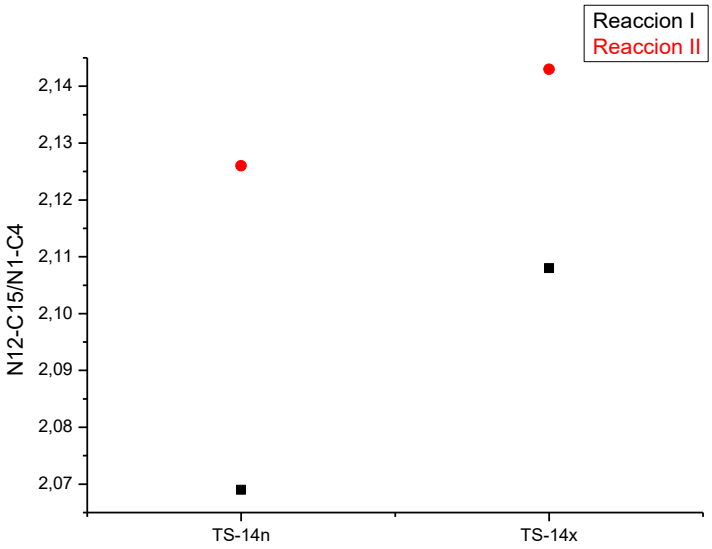
-Estado de Transición vía 1,4 aproximación *endo*: TS-14n.

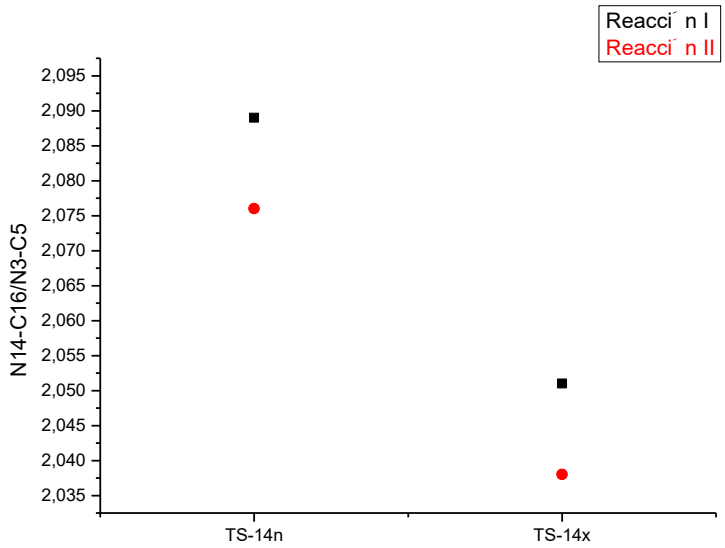
-Estado de Transición vía 1,4 aproximación *exo*: TS-14x.

-Producto vía 1,4: P14.



A continuación se representan gráficamente las diferencias que se han encontrado entre los valores de los nuevos enlaces formados en esta reacción con los obtenidos en la reacción original (Reacción I).

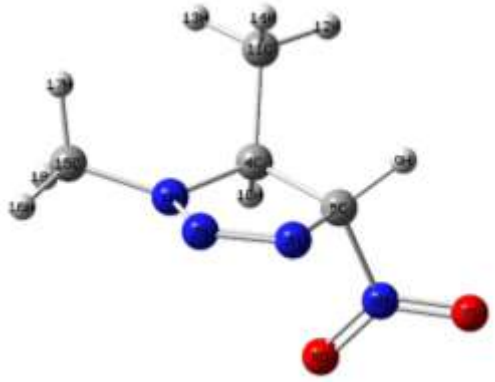




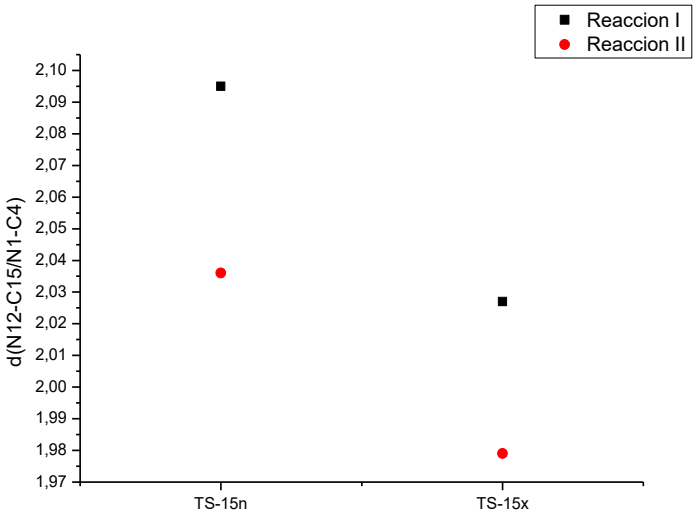
-Estado de Transición vía 1,5 aproximación *endo*: TS-15n.

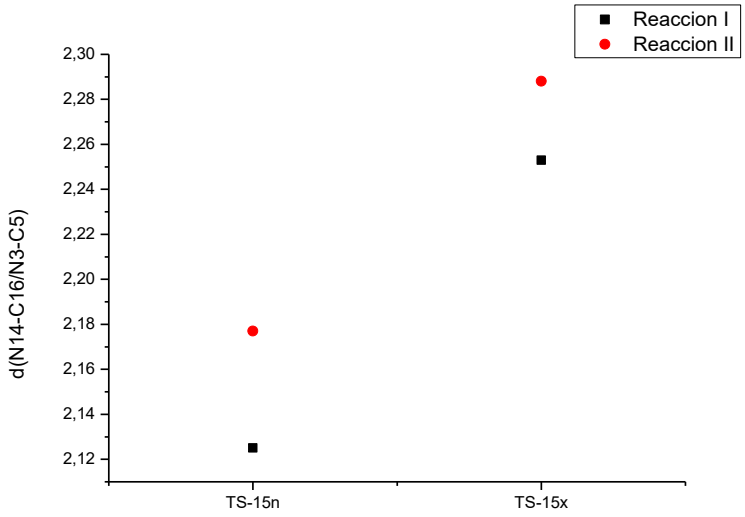
-Estado de Transición vía 1,5 aproximación *exo*: TS-15x.

-Producto vía 1,5: P15.



Se presentan las diferencias encontradas entre los enlaces, análogamente al caso anterior.





6.4. Anexo IV.

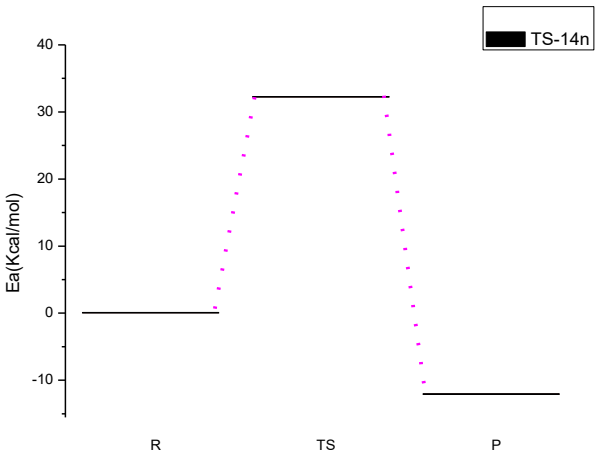
En el presente anexo se presentan las principales energías calculadas, para el método M062X/6-311+G(d,p) en los diferentes disolventes.

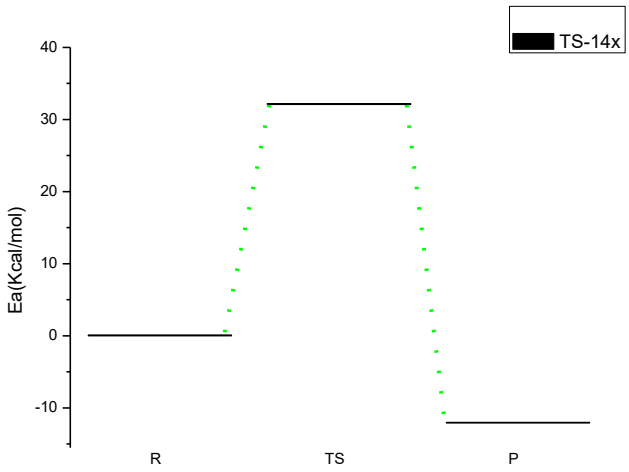
-Para el método M062X/6-311+G(d,p) en agua.

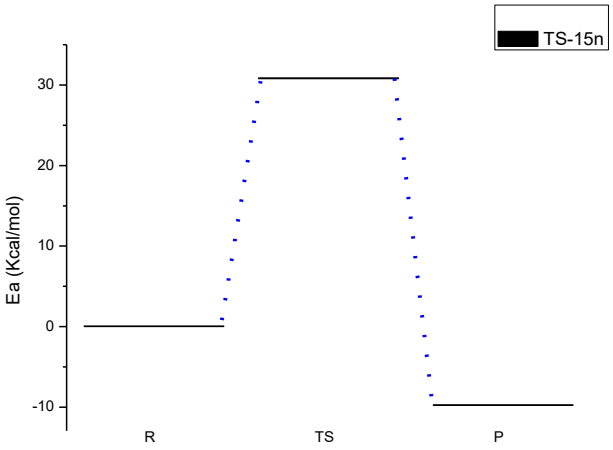
	G Hartrees	ΔG (Ea) Kcal/mol	Frec.i.	E(0) Hartrees	ΔE(0) kcal/mol	μ	H Hartrees	ΔH (Kcal/mol)
r1 (dipolo)	-395.705			-395.778		1.70	-395.67	
r2(dipolar)	-513.983			-514.084		5.93	-513.94	
r1+r2	-909.688	0.00		-909.862	0.00		-909.60	0.00
TS-14n	-909.635	33.5	-489.96	-909.833	18.5	5.37	-909.57	18.87
TS-14X	-909.635	33.0	-484.04	-909.834	18.0	2.50	-909.57	18.30
P14	-909.704	-10.1		-909.906	-27.4	4.05	-909.64	-24.61
TS-15n	-909.639	30.7	-476.49	-909.838	15.2	7.96	-909.58	15.50
TS-15X	-909.638	31.2	-478.62	-909.836	16.5	5.84	-909.57	16.86
P15	-909.701	-8.4		-909.904	-26.0	6.17	-909.64	-23.18

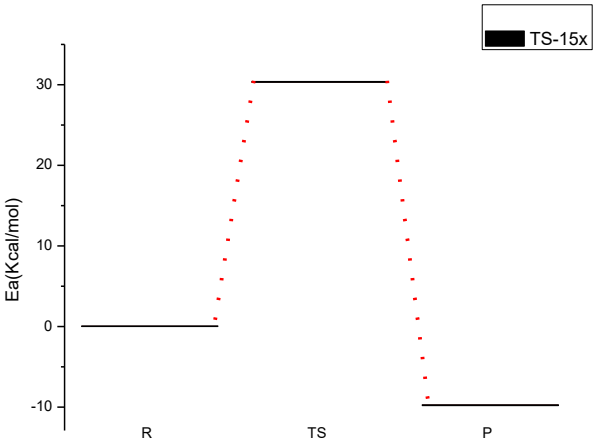
* Calculados obtenidos con el método M062X/6-311+G(d,p) y las condiciones de T= 298,15 K y P= 1atm con agua como disolvente.

A continuación, se adjuntan la representación de los diagramas de los perfiles de energía calculados para las diferentes posibilidades que ofrece el mecanismo.

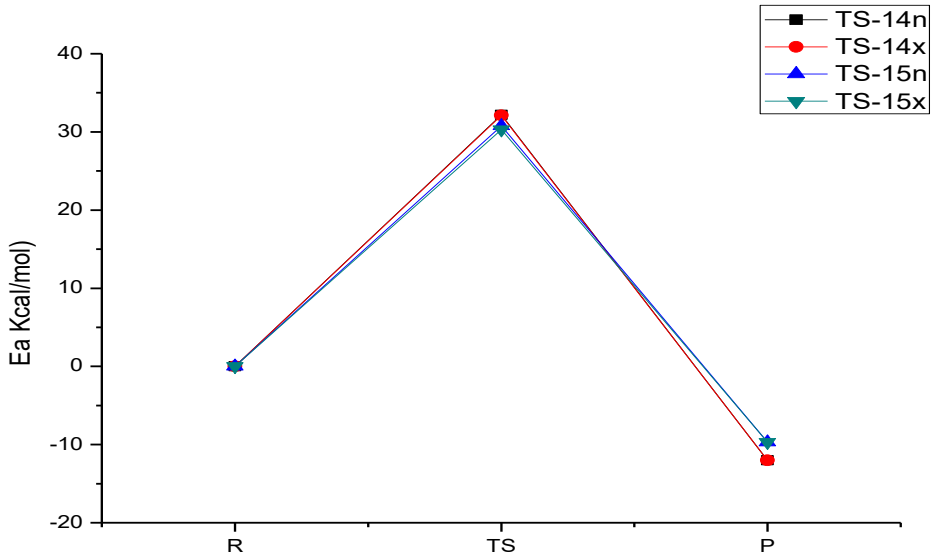



TS-14x
Ea(Kcal/mol)
40
30
20
10
0
-10
R
TS
P

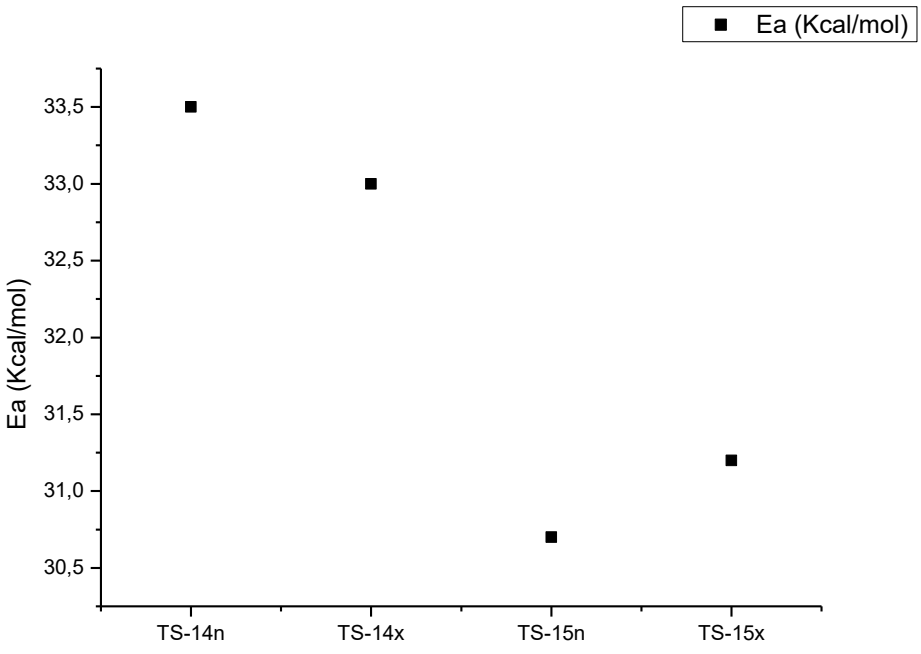

TS-15n
Ea (Kcal/mol)
30
20
10
0
-10
R
TS
P


TS-15x
Ea(Kcal/mol)
30
20
10
0
-10
R
TS
P

La representación gráfica de la comparación de los diferentes perfiles.



La comparación de las diferencias observadas para las energías de activación en los distintos estados de transición.

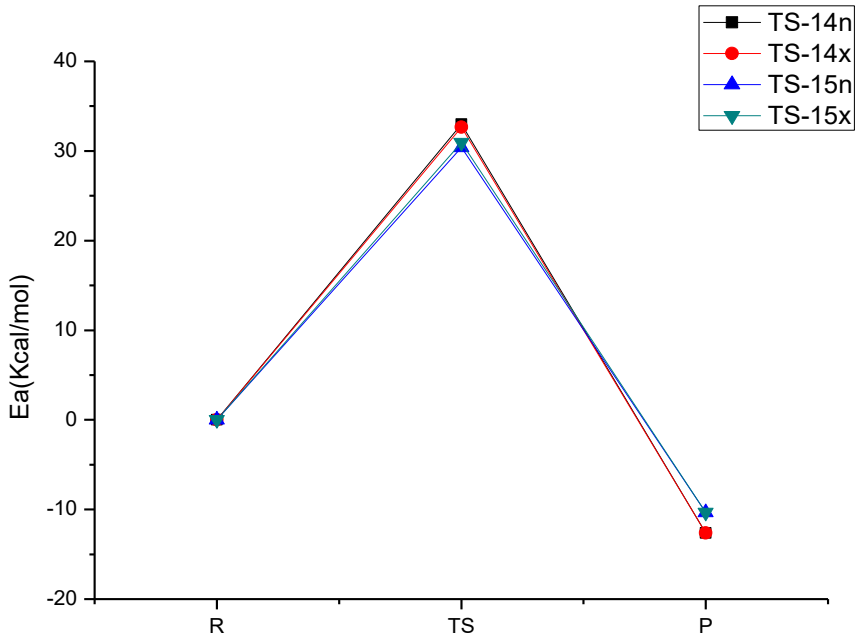


-Para el método M062X/6-311+G(d,p) en ACN.

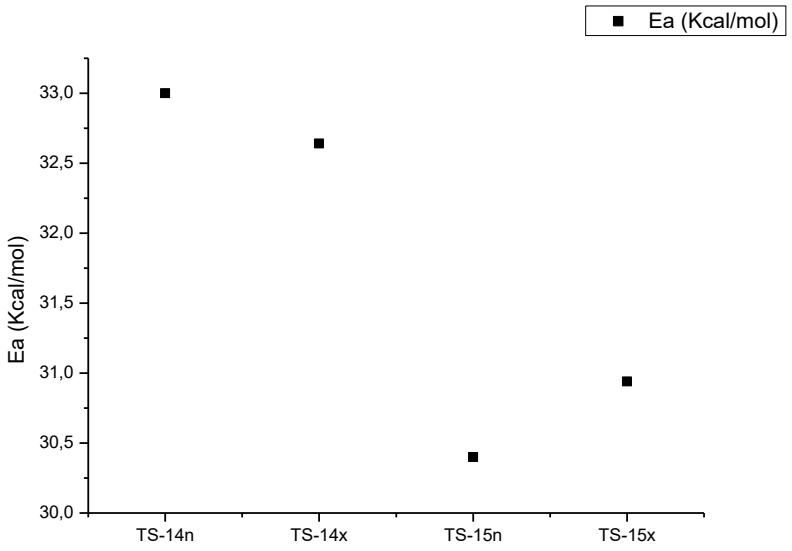
	G Hartrees	ΔG (Ea) Kcal/mol	Frec.i.	E(0) Hartrees	ΔE(0) kcal/mol	μ	H Hartrees	ΔH (Kcal/mol)
r1(dipolo)	-395.707			-395.780		1.70	-395.668	
r2(dipolar)	-513.990			-514.091		5.93	-513.943	
r1+r2	-909.697	0.00		-909.871	0.00		-909.611	0.00
TS-14n	-909.6	33.00	-489.96	-909.843	17.87	5.37	-909.582	18.34
TS-14X	-909.6	32.64	-484.04	-909.844	17.48	2.50	-909.582	17.90
P14	-909.7	-12.62		-909.919	-29.90	4.05	-909.654	-27.09
TS-15n	-909.6	30.40	-476.49	-909.848	14.81	7.96	-909.587	15.22
TS-15X	-909.6	30.94	-478.62	-909.846	16.10	5.84	-909.584	16.56
P15	-909.7	-10.32		-909.916	-28.01	6.17	-909.651	-25.10

* Calculados obtenidos con el método M062X/6-311+G(d,p) y las condiciones de T= 298,15 K y P= 1atm con acetonitrilo como disolvente.

A continuación, se representa la comparación energética de las diferentes vías.



La comparación de las diferencias observadas para las energías de activación en los distintos estados de transición.

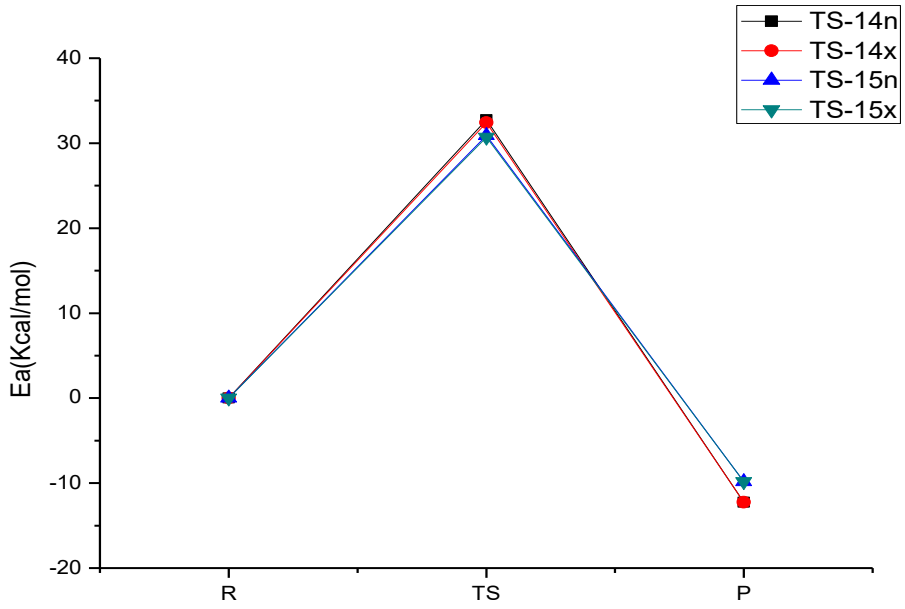


-Para el método M062X/6-311+G(d,p) en Cloroformo.

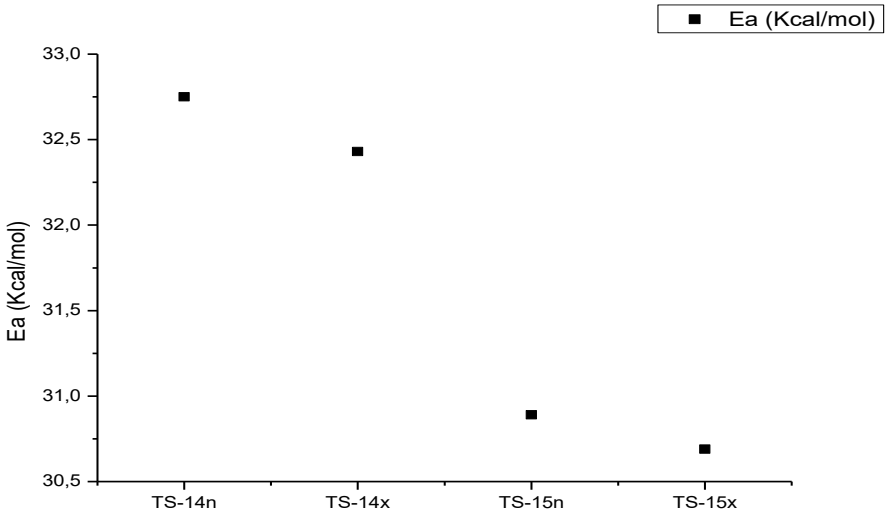
	G Hartrees	ΔG (Ea) Kcal/mol	Frec.i.	E(0) Hartrees	ΔE(0) kcal/mol	μ	H Hartrees	ΔH (Kcal/mol)
r1 (dipolo)	-395.678			-395.780		1.70	-395.631	
r2 (dipolar)	-514.017			-514.090		5.93	-513.977	
r1+r2	-909.695	0.00		-909.869	0.00		-909.608	0.00
TS-14n	-909.643	32.75	-489.96	-909.841	17.69	5.37	-909.580	18.09
TS-14X	-909.643	32.43	-484.04	-909.842	17.35	2.50	-909.580	17.69
P14	-909.714	-12.25		-909.916	-29.45	4.05	-909.651	-26.71
TS-15n	-909.646	30.89	-476.49	-909.845	15.37	7.96	-909.583	15.70
TS-15X	-909.646	30.69	-478.62	-909.844	15.93	5.84	-909.582	16.31
P15	-909.711	-9.83		-909.913	-27.45	6.17	-909.648	-24.61

* Calculados obtenidos con el método M062X/6-311+G(d,p) y las condiciones de T= 298,15 K y P= 1atm con cloroformo como disolvente.

A continuación, se representa la comparación energética de las diferentes vías.



La comparación de las diferencias observadas para las energías de activación en los distintos estados de transición.

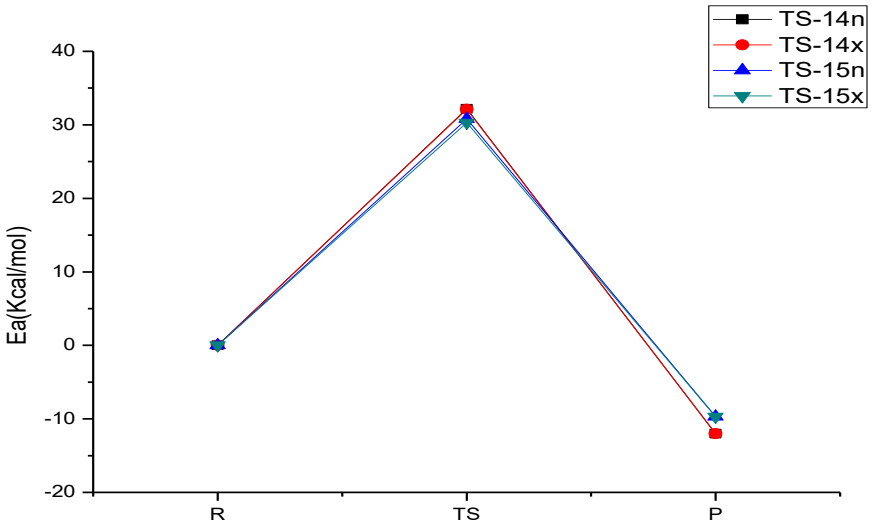


-Para el método M062X/6-311+G(d,p) en Tolueno.

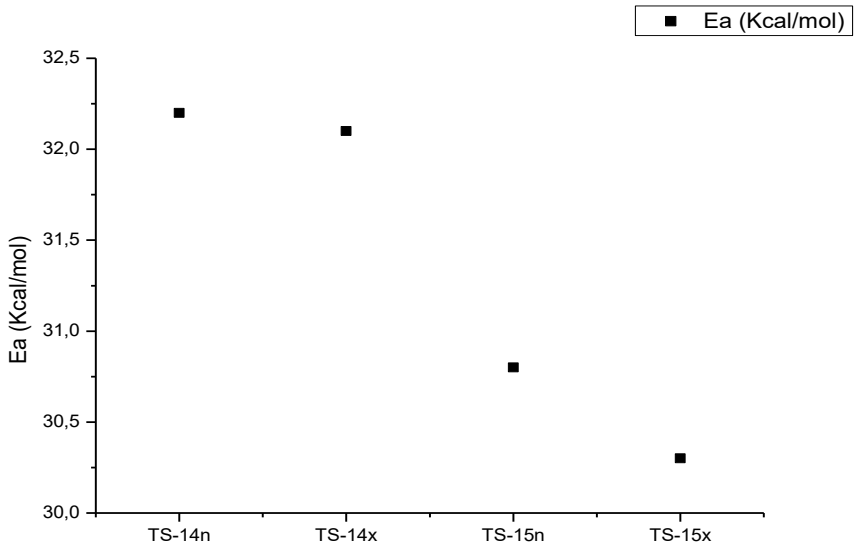
	G Hartrees	ΔG (Ea) Kcal/mol	Frec.i.	E(0) Hartrees	ΔE(0) kcal/mol	μ	H Hartrees	ΔH (Kcal/mol)
r1 (dipolo)	-395.705			-395.777		1.70	-395.665	
r2 (dipolar)	-513.986			-514.087		5.93	-513.939	
r1+r2	-909.691	0.00		-909.865	0.00		-909.604	0.00
TS-14n	-909.639	32.2	-489.96	-909.838	17.10	5.37	-909.576	17.49
TS-14X	-909.639	32.1	-484.04	-909.838	17.00	2.50	-909.576	17.34
P14	-909.710	-12.0		-909.911	-29.24	4.05	-909.646	-26.50
TS-15n	-909.642	30.8	-476.49	-909.840	15.26	7.96	-909.579	15.59
TS-15X	-909.642	30.3	-478.62	-909.840	15.54	5.84	-909.579	15.92
P15	-909.706	-9.7		-909.908	-27.31	6.17	-909.643	-24.48

* Calculados obtenidos con el método M062X/6-311+G(d,p) y las condiciones de T= 298,15 K y P= 1atm con tolueno como disolvente.

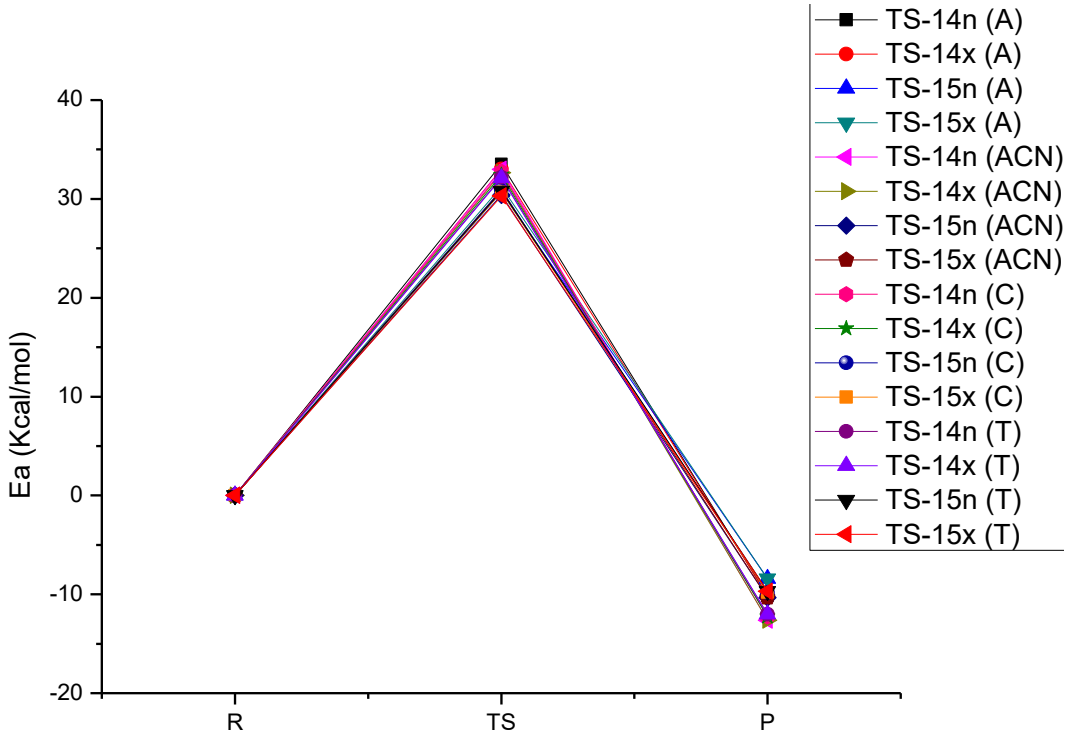
A continuación, se representa la comparación energética de las diferentes vías



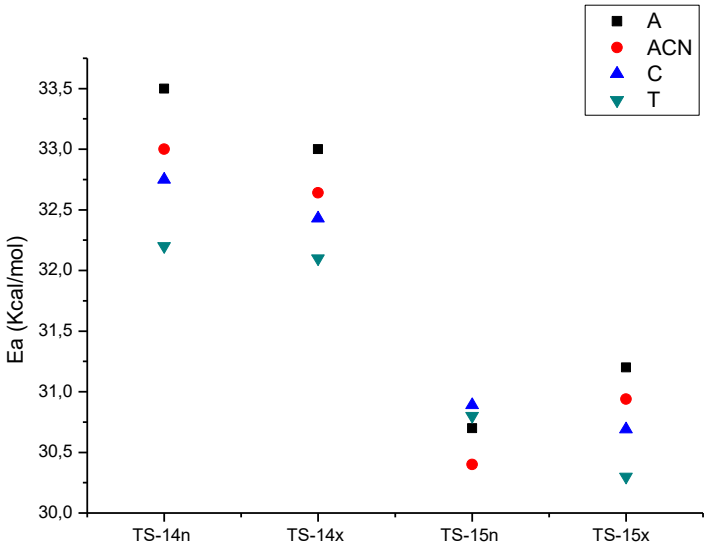
La comparación de las diferencias observadas para las energías de activación en los distintos estados de transición.



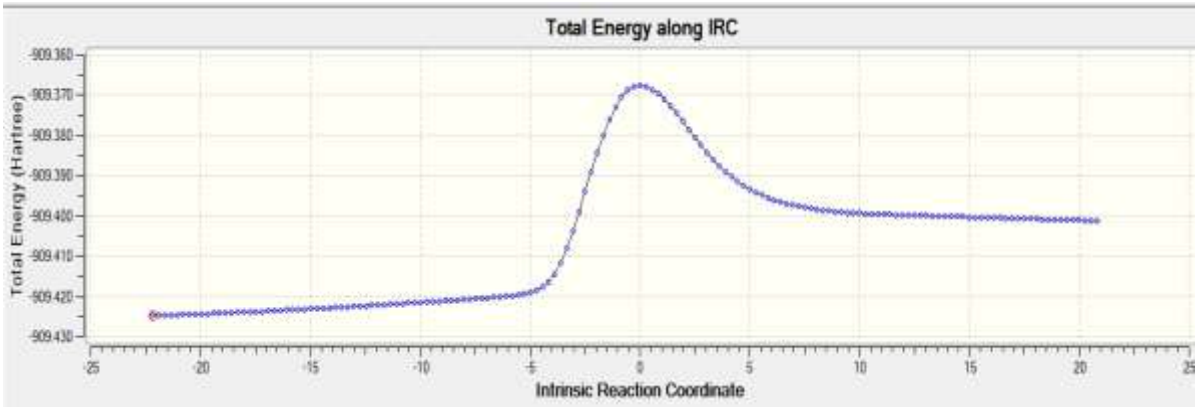
Para establecer una comparación global se adjunta la comparación de la totalidad de los perfiles calculados utilizando el método expuesto.



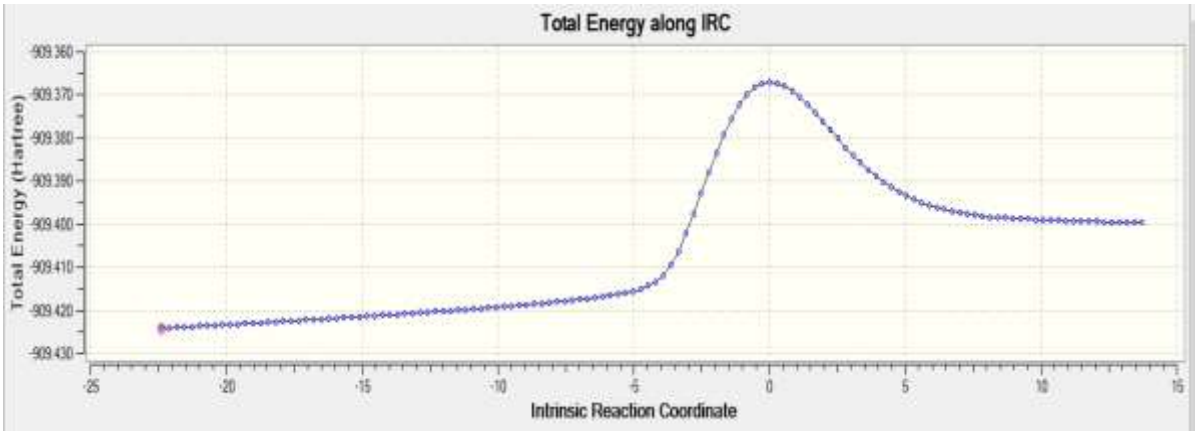
Análogamente, la compilación de las diferencias en las energías de activación de los estados de transición en los cuatro disolventes.



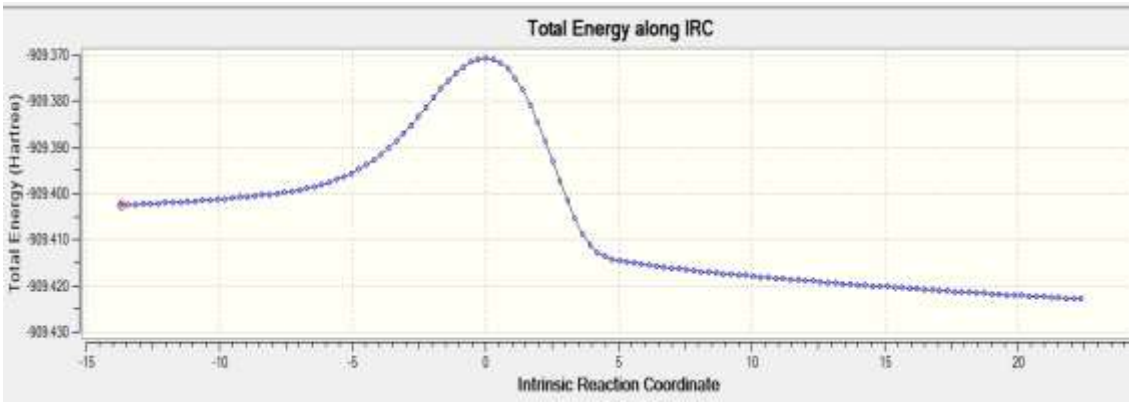
Finalmente se adjuntan los perfiles de los IRC obtenidos. En primer lugar, el IRC obtenido a partir del TS-14n:



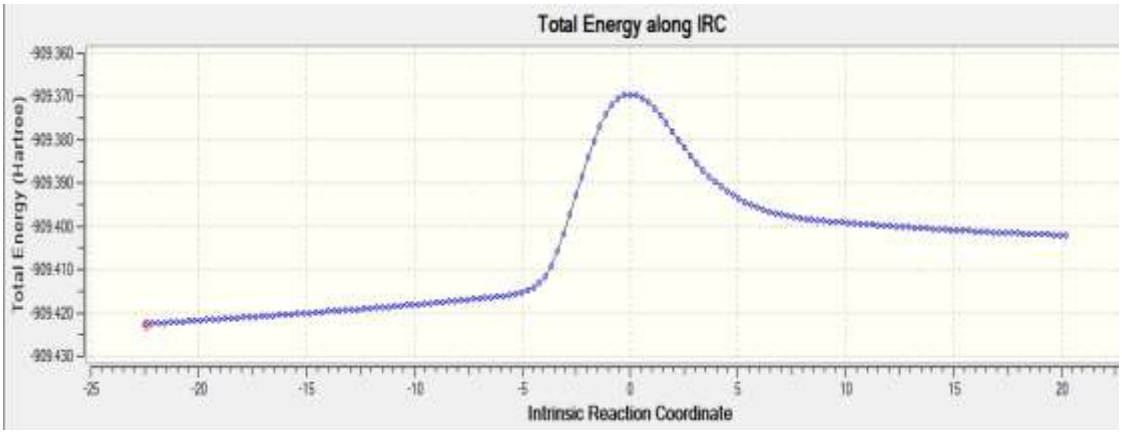
A continuación, el perfil obtenido a partir del TS-14x:



El perfil IRC obtenido a partir del TS-15n:



Finalmente, el perfil obtenido a partir del TS-15x:



6.5. Anexo V.

Este Anexo recopila las coordenadas cartesianas de los componentes de la reacción principal, registrados con el método M062X/6-31+G(d,p) en fase gas.

-Reactivo 1: Fenilazida (dipolo).

Número	Átomo	X	Y	Z
1	C	0.886235	-1.310.267	0.000051
2	C	-0.153846	-0.378279	0.000012
3	C	0.125079	0.990981	-0.000017
4	C	1.450794	1.418916	-0.000007
5	C	2.494133	0.495773	0.000031
6	C	2.204315	-0.869428	0.000061
7	H	0.641428	-2.366983	0.000073
8	H	-0.680667	1.719874	-0.000047
9	H	1.664807	2.482941	-0.000030
10	H	3.523946	0.836350	0.000039
11	H	3.009894	-1.596635	0.000091
12	N	-1.469418	-0.917623	0.000006
13	N	-2.394435	-0.099202	-0.000046
14	N	-3.307528	0.565151	-0.000090

-Reactivo 2: Nitroestireno (dipolarófilo).

Número	Átomo	X	Y	Z
1	C	0.616865	-0.449986	0.000193
2	H	0.924200	-1.493550	0.000550
3	C	1.591235	0.461231	-0.000191
4	H	1.504563	1.538055	-0.000623
5	C	-0.822130	-0.176297	0.000114
6	C	-1.703501	-1.265229	-0.000045
7	C	-1.351298	1.123816	0.000197
8	C	-3.081277	-1.065681	-0.000157
9	H	-1.300863	-2.274312	-0.000090
10	C	-2.725413	1.322729	0.000089
11	H	-0.688787	1.983613	0.000387
12	C	-3.594492	0.228873	-0.000096
13	H	-3.751138	-1.919057	-0.000288
14	H	-3.123173	2.332171	0.000165
15	H	-4.667738	0.388941	-0.000174
16	N	2.983521	0.034734	-0.000047
17	O	3.812860	0.931162	-0.000314
18	O	3.243377	-1.157202	0.000320

-Estado de Transición vía 1,4 aproximación *endo*: TS-14n.

Número	Átomo	X	Y	Z
1	C	2.043803	-0.322040	0.477141
2	C	1.949065	-1.619080	0.991144
3	C	2.808548	-2.603315	0.511752
4	C	3.737871	-2.306228	-0.484982
5	C	3.814865	-1.011275	-0.998016
6	C	2.978118	-0.010829	-0.513879
7	H	1.221339	-1.846212	1.765073
8	H	2.747640	-3.607792	0.918015
9	H	4.401786	-3.079585	-0.856435
10	H	4.537881	-0.773710	-1.771360
11	H	3.027890	1.006107	-0.892051
12	N	1.182755	0.734649	0.869122
13	N	0.368167	0.534613	1.824502
14	N	-0.756904	0.719353	2.045876
15	C	-0.205145	1.379578	-0.523824
16	C	-1.417384	1.214794	0.126647
17	C	-2.247317	0.021250	-0.130695
18	C	-3.638483	0.104308	-0.010891
19	C	-1.667992	-1.210124	-0.468160
20	C	-4.437136	-1.011954	-0.246079
21	H	-4.094239	1.051858	0.262635
22	C	-2.466839	-2.324043	-0.705032
23	H	-0.585340	-1.304810	-0.534458
24	C	-3.854503	-2.228308	-0.596881
25	H	-5.515553	-0.930952	-0.154483
26	H	-2.004885	-3.270642	-0.967157
27	H	-4.476513	-3.098635	-0.779206
28	N	0.378520	2.718707	-0.587417
29	O	1.239394	2.894480	-1.435333
30	O	-0.001978	3.555969	0.210909
31	H	0.152296	0.752974	-1.331332
32	H	-1.904219	2.110154	0.502101

-Estado de Transición vía 1,4 aproximación *exo*: TS-14x.

Número	Átomo	X	Y	Z
1	C	-2.169319	-0.718206	0.357749
2	C	-2.951255	0.119881	1.158424
3	C	-4.324871	0.168343	0.948413
4	C	-4.910621	-0.591945	-0.064036
5	C	-4.119774	-1.410896	-0.869092
6	C	-2.747173	-1.481218	-0.657908
7	H	-2.483042	0.724316	1.929829
8	H	-4.937836	0.812390	1.570157

9	H	-5.982143	-0.542663	-0.227073
10	H	-4.572269	-1.998699	-1.660698
11	H	-2.111796	-2.113844	-1.269292
12	N	-0.754561	-0.770350	0.458909
13	N	-0.201991	-0.400344	1.545081
14	N	0.724283	0.227344	1.863632
15	C	0.318107	0.560217	-0.775820
16	C	1.365654	0.943926	0.052513
17	H	1.348904	1.961949	0.428010
18	H	0.402110	-0.129249	-1.603851
19	N	-0.799064	1.475408	-0.936670
20	O	-1.508655	1.312043	-1.915735
21	O	-0.994683	2.306872	-0.060048
22	C	2.671396	0.257622	-0.038610
23	C	3.851349	0.968872	0.201596
24	C	2.749503	-1.109089	-0.339092
25	C	5.088149	0.334799	0.115847
26	H	3.796523	2.025107	0.450239
27	C	3.985734	-1.741320	-0.424609
28	H	1.836608	-1.68.031	-0.487003
29	C	5.159077	-1.020477	-0.201348
30	H	5.996728	0.899799	0.298072
31	H	4.033811	-2.800519	-0.656633
32	H	6.122703	-1.515322	-0.266304

-Producto vía 1,4: P14.

Número	Átomo	X	Y	Z
1	C	2.088487	-0.478103	0.047258
2	C	2.883007	-1.373426	0.770958
3	C	4.145403	-1.701307	0.291243
4	C	4.625209	-1.154679	-0.899561
5	C	3.826334	-0.264689	-1.610364
6	C	2.560233	0.081613	-1.142886
7	H	2.509727	-1.796257	1.695489
8	H	4.759886	-2.394113	0.857196
9	H	5.611722	-1.417745	-1.265313
10	H	4.185809	0.175704	-2.534612
11	H	1.958035	0.786744	-1.708134
12	N	0.799279	-0.145388	0.506190
13	N	0.384392	-0.483742	1.773986
14	N	-0.743244	-0.046985	2.028982
15	C	-0.088856	0.775874	-0.095164
16	C	-1.295570	0.685687	0.861676
17	C	-2.463687	-0.058970	0.255776
18	C	-3.560253	0.652560	-0.231969

19	C	-2.430135	-1.450055	0.133398
20	C	-4.617191	-0.020333	-0.842020
21	H	-3.587255	1.734783	-0.134691
22	C	-3.486810	-2.121133	-0.476434
23	H	-1.584714	-2.008854	0.526448
24	C	-4.580906	-1.407713	-0.965318
25	H	-5.468481	0.539169	-1.215971
26	H	-3.458150	-3.202308	-0.565245
27	H	-5.405042	-1.933110	-1.437022
28	N	0.475217	2.205754	-0.056341
29	O	0.127976	2.934812	-0.966445
30	O	1.167933	2.508676	0.889070
31	H	-0.315994	0.592145	-1.145193
32	H	-1.613922	1.676508	1.196777

-Estado de Transición vía 1,5 aproximación *endo*: TS-15n.

Número	Átomo	X	Y	Z
1	C	-0.913615	-1.475447	0.208373
2	C	-1.704306	-1.001800	1.259516
3	C	-3.089200	-1.041978	1.141810
4	C	-3.684724	-1.537443	-0.019388
5	C	-2.888864	-2.007310	-1.063157
6	C	-1.501547	-1.981496	-0.951403
7	H	-1.232963	-0.599967	2.152213
8	H	-3.705989	-0.675165	1.955948
9	H	-4.765965	-1.560885	-0.106732
10	H	-3.347962	-2.401364	-1.964008
11	H	-0.860799	-2.345818	-1.748529
12	N	0.495290	-1.350531	0.192647
13	N	1.137239	-1.286491	1.285723
14	N	2.064217	-0.732194	1.710466
15	C	1.246020	0.400255	-0.678824
16	C	2.416709	0.552644	0.055296
17	C	0.091947	1.288309	-0.457109
18	C	-0.918969	1.352759	-1.423903
19	C	-0.073938	1.995509	0.742723
20	C	-2.064241	2.112396	-1.204645
21	H	-0.807067	0.792364	-2.348207
22	C	-1.215168	2.761408	0.958059
23	H	0.682536	1.936656	1.520830
24	C	-2.214780	2.820016	-0.013124
25	H	-2.840825	2.147318	-1.961909
26	H	-1.329051	3.306085	1.889970
27	H	-3.107833	3.411925	0.159875
28	N	3.611948	-0.124179	-0.415073

29	O	4.677954	0.280480	0.020053
30	O	3.480971	-1.064364	-1.186563
31	H	2.656128	1.407625	0.669572
32	H	1.315599	-0.120862	-1.628623

-Estado de Transición vía 1,5 aproximación *exo*: TS-15x.

Número	Átomo	X	Y	Z
1	C	-1.644001	-0.802029	0.558810
2	C	-2.893849	-0.221530	0.329532
3	C	-3.931096	-1.017986	-0.143723
4	C	-3.715936	-2.370489	-0.414280
5	C	-2.457487	-2.932657	-0.204811
6	C	-1.415974	-2.151594	0.289982
7	H	-3.037166	0.841035	0.503839
8	H	-4.907071	-0.576712	-0.317060
9	H	-4.528432	-2.983316	-0.790580
10	H	-2.287910	-3.983619	-0.414894
11	H	-0.431181	-2.567703	0.479774
12	N	-0.518162	-0.043673	0.980324
13	N	-0.699395	1.017984	1.650241
14	N	-0.282794	2.094979	1.714078
15	C	0.689881	0.651486	-0.491788
16	H	-0.035111	0.356673	-1.247.398
17	C	0.760394	2.008127	-0.195423
18	H	1.656774	2.537845	0.093422
19	C	1.865220	-0.226727	-0.309593
20	C	2.073625	-1.289038	-1.194261
21	C	2.765254	-0.029719	0.745186
22	C	3.175263	-2.129032	-1.041784
23	H	1.371554	-1.451477	-2.007952
24	C	3.863984	-0.867896	0.896744
25	H	2.594324	0.772248	1.459261
26	C	4.073646	-1.918723	0.001798
27	H	3.330829	-2.946061	-1.739096
28	H	4.554919	-0.707414	1.718152
29	H	4.931323	-2.572606	0.122306
30	N	-0.241372	2.874463	-0.775610
31	O	0.026579	4.060628	-0.865390
32	O	-1.310871	2.372083	-1.109779

-Producto vía 1,5: P15.

Número	Átomo	X	Y	Z
1	C	-1.761628	-0.585912	0.051789
2	C	-2.788109	-1.201036	0.778785
3	C	-4.110733	-0.929760	0.450490
4	C	-4.427388	-0.056757	-0.591127
5	C	-3.399158	0.547843	-1.307384
6	C	-2.066341	0.291351	-0.992524
7	H	-2.542238	-1.884642	1.581982
8	H	-4.902227	-1.411454	1.015664
9	H	-5.463089	0.147059	-0.840275
10	H	-3.626677	1.229964	-2.120147
11	H	-1.276888	0.781143	-1.552035
12	N	-0.414700	-0.847688	0.363850
13	N	-0.077244	-1.680652	1.349725
14	N	1.155729	-1.850127	1.468566
15	C	0.757451	-0.279544	-0.301028
16	C	1.847912	-1.095100	0.405107
17	C	0.909008	1.209997	-0.074991
18	C	1.501562	1.998737	-1.061831
19	C	0.504290	1.792154	1.127339
20	C	1.693084	3.362483	-0.847687
21	H	1.810332	1.546698	-2.001678
22	C	0.695274	3.155224	1.340086
23	H	0.027842	1.180990	1.890216
24	C	1.290183	3.941801	0.354111
25	H	2.151232	3.971035	-1.620618
26	H	0.375259	3.603963	2.274842
27	H	1.434817	5.004323	0.520535
28	N	2.460686	-2.138405	-0.509664
29	O	3.646909	-2.350928	-0.376825
30	O	1.709524	-2.701401	-1.282244
31	H	2.685163	-0.522139	0.799495
32	H	0.731264	-0.519084	-1.369576