

Table 1 Refined Heavy Atom Derivative Parameters^a

Heavy Atom	Occupancy	Atomic Coordinates			Temperature Factor (Å ²)
		X	Y	Z	
Hg	0.763	0.398	0.491	0.929	36.1
	0.926	0.416	0.058	0.995	49.4
	0.930	0.892	0.218	0.364	58.3
	0.920	0.276	0.226	0.480	49.1
	1.066	0.751	0.196	0.699	70.9
	0.932	0.939	0.163	0.802	58.0
Pb	1.027	0.112	0.859	0.173	25.8
	0.192	0.198	0.430	0.405	80.1
	0.206	0.441	0.668	0.800	45.6
	0.958	0.842	0.369	0.822	10.9

^aThe overall figure of merit is 0.28 for 51,470 reflections with $F > 3\sigma$ in the resolution range of 3.0 Å to 50.0 Å.

Table 2 Merlot Molecular Replacement Results In Resolution Range of 4.0 to 8.0 Å

Cross Rotation							
Molecule Number	α	β	γ	% Max Value	RMS Number	Peak	S/N ^a
Mol 1	58.0	96.0	319.0	100.0	4.51	1	1.02
Mol 3	60.0	81.0	301.0	92.0	4.16	10	0.94
Mol 2	241.0	108.0	337.0	86.0	3.90	12	0.87
Mol 6	62.3	109.6	337.0	86.0	3.90	12	0.87
Mol 4	265.0	127.0	21.0	67.0	3.06	27	0.68
Mol 5	69.0	119.0	353.0	65.8	3.01	29	0.67
Translation for Y = 0.5 Section							
Intermolecular Vectors	2X (Å)	2Z (Å)	Peak Number	Solution in Fractional Coordinates			
				X	Z		
Mol 1- Mol 1'	6.0	27.0	1	0.061	0.101		
Mol 2- Mol 2'	59.0	3.0	1	0.425	0.511		
Mol 3- Mol 3'	73.0	70.0	1	0.571	0.761		
Mol 4- Mol 4'	18.0	97.0	1	0.695	0.861		
Mol 5- Mol 5'	48.0	37.0	1	0.869	0.638		
Mol 6- Mol 6'	13.0	64.0	9	0.136	0.238		

^aS/N = ratio of peak to first noise peak.