

Supporting Information

Parallel stacking interactions in square-planar transition metal complexes containing fused chelate and C₆-aromatic rings

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List of REFCODES

Fragment 1

<i>Refcode</i>	D_{CA}	D_{AA}	Δ
ADEXUD	3,971	5,466	1,495
AGICAU	4,038	5,182	1,144
AGICAU	3,996	5,182	1,186
ASEHEM	3,591	4,744	1,153
AVUKAD	3,911	5,274	1,363
AVUKAD	3,951	4,752	0,801
AXEHEQ	4,09	3,575	-0,515
AXEHEQ	4,751	3,835	-0,916
BZQXPD01	3,483	3,774	0,291
BZQXPD01	5,132	3,774	-1,358
CABLAU	3,742	4,822	1,08
CIQGOY	3,645	4,95	1,305
CIQGOY01	3,623	4,852	1,229
COHNET	4,284	3,718	-0,566
CUQUIN05	3,599	4,984	1,385
CUQUIN05	3,674	5,075	1,401
CURPOV	3,517	4,545	1,028
DAFKUQ	3,47	3,731	0,261
DIVJUO	3,767	3,634	-0,133
DUBSOI	3,697	3,712	0,015
DUPNEI	3,683	4,794	1,111
DUPTEO	3,65	4,787	1,137
DUPYIX	3,759	4,855	1,096
DUZWAW	3,721	4,574	0,853
EXIHOI	3,747	3,538	-0,209
GAFMAD	3,973	3,908	-0,065
GEVJAS	4,324	5,361	1,037
GICNIP	4,845	3,575	-1,27
GICNIP01	4,737	3,541	-1,196

GICNIP01	4,893	3,553	-1,34
GICNIP02	4,885	3,554	-1,331
GICNIP02	4,742	3,553	-1,189
GOCBUW	3,822	4,485	0,663
GOCBUW	3,494	4,08	0,586
HAXMAV	3,63	4,094	0,464
HAZCIV	4,278	3,687	-0,591
HECPOV	3,874	4,813	0,939
HECPOV	5,857	4,417	-1,44
HELGEK	4,199	3,512	-0,687
HENWEC	4,068	4,769	0,701
HQUIPD	3,733	4,77	1,037
IDULAV	3,625	4,486	0,861
ILIPID	3,585	3,598	0,013
ILIQAW	4,296	3,689	-0,607
IPUMOV	4,21	3,717	-0,493
ITEJUM	3,649	4,644	0,995
ITIKUS	3,884	5,366	1,482
ITIKUS	3,449	4,276	0,827
ITILED	3,517	4,327	0,81
ITILON	3,444	4,474	1,03
IVUCUY	3,623	4,308	0,685
JEKGAH	4,161	3,75	-0,411
JEXXEQ	3,688	4,83	1,142
JEXXEQ03	3,829	4,861	1,032
JISPEH	3,75	4,472	0,722
JISPUX	4,519	3,807	-0,712
JUHSUA	3,984	4,735	0,751
KACDID	3,731	4,417	0,686
KAFTIU	3,436	4,667	1,231
KAFTIU	3,859	5,42	1,561
LAGYID	5,728	4,043	-1,685
LAMBOR	4,317	4,806	0,489
LAPYAC	4,159	5,677	1,518
LAPYAC	3,757	4,577	0,82
LAPYAC	3,679	4,829	1,15
LIWNOV	3,908	5,191	1,283
LIWPOW	3,97	5,469	1,499
LIWPOW	3,693	4,934	1,241
LOFHUJ	3,566	3,676	0,11
LURMOB	3,569	3,98	0,411
MALXAZ	3,897	4,942	1,045
MAMJOA	3,794	4,931	1,137
MAMKER	3,551	3,75	0,199
MERBUG	3,906	5,062	1,156
MERCAN	3,903	4,708	0,805
MERCAN	4,013	5,081	1,068

MERCAN	3,602	4,082	0,48
MERCAN	5,074	4,082	-0,992
MERCER	3,837	4,952	1,115
MUMCIG	3,604	4,348	0,744
NACZIB	4,525	3,558	-0,967
NUQKIT01	3,601	4,653	1,052
ODOYUC	5,167	3,741	-1,426
OFOLIF	3,709	3,529	-0,18
OMISUY	4,395	3,488	-0,907
ORENAB	3,562	4,304	0,742
PAKBUZ	3,596	4,178	0,582
PMQONI10	3,783	3,989	0,206
PMQONI20	3,847	3,986	0,139
POQLOW01	5,715	4,195	-1,52
POQLOW01	4,315	3,795	-0,52
PORNOA	3,576	3,841	0,265
PUNBEF	4,109	4,5	0,391
RHQUPC01	3,673	4,211	0,538
SEHHES	3,685	4,291	0,606
SIFPAY	3,913	4,265	0,352
SIFPAY10	3,913	4,265	0,352
SOPKAJ	3,518	3,763	0,245
TAQJIF	3,628	4,977	1,349
TIXTUP	4,521	3,865	-0,656
TORJIT	3,944	4,839	0,895
TORYUU	4,536	3,633	-0,903
UDOPOT	4,046	3,733	-0,313
UFASOJ	3,686	4,704	1,018
UGUWUP	3,694	4,067	0,373
UHOCOJ	3,426	3,423	-0,003
UKUGAI	3,812	4,883	1,071
ULUSIE	3,481	4,585	1,104
VEGVIN	3,781	4,794	1,013
VERBUQ	3,815	5,186	1,371
VERBUQ	3,782	5,112	1,33
WATQAJ	4,303	3,772	-0,531
WESRAO	3,961	4,385	0,424
WEXKAL	4,862	4,111	-0,751
XAFLAS	3,423	4,051	0,628
XAFLEW	3,487	3,759	0,272
XAGKIZ	3,6	4,567	0,967
XERRAO	4,138	3,779	-0,359
XOKREV	5,007	3,606	-1,401
XORHIV	3,743	4,268	0,525
XORHIV	4,219	3,768	-0,451
YATYIB	4,017	3,44	-0,577
YOYKOM	4,124	5,239	1,115

YULDEP	4,009	5,536	1,527
ZADFIT	3,833	4,773	0,94
ZUNMUQ	4,217	4,484	0,267

Fragment 2

<i>Refcode</i>	D_{CA}	D_{AA}	Δ
ABOPOX	3,662	4,035	0,373
ABOPOX	3,663	4,487	0,824
ABOPOX	3,808	4,035	0,227
ACNBPD01	3,489	4,661	1,172
AQEGOS	3,696	3,723	0,027
AQEGOS	4,107	3,686	-0,421
AQEGOS	4,47	3,723	-0,747
ARITAW	3,862	5,128	1,266
ARITAW	3,567	4,202	0,635
ATOGAS	4,279	4,182	-0,097
ATOGAS	4,163	4,182	0,019
BIGRAL	3,581	3,749	0,168
BIGREP	3,559	4,465	0,906
COHNET	3,733	3,718	-0,015
COHNET	4,951	3,718	-1,233
DENCOP	3,632	4,964	1,332
DENCOP	3,502	4,689	1,187
DENCUV	3,699	5,052	1,353
DEYXIP	3,794	4,879	1,085
DIZYAN	5,468	4,131	-1,337
FEPLS	3,632	4,195	0,563
FIKXAZ	4,375	3,74	-0,635
FIKXAZ	3,985	3,82	-0,165
FIKXAZ	4,399	3,795	-0,604
FOCZUS	3,587	4,476	0,889
FUNKUU	3,676	4,857	1,181
FUNKUU	4,075	4,857	0,782
FUNKUU	3,748	4,26	0,512
GAJNAH	3,799	5,004	1,205
GAQPAP	3,986	5,102	1,116
GUWJUD	3,954	5,04	1,086
HIGBIJ	3,898	4,663	0,765
HIGBIJ	3,749	4,663	0,914
ICUMEY	3,496	4,778	1,282
ICUMEY	3,412	4	0,588
IHUBOD	4,233	5,138	0,905
IHUCAQ	4,137	5,038	0,901
IHUCEU	4,292	4,437	0,145

IJAQEP	3,456	4,137	0,681
INOQAE	4,024	4,691	0,667
JEBHOO	3,552	4,784	1,232
JEBHOO	3,72	5,068	1,348
JEVFOF	4,121	3,638	-0,483
JISPAD01	4,586	4,02	-0,566
JISPAD02	4,755	4,078	-0,677
KEXXIV01	3,592	4,387	0,795
KEXXIV01	3,827	4,387	0,56
KEXXIV01	3,893	4,482	0,589
KEXXIV01	3,724	4,482	0,758
KOFDOY	4,11	5,716	1,606
KOFDOY	3,587	4,5	0,913
KOFDOY	3,6	4,5	0,9
KOFDOY	4,112	5,725	1,613
KUDSAD	4,195	5,553	1,358
KUDSAD	4,053	4,821	0,768
KULGAZ	3,576	4,613	1,037
KULGIH	4,158	3,938	-0,22
KULHEF	4,484	5,244	0,76
KULHEF	4,019	5,018	0,999
KUZROM	4,446	3,99	-0,456
LADGAZ	4,147	5,212	1,065
LALCIK	3,822	5,035	1,213
MIMLUP	5,547	4,036	-1,511
NAMNIY	3,992	5,385	1,393
NEFBIJ	4,553	4,29	-0,263
NEXHUU	4,051	4,953	0,902
NEXHUU	4,12	4,953	0,833
OGAHEK	4,854	3,851	-1,003
OGIGOA	3,819	4,439	0,62
OGIGOA	3,833	4,439	0,606
OHONIJ	3,763	3,883	0,12
OJIMAW	4,603	4,267	-0,336
OJIMEA	4,073	3,812	-0,261
OVERUD	4,229	4,638	0,409
OWEVOC	3,687	4,119	0,432
OWEWOD	3,979	3,612	-0,367
OWEXAQ	3,617	4,866	1,249
PAZPCP	3,735	4,087	0,352
PAZPCP	5,439	4,087	-1,352
PECHIO	3,903	3,578	-0,325
PECTEW	3,824	4,535	0,711
PECTEW	4,028	4,489	0,461
POKRUD	3,925	4,284	0,359
PORNUG	3,937	3,915	-0,022
QAQPUU	3,834	4,818	0,984

QAQPUU	3,652	4,331	0,679
QEFON	3,858	3,681	-0,177
RANVAD	3,775	4,735	0,96
RIYJUF	3,778	5,18	1,402
SARRUZ	3,446	4,528	1,082
SARRUZ	3,439	4,542	1,103
SARRUZ	3,709	5,11	1,401
SARRUZ	3,688	5,11	1,422
SEMDEU	4,776	3,793	-0,983
SICRUS	4,102	3,813	-0,289
SICSAZ	3,588	4,866	1,278
SICSAZ	3,797	4,015	0,218
SICSAZ	3,597	4,899	1,302
SICSAZ	5,016	4,015	-1,001
SICSIH	4,171	5,1	0,929
SICSIH	3,703	4,988	1,285
SICSIH	4,131	4,988	0,857
SICSIH	3,743	5,1	1,357
SICSON	3,502	4,509	1,007
SICSON	3,765	5,136	1,371
SICSUT	3,972	5,588	1,616
SICSUT	3,457	4,384	0,927
SITTAR	3,895	4,752	0,857
SITTIZ	3,515	4,526	1,011
SIWCAD	3,691	4,454	0,763
SIWDAE	4,261	3,659	-0,602
SIWDUY	3,981	5,223	1,242
SOHDUO	3,598	4,845	1,247
SOHDUO01	3,6	4,832	1,232
SOHDUO02	3,583	4,884	1,301
SOJNIP	3,634	3,808	0,174
SOJNIP	3,681	3,828	0,147
SOJNIP	3,712	3,689	-0,023
SOJNIP	3,859	3,808	-0,051
SOJNIP	4,259	3,808	-0,451
SOJNIP	4,152	3,828	-0,324
SOJNIP	4,769	3,689	-1,08
SOJNOV	3,849	4,056	0,207
SOJNOV	3,76	4,172	0,412
SOJNOV	3,466	4,056	0,59
SOJNOV	3,914	4,172	0,258
TAMJIB	3,61	4,959	1,349
TAMJIB	3,691	4,672	0,981
TAMJIB	3,474	4,672	1,198
TAMJIB	3,812	4,959	1,147
TOGMAD	4,205	5,317	1,112
TOMGEI	4,007	5,525	1,518

TOMGEI	3,964	5,525	1,561
TOMGEI	3,898	4,11	0,212
TOMGEI	3,852	4,11	0,258
TOMGIM	4,97	3,936	-1,034
TOMGOS	5,71	4,285	-1,425
TOMGOS	5,236	4,137	-1,099
TUKWAY	4,083	4,836	0,753
UDISOQ	4,747	3,928	-0,819
VOVGES	3,505	4,091	0,586
WATJIL	3,746	4,132	0,386
WATJIL	3,804	5,28	1,476
WAYCII	5,693	4,191	-1,502
WELKUU	3,566	4,774	1,208
WELKUU	4,549	4,09	-0,459
XOKBIJ	4,032	5,496	1,464
XUMZUA	4,15	3,466	-0,684
XUXJUV	3,862	3,83	-0,032
XUXJUV	4,872	3,83	-1,042
YALLUT	4,237	5,65	1,413
YUBJAG	4,203	4,874	0,671
YUBJAG	3,665	4,874	1,209

Fragment 3

<i>Refcode</i>	D_{CA}	D_{AA}	Δ
AMSCNII1	3,513	4,768	1,255
AWAZUT	4,16	4,268	0,108
BEJIK	4,323	5,505	1,182
BIPBAE	3,666	3,79	0,124
BIZBAO	3,532	5,041	1,509
BOVQEJ	3,486	4,827	1,341
COMCUD	3,56	4,911	1,351
DELVUM	4,075	4,85	0,775
DEPLAL03	4,166	4,317	0,151
DEXNAV01	3,704	5,181	1,477
DEYVUZ	3,667	4,903	1,236
DEYVUZ01	3,658	4,894	1,236
DILDOS	3,71	3,906	0,196
DIMPUK10	4,505	3,957	-0,548
DIMROG10	3,845	3,615	-0,23
DUHGAP	5,245	4,122	-1,123
DUNPIL	4,014	3,738	-0,276
EMEMAL	4,035	3,925	-0,11
EMEMOZ	3,747	3,959	0,212
FETLEW	4,715	4,004	-0,711

FISYAI	4,525	4,256	-0,269
FIWXEO	3,709	4,487	0,778
FUXVAV	3,713	4,079	0,366
GICSER	3,733	3,77	0,037
GUKQUY	3,785	3,84	0,055
HEPHAM	3,648	5,164	1,516
HMAPNI	4,036	5,078	1,042
HUJWEO	3,874	4,985	1,111
ICUHEU	3,755	4,159	0,404
IDONEV	3,957	4,692	0,735
IMUCOJ	3,576	4,733	1,157
JIJVON	3,911	5,445	1,534
JIMYIO	3,41	4,621	1,211
JIMYOU	3,735	5,351	1,616
KEFJOV	3,745	3,617	-0,128
KEFJUB	3,767	4,587	0,82
KIWNEJ	6,038	4,33	-1,708
KUSCIL	3,404	4,645	1,241
KUSCIL	3,589	4,153	0,564
LAKCAD	3,667	3,603	-0,064
LALSUM	3,701	3,76	0,059
LAPXUW	3,584	5,167	1,583
LEXWAM	3,723	4,644	0,921
LEXWAM	3,542	4,644	1,102
LITDUN	3,56	4,57	1,01
LITDUN	3,55	4,76	1,21
MAFXIC	4,395	4,526	0,131
MAHVAT	4,348	5,505	1,157
MIGBEK	3,629	4,366	0,737
MIGCUB	4,152	5,729	1,577
MIRVUF	3,758	3,637	-0,121
MORGAC	3,552	4,974	1,422
MOZRUP	3,93	5,487	1,557
MOZRUP	3,792	5,073	1,281
MUBZIT	3,877	5,43	1,553
MUBZIT	3,716	5,023	1,307
NEXFOM	3,656	5,15	1,494
NISALO02	3,693	4,991	1,298
NISALO02	4,039	5,753	1,714
NOZMOE	3,701	5,211	1,51
NUGLEH	5,363	4,054	-1,309
NUMJEK	4,27	3,56	-0,71
OWODUA	3,651	3,654	0,003
OWODUA	4,356	3,654	-0,702
QERNUW	4,244	4,131	-0,113
QEZQUI	4,102	5,166	1,064
QIVVOG01	3,961	4,31	0,349

QOGBOE	3,738	4,081	0,343
QOLMOU	4,335	3,501	-0,834
QUGREP	4,044	5,354	1,31
REBVUP	3,81	5,212	1,402
ROMTUJ	3,502	4,86	1,358
SALCOP01	3,504	4,918	1,414
SAOXPD	3,542	4,916	1,374
SAPCIW	3,561	3,952	0,391
SAPCIW	5,553	3,952	-1,601
SUSQOM	3,596	4,072	0,476
TEBSCO10	4,423	4,03	-0,393
TONHAF	3,694	5,124	1,43
UGENIE	3,619	4,514	0,895
VECQEZ	3,59	4,857	1,267
VETTUJ	3,92	3,824	-0,096
VOPCIM	3,601	4,881	1,28
WABDEK	3,829	5,42	1,591
WAGZUB	3,972	5,062	1,09
WIPQUH	3,617	4,708	1,091
WOGSIV	3,885	4,466	0,581
XEDBEN03	3,589	5,03	1,441
XEDBEN03	3,757	3,693	-0,064
XICGUM	5,208	3,82	-1,388
XIRZAA	4,901	4,123	-0,778
XOBSUD	3,749	4,775	1,026
YEWHUE	4,993	3,798	-1,195
ZOPYUY	4,103	4,251	0,148