

Apéndice 1

Ángulos de torsión de los compuestos obtenidos en la búsqueda de la CSD

<i>Refcode</i>	τ_1	τ_2	τ_3	τ_4	τ_5	τ_6	τ_7	τ_8
ACAWEG-1	-61,347	-31,492	86,254	-5,011	-31,61	-61,383	100,236	13,612
ACAWEG-2	-67,56	2,551	-69,605	46,262	-69,441	26,613	42,596	90,296
ACAWEG-3	-61,383	-31,61	86,378	-5,071	-31,57	-61,291	100,154	13,65
ACAWEG-4	-67,56	42,596	-63,85	19,539	46,055	-63,849	-0,86	89,47
ACAWEG-5	-69,605	46,262	21,139	-69,652	46,055	-63,849	84,745	3,991
ACAWEG-6	-61,35	-31,49	-5,17	86,38	-31,57	-61,29	13,52	100,25
ACAWEG-7	31,48	61,35	13,61	-100,24	61,38	31,56	5,09	-86,28
ACAWEG-8	31,56	61,38	-13,65	-100,15	61,29	31,44	5,26	-86,41
ACAWEG-9	31,48	61,35	-100,25	-13,52	61,29	31,44	-86,29	5,2
ACAWEG-10	-46,22	63,85	-84,75	-3,99	69,6	-46,04	-21,44	69,9
ACAWEG-11	-46,04	69,6	-90,3	-2,55	67,56	-42,61	-26,58	69,22
ACAWEG-12	-46,22	63,85	0,86	-89,47	67,56	-42,61	63,82	-19,36
ADIBUK	103,513	-109,381	50,24	40,478	-103,513	109,381	-50,24	-40,478
ADICAR	116,574	-92,247	37,54	58,772	-116,573	92,247	-37,54	-58,772
ADICEV	92,113	1,147	-37,751	92,123	-92,113	-1,147	37,751	-92,123
ADICIZ	21,261	85,595	-96,748	59,425	-21,261	-85,595	96,748	-59,425
BICJAY	51,906	68,303	-92,944	85,122	-51,906	-68,303	92,944	-85,122
BISCEL	80,213	-80,213	38,858	38,858	-80,213	80,213	-38,858	-38,858
BOWBIY	28,117	-48,768	111,418	-80,648	28,117	-48,768	111,418	-80,648
BOXBIZ	131,521	-66,733	9,028	87,288	-131,521	66,733	-9,028	-87,288
BUBQOE-1	110,72	-48,448	-49,929	95,717	-23,453	-113,228	82,86	-51,971
BUBQOE-2	-104,206	94,687	-37,307	-74,33	104,206	-94,687	37,308	74,33
BUBQOE-3	-153,986	60,828	9,489	-104,875	134,318	-92,647	44,681	76,434
CAJTOW	47,991	55,305	-56,442	77,254	-47,991	-55,305	56,442	-77,254
CLPSSB	-53,147	-67,767	98,634	-86,895	53,147	67,767	-98,634	86,895
DBUPCU-1	-51,796	127,122	-95,858	-1,341	51,796	-127,122	95,858	1,341
DBUPCU-2	-124,584	48,219	-0,448	-96,432	124,584	-48,219	0,448	96,432
DPINRE-1	75,923	50,95	-79,236	111,448	-75,923	-50,95	79,236	-111,448
DPINRE-2	-54,18	-68,314	104,87	-92,232	54,18	68,314	-104,87	92,232
DPPOPBI0-1	-50,083	-72,893	108,86	-66,504	50,083	72,893	-108,86	66,504
DPPOPBI0-2	-99,787	72,867	-11,669	-68,007	99,787	-72,867	11,669	68,007
ECIGUS	-75,363	125,747	-74,6	-16,465	80,755	-128,364	77,382	10,751
GAWZAF-1	-66,621	123,436	-82,687	-8,815	66,621	-123,436	82,687	8,815
GAWZAF-2	-127,749	77,453	-19,264	-77,046	127,749	-77,453	19,264	77,046
GIDMIP	-26,548	-104,815	125,118	-54,742	26,548	104,815	-125,118	54,742
GOMPIH	53,383	70,97	-101,34	83,134	-53,383	-70,97	101,34	-83,134
GOPPAC-1	-12,727	22,968	-30,326	11,252	12,727	-22,968	30,326	-11,252
GOPPAC-2	27,914	-17,838	-8,475	32,305	-27,914	17,838	8,475	-32,305
GOPPAC01-1	-12,704	22,906	-30,221	11,174	12,704	-22,906	30,221	-11,174
GOPPAC01-2	27,931	-17,93	-8,298	32,188	-27,931	17,93	8,298	-32,188
HEQCAH-1	-27,793	27,739	-26,697	26,642	-27,793	27,739	-26,697	26,642
HEQCAH-2	63,21	-95,85	111,86	-86,02	62,96	-67,1	75,66	-59,92
HEQCAH-3	62,96	-67,1	75,66	-59,92	63,21	-95,85	111,86	-86,02
HEQCAH-4	-63,462	59,669	-42,093	45,625	-63,462	59,669	-42,093	45,625
HEQCAH-5	-117,784	-4,287	67,317	-57,085	-3,54	142,33	-114,049	95,235

HEQCAH-6	131,266	-9,198	-52,661	59,181	4,814	-126,383	89,972	-93,289
HEQCAH-7	58,115	-72,968	70,327	-25,429	-1,658	17,683	0,234	-45,747
HEQCAH-8	-161,383	2,581	51,09	-57,633	-4,902	75,021	-48,054	128,882
HEQCAH-9	-66,55	39,87	-41,46	64,92	-50,29	8,52	-19	66,4
HEQCAH-10	51,84	-84,53	72,18	14,38	-36,8	7,21	21,54	-43,85
HOYKIP	-98,378	134,585	-67,029	-52,103	98,378	-134,585	67,029	52,103
HOYKOV	-94,463	137,659	-71,807	-48,62	94,463	-137,659	71,807	48,62
HOYKUB	-94,178	138,46	-72,124	-47,293	94,178	-138,46	72,124	47,293
HOYLAI	-95,896	136,343	-70,178	-50,679	95,896	-136,343	70,178	50,679
HOYLEM	-96,996	135,562	-68,601	-53,142	96,996	-135,562	68,601	53,142
HOYLIQ	-97,419	131,609	-65,846	-53,606	97,419	-131,609	65,846	53,606
HOYLOW	-96,069	128,966	-63,012	-53,696	96,069	-128,966	63,012	53,696
IFEJOS	-18,112	38,598	-29,721	-13,289	18,112	-38,598	29,721	13,289
JORXUJ	48,716	-49,756	101,913	-101,913	49,756	-48,716	100,668	-100,668
JOSPUC	115,05	-117,112	43,933	43,716	-116,999	114,955	-41,611	-41,775
JOSPUC10	114,994	-117,187	43,763	43,763	-117,187	114,994	-41,55	-41,55
JUMKEH	-32,781	42,556	-97,613	71,501	-16,263	36,062	-99,348	84,844
KEGHAF	16,718	-3,762	74,136	-94,182	16,718	-3,762	74,136	-94,182
LEHLOZ	22,22	39,153	22,728	-101,392	22,22	39,153	22,728	-101,392
LEYRUC	94,914	-7,766	-38,572	-22,379	94,914	-7,766	-38,573	-22,379
MEFKAJ	-39,359	38,413	34,309	-48,724	-21,84	32,419	30,39	-33,849
MEFKEN	-2,844	47,089	6,38	-27,547	-35,255	23,995	51,045	-80,874
MPCTRE	-59,997	-59,997	94,902	-94,902	59,997	59,997	-94,902	94,902
NAGKAH	10,403	88,569	-93,962	29,14	-10,403	-88,569	93,962	-29,14
NAPRIF	3,689	-86,085	95,839	-29,421	-3,689	86,085	-95,839	29,421
NIMWAH	21,312	30,019	-113,785	35,48	24,731	28,243	-113,906	37,971
NIMWOV	33,475	25,602	-117,304	36,3	23,521	28,333	-110,287	26,65
NULZID	-26,03	16,873	-85,546	109,412	-26,03	16,873	-85,546	109,412
NULZOJ	32,149	-29,319	91,935	-98,674	22,168	-19,921	101,348	-108,829
PHACCR	37,728	44,664	-82,148	0,152	59,89	-57,15	5,96	-14,732
PHACCR01	-18,645	74,666	-15,264	-82,651	55,441	44,385	-25,601	-27,22
PHBPMN	-74,87	-31,927	75,769	-105,285	74,87	31,927	-75,769	105,285
POWCOT	11,647	35,216	33,317	-106,27	12,555	36,115	30,963	-103,764
QEDKAL	-110,046	91,852	-17,094	-61,059	110,046	-91,852	17,094	61,059
QOBKOH	37,484	-84,635	124,263	-57,008	37,484	-84,635	124,263	-57,008
RELLOJ-1	14,09	-87,049	80,729	2,448	-14,09	87,049	-80,729	-2,448
RELLOJ-2	18,656	-100,028	91,326	5,427	-18,656	100,028	-91,327	-5,426
RELLUP-1	-48,011	128,576	-72,119	-12,339	32,24	-100,106	109,185	-17,876
RELLUP-2	-16,791	-19,242	18,906	-25,046	16,79	19,242	-18,906	25,046
RUQHUG	-32,666	-33,635	-24,863	97,492	-22,558	-43,843	-20,157	103,379
SIRCEB-1	36,847	-35,91	-73,579	75,621	32,678	-33,693	-72,997	71,595
SIRCEB-2	35,91	-36,847	117,488	-113,318	32,678	-33,693	116,116	-115,336
SIRCEB-3	-32,678	33,693	165,625	154,323	32,678	-33,693	-165,625	-154,323
SIRCEB-4	-36,847	35,91	152,068	164,463	36,847	-35,91	-152,068	-164,463
SOSWIG	41,825	-116,985	93,82	-9,813	-41,825	116,985	-93,82	9,813
SUZCUL	116,298	-78,756	4,099	70,915	-116,298	78,756	-4,099	-70,915
TATYES	-82,267	-11,993	29,912	-89,989	82,267	11,993	-29,912	89,99
TAVYOE	16,105	-16,749	12,371	4,786	-16,105	16,749	-12,371	-4,786
TAVYUK	-35,145	33,05	-9,399	-25,615	35,145	-33,05	9,399	25,615
TIQMUB-1	61,029	-76,964	109,813	-74,655	9,094	11,784	45,772	-82,028
TIQMUB-2	62,436	-73,424	104,599	-84,056	7,026	40,196	15,033	-79,99
TIQMUB-3	-45,112	48,499	-31,458	-17,339	45,112	-48,499	31,458	17,339

TIRXUN	64,589	-125,283	85,252	-7,64	-64,589	125,283	-85,252	7,64
TIXKEQ	-23,008	4,513	-70,488	104,005	-30,835	8,052	-70,229	98,015
TIXLER	-129,234	53,056	-11,279	-97,807	129,234	-53,056	11,279	97,807
VACJIS	-0,241	9,302	-26,444	21,31	0,241	-9,302	26,444	-21,31
VACJOY-1	58,992	56,021	-77,499	91,773	-58,992	-56,021	77,499	-91,773
VACJOY-2	10,112	28,516	-98,808	40,1	11,013	42,075	-116,884	49,261
VAQNAC	-19,271	-1,031	-64,929	96,621	-9,531	-5,561	-68,295	107,817
VEHMOK	41,239	64,004	-104,273	81,059	-41,239	-64,004	104,273	-81,059
VEHNAX	63,866	42,75	-82,1	-29,379	63,866	42,75	-82,1	-29,379
VELMEE	-24,303	70,752	-60,683	-8,334	24,303	-70,752	60,683	8,334
WACRIB	-39,332	58,601	-40,737	28,719	-56,274	71,721	-46,359	22,161
WACROH-1	27,096	-39,507	-31,538	91,24	-42,349	15,705	-56,997	49,403
WACROH-2	35,292	-40,614	78,724	-25,347	-42,349	15,705	63,621	-81,833
WACROH-3	35,292	-40,614	-37,7	85,769	-39,507	0	-67,504	39,747
XAHHET	100,607	-95,891	44,217	49,896	-100,607	95,891	-44,217	-49,896
XAPREL-1	24,74	82,55	-106,58	-10,72	12,54	58,99	-68,18	-16,3
XAPREL-2	24,74	82,55	-26,53	-89,72	38,69	55,58	2,78	-89,75
XAPREL-3	58,99	12,54	-86,09	0,9	38,69	55,58	-114,45	5,33
XAWQAN-1	-48,037	-69,958	94,9	-69,353	48,037	69,958	-94,9	69,353
XAWQAN-2	57,252	57,39	-82,249	77,604	-57,252	-57,39	82,249	-77,604
XAWQAN-3	-16,937	19,621	57,738	-67,641	7,765	-27,022	92,372	-60,98
XAWQAN-4	-0,557	12,323	-81,136	60,174	2,064	22,582	-92,189	66,131
XEPRUF-1	31,22	54,79	-97,75	-7,02	50,44	32,27	-73,17	9,08
XEPRUF-2	-33,62	59,27	-86,78	3,43	55,16	-34,83	-27,9	61,78
XEPRUF-3	28,43	51,93	-5,92	-93,06	50,44	32,27	7,43	-80,07
XEPRUF-4	-39,37	48,76	9,84	-83,14	55,16	-34,83	61,06	-19,29
XEPRUF-5	28,43	51,93	-90,19	-12,02	54,79	31,22	-80,93	10,2
XEPRUF-6	-33,62	59,27	0,45	-75,39	48,76	-39,37	70,1	-28,38
XEPRUF-7	-50,44	-32,27	83,17	-9,08	-31,22	-54,79	97,75	18,37
XEPRUF-8	-54,79	-71,22	80,93	-10,2	-28,43	-51,93	90,19	12,02
XIKSIT	30,213	-88,964	75,666	8,313	-30,213	88,964	-75,666	-8,313
YEYJIV	-10,431	-21,477	115,078	-54,328	-11,139	-25,18	123,687	-58,833
YEYJOB	-31,057	5,946	-71,995	118,304	-31,057	5,946	-71,995	118,304
YOMDOT	-7,505	-92,173	99,913	-27,678	7,505	92,173	-99,913	27,678
ZAZZUV	33,078	-34,239	95,498	-94,011	39,102	-40,981	98,965	-91,55
ZIRMES	166,043	4,759	-6,639	169,054	-166,043	-4,759	6,639	-169,054
ZOWMON	-67,991	-35,907	59,408	-94,195	67,991	35,907	-59,408	94,195
ZOZJUT	-77,473	25,185	-6,79	-67,003	77,473	-25,185	6,79	67,003
ZUHCAG	133,601	-84,189	21,342	73,284	-133,601	84,189	-21,342	-73,284
ZUHCUA-1	53,037	50,64	-94,4	90,103	-53,037	-50,64	94,4	-90,103
ZUHCUA-2	25,393	71,54	-93,674	66,626	-25,393	-71,54	93,674	-66,626