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APPENDIX

APPENDIX

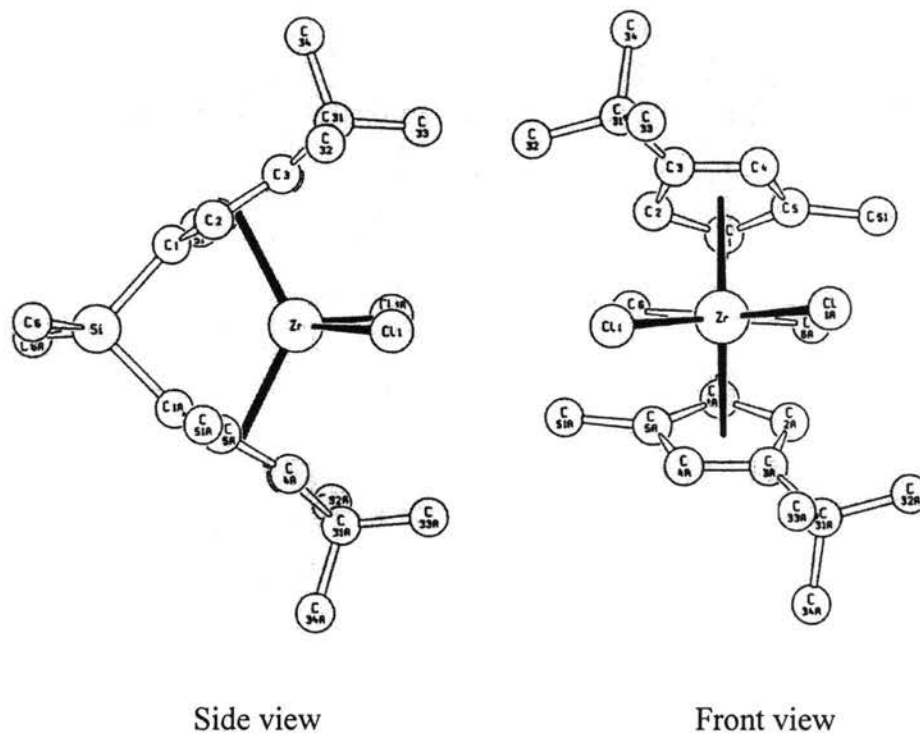


Figure A. The X-ray structure of zirconocene **structure 3**.

Table A. The atomic coordinates ($\times 10^4$) and isotropic thermal parameters for zirconocene **structure 3** from X-ray data.

	<i>x</i>	<i>y</i>	<i>z</i>	U^a
Zr(1)	0	6974(1)	7500	33(1)
Cl(1)	815(1)	5357(1)	8283(1)	79(1)
Si(1)	0	10347(1)	7500	46(1)
C(1)	367(2)	9053(3)	6609(2)	36(1)
C(2)	1030(2)	8329(3)	6807(2)	38(1)
C(3)	1070(2)	7172(3)	6198(2)	36(1)
C(4)	405(2)	7125(3)	5667(2)	33(1)
C(5)	-30(2)	8261(3)	5902(2)	34(1)
C(6)	743(2)	11429(4)	7995(3)	73(2)
C(31)	1736(2)	6271(4)	5998(3)	47(1)
C(32)	2320(2)	6421(5)	6801(4)	75(2)
C(33)	1501(2)	4784(4)	5899(3)	57(1)
C(34)	2053(2)	6739(4)	5002(3)	62(1)
C(51)	-760(2)	8564(4)	5438(3)	47(1)

^a Equivalent isotropic U defined as one third of the trace of the orthogonalised U_{ij} tensor ($\text{\AA}^2 \times 10^3$)

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