

# Intimate Interactions with Carbonyl Groups: Dipole–Dipole or $n \rightarrow \pi^*$ ?

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**Table S1.** Data used in Figure 1A.

<b>CCDC Refcode</b>	<b>Dihedral Angle</b>
ISAHEP	138.14
HEYGAT	-164.26
JISCEU	32.24
REFLUJ	-27.33
ZULWEI	-139.85
IYIYAQ	-0.91
CORJUP	-65.16
LABRIQ	-76.09
TOHVUI	29.77
HEPVUT	-128.25
YARJOQ	-42.73
BAZGOZ	-133.59
YAKZIU	64.13
HOKMAW01	-102.67
TOHVIW	29.42
RIGVEJ	176.53
YERDOO	-60.94
SIMVEQ	-173.92
HOKMUQ	-21.60
TIHGEX	23.78
HOKMUQ	83.69
QOHCUM	-34.19
IDALAA	12.26
VATNOU	-114.75
ZUBBUT	105.90
HOKNAX	-19.65
JEYKOO	-130.86
ESATOH	-10.21
ESATUN	18.78
HEXWAJ	-161.21
BAZGOZ	-109.62
GALDED	56.69
POQZOL	82.24
HOKMIE	15.97
TAPPUV	39.46
HOKMOK	177.32
TITTOG	126.80
NIWRAN	60.03
SIBTIH	147.47

VIGXAK	-31.13
RAZLEK	69.53
YERDAA	134.18
GORBOE	-55.12
IDALAA	-7.93
KISPUY	130.88
UGUMUE01	-41.74
HOKMOK	-93.44
HOKMIE	-82.23
PANLAS	-62.26
PEYMUC	22.49
XOSLEX	-86.37
YEXQIB	-155.24
OGENOE	-116.00
IWAMEY	-118.14
ZESZOM	-173.84
ZIZYUC	147.29
JIGYED	-16.73
WESMAJ	-173.95
VOHNUC	6.31
TFACET	117.90
NAGWAT	-167.00
VEVSIZ	7.38
UKOKIO01	-66.30
ODUSEM	-20.12
UKOKIO01	-94.01
PFBZAC01	7.00
PFBZAC	-8.25
WESBEB	-74.85
WESBOL	8.19
CIJLOW	-38.85
GADXIT	-179.92
TEFNUN	169.15
VEVSIZ	-17.41
JASHOA	61.40
ESATUN	-121.93
UKOKIO01	-52.34
NAGVUM	23.64
QORSUM	36.61
MIDXIH01	-162.50
MIDXIH	-162.84
PAPTUW	96.09
JOPYES	-8.57

ZOZVIT	93.80
NOTNIT	-100.65
MIHXAD	-26.35
HEYGAT	109.38
ASOGIY	-154.15
NADRIU	146.11
UDEHER	-64.27
FMESIB	21.38
JAYGUM	153.10
QODYAJ	-117.95
ILEMIV	-77.26
LEKMIX	-104.75
MIJCUE	62.82
MIJCUE	-34.56
HEKZEC	-104.24
MAVBOB	-130.17
WIFGUO	-158.80
DISQIG	84.76
LEZRAK	-50.69
OKATID	129.95
TAHYUX	106.54
SITZOK	69.41
UDEHER	138.36
GETLEX	17.86
WOJLIQ	-82.49
WOJLIQ01	-82.49
SATQUA01	175.11
MIHXAD	-58.09
MAYTAH	-80.64
DILDIL	8.12
VINCOL	-62.04
MEBCAX	-94.40
JEKMAO	57.95
MIKYAG	113.64
VOHLUA	-46.29
VOHMAH	100.09
SOBQIK	-2.41
UFOTIS	168.79
LIBWEZ	96.13
REVPOY	-163.20
VIPROC	33.18
IHENIS	112.85
GAGPIO	-58.83

UFOTIS	107.10
LIWJIL	115.89
PILLIG	36.41
EQOPAB	6.47
TUGWUN	173.13
VOHLUA	-34.06
HIGLAL	140.84
XEKLOP	111.77
JEKMAO	-55.84
RADYEA	-12.53
BOVBIY	-60.08
MEBCAX	-63.15
CECBAO	75.79
PEJLAR	89.33
DAQLUD	-110.17
YOHDEE	-18.23
COJRAV	-175.22
DOJXEG	-75.29
DATKAL	-74.18
BIKHIN01	-2.58
ODOTOR	46.76
SUKKUE	38.93
PAHHUC	1.60
MAJVOJ	-23.37
KEYNUX	26.63
IZONEQ	2.21
LESJUP	-63.54
MAQVEF	20.03
QEYFOP	-162.68
POQZOL	40.03
FURACL01	0.49
CONLEX	-168.72
JIKBUA	147.99
KITSOV	169.25
SOWQIE	126.39
JIKBUA	-158.48
QEGKAO	-153.09
AFUPUN	-162.13
RAZLEK	-89.58
TAPPUV	-141.90
UBEREY	5.36
UBEREY	-13.08
UBEREY	39.99

UBEREY	28.24
UBEREY	-20.05

**Table S2.** Data used in Figure 1B.

<b>CCDC Refcode</b>	<b>Dihedral Angle</b>
VOJJUA	-62.05
GIVLIH	10.70
RAKTUT	85.54
JINFUH	-88.86
CEQBUW	161.37
REZCOP	-118.51
IDAZOD	8.87
FOVVES	138.48
ERESAV	-79.89
ICSALA	-48.84
LAWDET	122.16
SAMBOY	173.50
SIMYOD	-65.57
KIKGOB	13.54
ODASOB	-176.99
LIWJUX	-96.60
IZONOA	167.12
PONSOB	179.91
AZADAG01	-139.07
JEKWUS	-106.40
NORKUB	61.37
PIKMIF	-69.37
HIJBOR	61.59
MURTAU	166.52
ROFTEM	50.57
PIKMIF	7.84
FAMDUS	-5.86
SAQKUR	178.14
CEYXEK	-20.22
QELXUA	-152.76
YICJAW	158.49
WAMNOO	37.94
VEMXIU	149.15
WALXIR	13.33
RIZTAV	-133.18
AFIIQI	30.86
TETFEE	-51.83

VOQZAD	-93.57
WEGPEE	150.40
TIGXEN	20.70
TUWDUK	135.70
VERZIB	-163.46
CNIXQX	-35.10
DIWSIM	-127.28
GENBIL	116.13
POTCAD	-21.77
ERESEZ	-73.76
JEWTAG	-146.03
MIPKOM	-20.30
YICJAW	-82.04
LIVQIR	-152.55
TORHAK	36.89
KEFTOF	92.20
TORHAK	-148.95
QIQXET	58.99
BUHQOK	24.82
KEFTOF	174.45
UCOGEZ	125.34
MELQUQ	-45.32
MIGVUU	133.96
LUDJEZ	63.20
ODATIX	-10.93
SIMQOV	-112.39
MIGTIG	-153.19
WEJSOT	27.27
FOFKER	-169.25
MOPCIE	-163.04
FOCDEH	-36.34
DEZXIP	-33.31
HOMXOW	-19.20
YIQGAH03	19.45
QAFVAU	174.03
YIQGAH02	20.91
XAPWUG	70.75
AJAHEY	-177.39
KUCDAN	166.57
GANKEL	146.63
XEPRIU	1.19
RAVMUW	129.92

EDEGIE	171.75
CHPCBO	-85.51
WIZQIF01	27.60
WIZQIF	26.57
MCHTEP17	32.03
RUNQEW	42.95
OKOBEV	-170.09
IRUCON	168.33
WEJCAQ	-123.69
SIYYII	57.74
AVEHOY	58.89
FEHTAO	166.63
HEVMOK	-131.08
CIKTIA	161.22
BICXUG	-29.55
ZEXSUQ	87.83
MCHTEP06	54.14
BIKBAZ	62.46
MOBD AJ	75.24
HIPNOJ	-94.84
QAMFAL	117.59
MCHTEP09	54.00
CAXPOG	140.70
KOVWUN	-128.23
MCHTEP08	53.98
LITHIG	163.44
MIBGIO	-23.20
LOKROT	-14.46
MCHTEP03	53.88
VEQWEU	-124.04
QOGYUH	-89.00
XATLOT	-147.12
MCHTEP07	53.84
NELVOP	-4.77
HODSUO	62.32
MAYTUC	-24.03
QAMFAL	-48.28
RAJDUC	27.10
WATQUD	38.63
HEKPAO	7.07
EFOLUH	-150.58
IQORUB	-88.92
QUQDEL	32.55

KIYBAW	-116.38
ZIKLEK	46.99
TOHJOP	153.14
NAZMOR	157.18
YERXEZ	6.03
GUKBUJ	31.64
PUTFIT	-141.81
VERKAE	-129.73
OCAFEE	179.67
BIKBAZ	-11.60
TUCLOS	-148.18
JESXIO	-158.50
XODBEY	-81.05
XODBEY01	-81.05
SEZDOR	-6.04
NOQYUO	76.38
BANQUD	65.66
PARTOR10	-179.39
HOPPIC	172.25
OKOBEV	46.28
HOPPIC	169.46
QOWNAR	0.00
BUTRAJ	-170.83
DACQOO	173.73
HEVWIO	-157.15
FACWEM	-141.08
SAYYAT	-159.34
XEGWIP	128.19
FAQFEJ	-122.31
WATREP03	-117.13
NUQVEA	23.73
TEVJUZ	39.25
BAVMIU	83.57
PEZQAN	-118.87
PEZQAN01	-118.66
REXRUI	164.62
JIYRAK	-177.46
DCACON	-167.38
GINKUK	117.93
YODFON	-108.59
NAFBUR	-116.91
WATREP02	-117.51
XEGWIP	-44.62

ECECUL	16.49
RIHFAQ	166.66
NAFBUR	-124.11
JEQVUX01	170.43
JUFDIX	80.22
HATTOM	-122.54
ECHNYL	59.45
VUYWIV	-151.16
RAGBAD	-117.47
VABREV	-164.90
YAMTEM	-55.86
JUTFUZ	150.84
JUTFUZ10	150.84
DUZSOG	115.67
ACUJEN	-124.39
JONTEL	-122.64
YITFEN	110.53
BANTEQ	-74.94
WOGXUM	-70.50
GALDON	22.70
SIFKEX	-178.31
LAKJOW	-15.54
REVLUA	89.44
RESWOB	166.58
VARGIF	117.49
DAMGED	-48.85
REVLUA	-42.52
CEYXEK	-21.23
DORXIS	-34.39
DOZJEH	-75.47
EFUFER	27.68
HACCET	-50.34
LETHIB	149.05
WAMNOO	144.05
XAKSUX	56.61

**Table S3.** Data used in Figure 1C.

<b>CCDC Refcode</b>	<b>Dihedral Angle</b>
OGARIY	60.46
RALTII	15.48
OGAREU	-119.56
HAGKUV	-84.39
JISKEC	-173.71
CILJIQ01	-59.63
OGAREU	120.07
TUDQUE	59.27
TIWYII	-49.49
YIRNUI	-177.20
JAWCIT	-153.21
IZOPAO	164.10
HOPDAS	-80.76
NELXOS	-107.95
IDOZAD	-140.73
MAVMAY	-78.90
KOMREK	-145.24
HOFMUK	-13.42
MIBGOU	-175.72
ACIQIM	-24.23
AXEJUI	-160.61
QOQQIW	132.03
MIFJOA	-37.36
VUKTEA	164.13
NIQRIP	63.72
ZUKPUQ	152.13
UMUMIY	-4.95
VOQRAV	20.77
MAYHIE	-173.52
CARJIP	-82.65
KIXVIX	-83.97
ZUKKUL	-112.58
XIKMEK	-122.53
HOTBIB	25.83
IBEXOD	167.67
TIWYII	-97.54
QOSZII	-164.63
PEFZAC	45.93
ZUMTIK	-25.32

JARHUG	-145.89
MAQHAO	-113.88
RAKHER	143.22
DBTCHY	110.70
RAPVAG	-170.09
IXOJAG	7.03
EFAXEO	-170.23
BPENTA	173.44
IXOJAG	18.74
TEVYOI	-170.46
CEFYIW	-70.64
QAVCEW	-156.70
QERVOY	134.61
CEZGAQ	-158.17
GAYYUA	177.99
WIXTIH	143.80
IBUPIE	125.57
SIJTIO	-57.48
BIWBUF	-157.76
IFAHIH	92.95
XAGFOB	-179.45
IDEKOR	-40.66
JESTEY	-176.72
EZAPUQ	178.46
TEWFUW	19.29
YIBDES	-156.92
YIBDES10	-156.92
JESTEY	121.17
CIPWUU	-95.06
SATPOT	-137.84
ABAXES	-4.83
YEHKIF	-105.93
LICJIR	-87.97
COCDIH	113.85
TUZWOA	-8.91
QARDOC	-31.26
DEMGUY	142.61
HABPEF	169.48
BENBCL	-176.63
EFAXEO	90.57
CILLIS	-23.38
BAWJAL	120.40
GULFIC	-165.46

VOBCIZ	3.81
COPCAL10	9.11
NIKSUW	126.79
PEHWAB	-173.12
VOBCIZ	58.82
XEHCIW	-65.88
KILCUD	-57.81
PEQHEY	-53.64
ECECOF	14.55
CEGNIL	-84.14
KOYREV	44.60
KOMREK	144.87
DIZGEY	-147.58
LAMWUS	145.17
DOGZUU	55.28
EGIYIC	10.30
XICNON	65.76
QELFET	175.37
IFIHIO	150.23
NASGOE	-139.23
NASGOE	139.54
OLASOJ	-0.15
OLASOJ	0.89
OLASOJ	8.11
MAJDUX	43.52
OLASID	137.02
OLASID	-0.06
DPHPZL	-161.80
BOPDIU	74.70
OLASOJ	-2.00
OLASOJ	0.73
OLASOJ	-7.40
QAYHUU	-26.75

**Table S4.** Data used in Figure 1D.

<b>CCDC Refcode</b>	<b>Dihedral Angle</b>
ADUGIP	145.24
BAQVIZ	166.76
CBIOXO01	-98.73
CIJSIX	-11.68
FEXCUH	-74.50
GIVLIH	175.16
HACXAL	177.36
HOKXOV	-4.78
IGALOS	155.25
IHXNAQ	120.90
IOBNZA	169.81
IOBNZA01	149.74
IXOKAH	-110.33
JEWYIU	-174.43
LEQBEP	175.89
MOFSUW	-59.17
NEJDEL	-112.32
POBREE	-53.44
QETWOB	4.29
QETWOB	-3.90
QEXMIQ	121.19
QIFFER	-158.51
QIFFER	-147.15
ROGNAD	-3.67
SANZUC	116.77
TATDEX	122.25
TATDEX	-120.74
VEJLEC	-168.06
VEJLIG	-119.55



**Table S5.** Data used in Figures 3A and 4A.

CCDC Refcode	$d$ (Å)	$\theta$ (°)	$\Delta$ (Å)	$\Theta$ (°)
GEMPEU	2.93	90.29	0.000	0.00
RIGGAQ	2.87	90.82	-0.006	-0.33
WIHQUA	2.84	89.96	0.016	0.94
WURCER	3.06	97.27	0.040	2.29
WURCER	2.91	87.96	0.043	2.48

**Table S6.** Data used in Figures 3B and 4B.

CCDC Refcode	$d$ (Å)	$\theta$ (°)	$\Delta$ (Å)	$\Theta$ (°)
AREWID	3.42	102.73	0.004	0.24
AZGUCM10	3.43	104.53	0.007	0.42
BEKSEP	3.38	100.28	0.063	3.59
BERVOJ	3.32	114.98	0.076	4.33
BIYZAL	3.29	86.11	0.042	2.41
BIYZEP	3.29	84.74	0.038	2.17
BIZJUQ	3.33	89.44	0.041	2.35
CAGLCL10	3.39	92.48	0.016	0.91
CAWCAE	3.28	86.75	0.033	1.87
CERGUC	3.22	110.97	0.101	5.79
COBYEX	3.32	99.49	-0.005	-0.28
COBYOH	3.33	100.69	0.015	0.85
COKCIO	3.24	92.87	-0.035	-2.02
CYTOSC	3.40	102.24	0.035	2.01
CYTOSC02	3.35	101.43	0.034	1.96
DASQEU	3.28	97.55	0.023	1.30
DEJYIB	3.34	71.66	0.016	0.89
DETZOS	3.40	84.69	0.022	1.26
DGLYHC02	3.45	97.25	0.029	1.65
DIWQUW	3.37	97.55	0.039	2.22
DOCYTC	3.35	91.79	0.016	0.94
ECECIY	3.36	87.53	0.044	2.49
ELIYIH	3.25	101.05	0.000	0.00
ENANLC	3.34	101.94	0.069	3.95
ENCOCT	3.41	101.05	0.033	1.92
ENCOCT01	3.41	95.94	0.030	1.71
ETCYTC	3.30	101.81	0.026	1.47
FAXFUF10	3.38	103.23	0.000	0.00

FAYQIF	3.42	90.93	0.013	0.75
FAYQOL	3.32	95.41	0.030	1.73
GEQFUD	3.48	99.87	0.008	0.48
GIFFUX	3.43	101.65	0.042	2.42
GIQCEO	3.31	94.57	0.073	4.17
GOLSEG	3.42	94.39	0.028	1.61
GONHOG	3.40	93.70	0.035	2.03
HAZGIZ	3.27	87.24	0.043	2.47
HEMSAT	3.43	91.74	0.029	1.68
HISTDC10	3.39	100.21	0.029	1.68
HONRAE	3.41	79.53	-0.021	-1.18
HVALAC	3.40	86.29	0.030	1.74
HXFAVC	3.32	81.92	0.048	2.73
IBAZIV	3.29	99.75	-0.008	-0.47
IBAZIV	3.19	98.50	0.002	0.14
IBAZIV	3.42	97.45	-0.007	-0.42
IFURAD	3.37	97.64	0.067	3.82
JAXKOI	3.41	94.96	0.046	2.62
JENHAL	3.41	97.20	0.035	1.99
JUBJOF	3.17	95.39	0.040	2.32
JUNQOY	3.33	81.07	0.012	0.67
KABJUS	3.34	100.19	0.033	1.87
LAPVIH	3.35	91.44	0.019	1.12
LAPVIH	3.25	86.50	0.004	0.23
LAXTOU	3.40	106.44	-0.001	-0.05
LEPLUN	3.21	97.46	0.050	2.89
LIGLES	3.41	91.41	0.011	0.61
LOBZOS	3.38	84.60	-0.017	-1.00
LTYRHC10	3.19	91.63	0.042	2.43
MAWGEX	3.46	103.86	0.014	0.79
MODSAA	3.28	88.95	0.045	2.59
NAVSAF	3.23	99.83	0.008	0.47
NAVTUA	3.09	50.91	0.060	3.44
NAWGIB	3.40	95.68	-0.007	-0.37
NECVUN	3.23	161.47	0.058	3.33
NILXUB	3.41	81.82	0.020	1.14
NIYXID	3.47	13.88	-0.098	-5.62
NUMJUA	3.38	85.01	0.043	2.48
ODAWEW	3.29	99.98	0.027	1.55
PASKOK	3.30	94.53	0.059	3.39
PINFEX	2.25	104.78	0.000	0.00
PMABUO	3.43	92.56	0.039	2.22
POFHEX	3.36	90.76	0.007	0.41

POFHEX	3.26	86.56	-0.003	-0.18
POFTIO	3.27	95.15	0.046	2.61
POSTAS	3.42	81.77	0.010	0.56
POSTEW	3.32	85.47	0.016	0.94
PYMOCL	3.28	96.78	0.016	0.90
QABCAX	3.33	93.89	0.065	3.74
QENMAX	3.34	100.50	0.002	0.14
QENMAX	3.37	93.24	0.019	1.10
QETBIB	3.36	95.20	0.006	0.33
QETBIB	3.36	100.06	0.020	1.17
QOBYAI	3.73	103.63	0.005	0.29
QOBYEM	3.17	97.67	0.004	0.24
QOFMAA	3.40	104.51	0.015	0.86
QQDOQ	3.43	92.66	0.012	0.66
RAVMAC	3.66	89.19	-0.032	-1.82
RIFJAS	3.11	98.16	-0.005	-0.28
SISWIB	3.42	93.97	0.027	1.57
SISWIB	3.22	92.69	0.016	0.93
SISWIB	3.27	92.77	0.013	0.75
TAVLUX	3.44	95.42	0.022	1.27
TEZZUU	3.37	94.88	0.019	1.09
TICKIZ	3.41	95.58	0.062	3.54
TRGLCO10	3.36	88.03	-0.009	-0.51
UKAZIP	3.26	93.52	0.023	1.32
UKAZOV	3.25	93.58	0.023	1.33
UKAZUT	3.27	94.99	0.048	2.74
UKEMAY	3.38	87.98	0.010	0.58
UKEMAY	3.36	98.66	-0.010	-0.58
VABFIN	3.39	98.30	0.047	2.67
VIDQUU	3.39	98.54	0.040	2.28
WABTOI	3.38	88.37	0.041	2.37
WEPSAM	3.45	86.44	0.023	1.32
WIKTUF	3.29	94.27	0.060	3.42
WUGJEN	3.39	19.46	-0.030	-1.70
WUGNIV	3.37	107.68	0.013	0.73
XALDAP	3.41	81.76	0.013	0.77
XIKXUL	3.30	93.70	0.016	0.90
XIKXUL	3.19	91.58	0.037	2.14
XIKXUL	3.44	94.54	0.017	0.98
XISHAJ	3.32	101.19	0.022	1.25
XIWBEK	3.49	93.46	0.006	0.33
YAMSIP	3.43	85.19	0.011	0.64
YAZNES	3.28	97.71	-0.129	-7.40

YIBQIK	3.27	98.81	0.027	1.55
YICJOJ	3.19	97.94	0.017	0.95
YOPZOS	3.40	79.84	0.000	0.00
YUKLAR	3.42	87.94	0.032	1.85
SITBIH	3.32	108.86	0.000	0.00
SITBIH	3.39	111.16	0.000	0.00
TASPUZ	3.08	99.53	-0.009	-0.52
TASPUZ	3.10	88.52	0.009	0.52
TASPUZ	3.36	99.43	0.004	0.24
TASPUZ	3.29	109.04	-0.004	-0.24
RIFJAS	3.28	102.62	0.007	0.38
RIFJAS	3.45	63.57	0.007	0.38
NEYHOP	3.26	92.71	-0.007	-0.42
NEYHOP	3.32	97.57	0.007	0.42
NEYHOP	3.17	96.35	-0.005	-0.28
NEYHOP	3.23	99.15	0.005	0.28

**Table S7.** Data used in Figures 3C and 4C.

<b>CCDC Refcode</b>	<b><i>d</i> (Å)</b>	<b><i>θ</i> (°)</b>	<b><i>Δ</i> (Å)</b>	<b><i>Θ</i> (°)</b>
AQANEL	3.53	107.78	0.019	1.08
MEGGAH	3.43	90.86	0.005	0.28
MEGGEL	3.49	94.07	0.045	2.57
VAGYEI	3.38	110.11	0.000	0.00
AZGUBH	3.52	102.87	0.018	1.04
DIBHET	3.48	86.13	-0.014	-0.79
FONNAX	3.41	94.05	0.007	0.37
RANYUB	3.33	95.48	0.028	1.60
HEXWEN	3.44	101.14	0.017	1.00
LAXTUA	3.54	108.46	-0.013	-0.76
LEJYEF	3.27	95.47	0.010	0.56
CPYRZD	3.49	88.48	0.008	0.43
CYSTIN10	3.28	103.24	0.092	5.28
DEFLOP	3.50	85.58	-0.002	-0.09
DOTMEE	3.09	82.87	0.016	0.92
OXENCO01	3.47	92.85	0.040	2.28
SIXCIM	3.52	87.88	0.057	3.29
VOWSOP	3.48	103.01	0.016	0.90
XOTQOM	3.40	90.84	-0.005	-0.28
GIDROB	3.46	98.25	-0.026	-1.50
VAGYEI	3.31	107.54	0.000	0.00
EGZEWE	3.48	100.81	-0.007	-0.42
EGZEWE	3.53	97.10	-0.003	-0.19
TASPOT	3.20	91.89	0.005	0.29
TASPOT	3.21	99.23	-0.005	-0.29
TASPOT	3.40	100.23	0.002	0.14
TASPOT	3.41	108.34	0.002	0.14

**Table S8.** Data used in Figures 3D and 4D.

<b>CCDC Refcode</b>	<b><i>d</i> (Å)</b>	<b><i>θ</i> (°)</b>	<b><i>Δ</i> (Å)</b>	<b><i>Θ</i> (°)</b>
HIQPIG	3.63	96.48	0.043	2.46
LAXVAI	3.55	98.70	0.011	0.61
RADKOX01	3.66	91.86	0.019	1.08
UGUBIH	3.65	99.88	0.035	2.02
GAPHUA	3.53	97.70	0.024	1.39
TENCOG10	3.68	95.62	0.009	0.53
GAPHUA	3.68	98.80	-0.002	-0.14

**Table S9.** Data used in Figure 5.

<b>CCDC Refcode</b>	<b><i>d</i> (Å)</b>	<b><i>θ</i> (°)</b>	<b><i>Δ</i> (Å)</b>	<b><i>Θ</i> (°)</b>
ACAMCL	4.39	86.25	-0.009	-0.41
ACAMNI	4.39	91.11	0.005	0.23
ACIHAW	4.36	63.52	-0.044	-2.05
ALUNIE	4.42	52.05	-0.021	-0.99
AREWID	4.42	44.70	0.005	0.24
BAQTUJ	4.35	157.33	0.007	0.33
BEFYOB	4.36	155.13	0.031	1.45
BEFYOB	4.40	52.43	0.023	1.08
BEKYOF	4.39	97.19	0.053	2.43
BETANC01	4.41	126.67	0.005	0.24
BIYZAL	4.44	151.33	-0.052	-2.41
BIYZEP	4.43	151.33	-0.047	-2.17
BUCRAS	4.36	163.70	0.006	0.28
BUTPIP	4.39	112.43	0.017	0.79
BUTPIP01	4.38	99.85	0.064	2.94
CBMCHL01	4.37	159.29	0.000	0.00
CBMCHL10	4.42	158.59	0.000	0.00
CEJTIV	4.41	89.83	0.009	0.42
CEWQOL	4.42	131.00	0.007	0.33
CEYVIL	4.44	50.18	0.000	0.00
CYSTCL02	4.44	58.01	0.013	0.62
CYSTCL03	4.43	58.54	0.012	0.57
DAZQOL	4.36	59.35	0.032	1.48

DESKUI	4.42	61.10	-0.002	-0.09
DESKUI	4.42	61.10	-0.002	-0.09
DIGMAI	4.39	61.45	-0.009	-0.41
DIYJUQ11	4.44	34.52	0.035	1.64
DIYJUQ11	4.43	90.17	0.048	2.28
EGOFUB	4.38	146.22	0.000	0.00
EKAMIM	4.44	75.36	0.030	1.38
EKAMIM	4.42	106.24	0.012	0.56
FAXFUF10	4.42	44.91	0.000	0.00
FEQYUW	4.38	112.58	0.018	0.86
FEVFES	4.42	165.94	-0.006	-0.29
FIKSOI	4.41	31.19	-0.022	-1.02
FIMKAO	4.35	158.27	0.026	1.21
FUDYIM	4.37	83.77	0.016	0.76
FUQHEE	4.43	91.69	0.017	0.81
GIPROM	4.38	130.87	-0.203	-9.44
GIWRIN	4.37	102.78	-0.056	-2.52
GLGLMO	4.42	42.71	-0.019	-0.88
GLYHCL	4.39	115.80	-0.008	-0.38
GOKXAF	4.37	136.44	0.099	4.64
GOMDER	4.42	99.20	0.035	1.63
GOMDER	4.43	60.01	-0.035	-1.63
GOMDER	4.40	72.93	-0.032	-1.48
GUQCEA	4.42	32.76	-0.003	-0.14
GUYRIB	4.39	101.51	0.017	0.79
HEBMEG	4.36	161.47	-0.010	-0.46
HIBZOH	4.39	82.64	0.018	0.86
HISTCM01	4.36	59.35	-0.038	-1.77
HISTCM12	4.38	59.70	-0.023	-1.07
HIWJOM	4.36	127.90	0.000	0.00
IKALOV	4.36	147.55	0.032	1.53
ILIHAM	4.37	126.63	0.025	1.18
JOQSOX	4.44	163.04	-0.026	-1.22
JUBFAN	4.36	151.28	0.057	2.63
KAGLUA	4.37	86.54	-0.008	-0.37
KAVLOI	4.37	148.67	0.011	0.50
KISSAH	4.44	58.42	0.003	0.14
KORBAU	4.45	81.56	0.034	1.58
KUGREJ	4.38	46.45	0.102	4.78
LCITHC01	4.42	59.53	0.023	1.09
LEPLUN	4.35	143.80	-0.026	-1.23

LGLUTA	4.41	62.09	-0.043	-2.02
LGLUTA02	4.38	62.40	-0.046	-2.16
LUXHUH	4.36	150.31	-0.001	-0.05
LYSCLH11	4.39	153.27	-0.036	-1.66
LYSCLH11	4.45	69.42	0.036	1.66
MAJJAJ	4.36	161.87	0.083	3.99
MAJJAJ	4.39	162.72	0.082	3.92
MAVDUJ	4.42	67.92	0.027	1.25
MIBHOV	4.40	117.13	0.027	1.27
NABJAB	4.40	72.18	-0.042	-1.95
NABSIT	4.37	173.47	-0.038	-1.81
NAFZIE	4.45	84.50	0.026	1.21
NASREE	4.44	117.30	-0.007	-0.34
NILFUJ	4.40	103.28	-0.076	-3.60
NILXUB	4.38	50.66	-0.024	-1.14
NUQZEE	4.43	75.38	-0.023	-1.08
NUTQOI	4.41	153.43	0.049	2.29
PENICS10	4.40	49.25	0.020	0.96
PIXSUL	4.36	108.82	-0.016	-0.74
PUHNIP	4.44	84.56	0.008	0.38
PUNQEU	4.36	91.51	0.013	0.62
QESFOJ	4.38	125.64	-0.037	-1.74
QOCZEN	4.44	148.24	-0.019	-0.98
QQQAQS01	4.39	138.70	0.024	1.12
RIJXAJ	4.35	87.12	0.224	10.70
ROBYEM	4.44	89.94	0.018	0.85
ROLYIA	4.40	43.14	-0.003	-0.14
SARCAC01	4.41	57.57	-0.010	-0.46
SEQHEB	4.39	122.46	0.035	1.63
SETMOT	4.43	155.84	-0.092	-4.40
SISWIB	4.43	40.64	-0.016	-0.75
SOPVOI	4.43	99.97	0.057	2.66
SOPVOI	4.44	95.59	0.016	0.77
STIZOL	4.44	41.43	-0.020	-0.93
TEJGAQ	4.38	108.96	-0.010	-0.47
TICLOG	4.42	50.98	0.047	2.19
UCOLEE	4.39	93.68	-0.051	-2.39
VALHCL11	4.43	53.11	-0.011	-0.53
VEDFAL	4.44	52.24	0.057	2.64
VITKUE	4.35	146.58	-0.029	-1.31
VITYON	4.44	115.54	-0.020	-0.94



VIWNIZ	4.38	13.87	-0.002	-0.09
VIXJUH	4.42	66.75	-0.004	-0.19
VUSRUW	4.37	59.67	-0.046	-2.13
WEWTAU	4.40	72.62	-0.001	-0.05
WEZVUS	4.41	116.30	0.012	0.57
WIKTUF	4.37	51.98	0.071	3.42
WIWZOS	4.38	150.93	0.042	1.96
WIWZOS	4.43	151.29	0.008	0.38
WIYMEW	4.35	54.88	0.047	2.12
WUGNIV	4.43	97.60	-0.016	-0.73
WUQHIZ	4.38	64.12	0.012	0.58
XALDAP	4.38	50.67	-0.016	-0.77
XAMFOG	4.42	46.59	0.064	2.99
XAVGAD	4.42	95.30	-0.016	-0.75
XECDAL	4.37	157.81	-0.011	-0.51
XECFIV	4.43	105.82	-0.015	-0.71
XIKXUL	4.42	40.73	-0.019	-0.90
XIYSAA	4.38	81.03	-0.006	-0.29
XUQCOB	4.37	117.49	0.044	2.10
YAMSIP	4.43	51.50	-0.014	-0.64
YAMSIP	4.36	156.10	-0.021	-0.97
YAPBOH	4.37	51.79	0.106	4.98
YEFTUZ	4.40	49.32	-0.003	-0.14
YERMEO	4.43	107.14	0.002	0.10
YICHUN	4.43	51.40	0.026	1.27
ZEZJUJ	4.43	60.98	0.016	0.75
ZOZVOZ	4.37	156.28	0.019	0.90
ZOZWAM	4.38	169.45	-0.034	-1.65
JOBHEO	4.41	82.45	0.044	2.07
MODSAA	4.40	47.26	0.054	2.59
QOCWAH	4.36	135.78	-0.004	-0.19
TADLAL01	4.35	66.57	-0.177	-8.41